Rigorous Derivation of the Wave Kinetic Equation for β-FPUT System

by

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To my family

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LIST OF NOTATIONS

Wave Kinetic Theory Basics

Symbol	Meaning	Comments	Reference
N	Number of particles		Section 1.4.
β	Strength of nonlinearity	$\beta = N^{-\gamma}$	Section 1.4.
γ	Scaling law	$\gamma \in (0,1)$	Section 1.4.
T_{kin}	Kinetic Time	$T_{\text{kin}} = \beta^{-2}$	Section 1.4.
$\mathbb{Z}_N$	Lattice space	$\mathbb{Z}_N = N^{-1}\mathbb{Z}$	Section 1.4.
k	Wave number on lattice	$k \in \mathbb{Z}_N \cap (0,1)$	Section 1.4.
$\omega(k)$	Dispersion relation	$\omega(k) = 2\lvert\sin(\pi k)\rvert$	Section 1.4.
Ω	Resonance factor		Section 2.2.
$\widetilde{\Omega}$	Nonlinear frequency shifts		Section 2.4.
$\mathcal{K}$	Collision kernel		See (KIN).

Trees, Couples, and Molecules

Symbol	Meaning	Reference
$\mathcal{T}$	Ternary tree	Definition 2.1.
$\mathfrak{r}, \mathfrak{n}, \mathfrak{l}$	Root, node, leaf	Definition 2.1.
$\mathcal{N}$	Set of branching nodes	Definition 2.1.
$\mathcal{L}$	Set of leaves	Definition 2.1.
$\lvert\mathcal{T}\rvert$	Scale of a tree	Definition 2.1.
$\zeta, \zeta_{\mathfrak{n}}$	Signs	Definition 2.1.
$c_k^{\mathcal{T}}$	Iterate expression for trees	Section 2.4.
$\mathcal{Q}$	Couple	Definition 2.4.
$\mathscr{P}$	Partition (of leaves in a couple)	Definition 2.4.
$\lvert\mathcal{Q}\rvert$	Scale of a Couple	Definition 2.4.
$\mathscr{D}, \mathscr{E}$	Decorations of a tree or couple	Definitions 2.1 and 2.4.
$\mathcal{K}_{\mathcal{Q}}$	Contribution of each couple	Definition 2.9.
$\mathbb{M}$	Molecule	Definition 2.11.
v, ℓ	Atom, bond	Definition 2.11.

ABSTRACT

The Fermi–Pasta–Ulam–Tsingou (FPUT) chain, a one-dimensional lattice of N oscillators, was originally studied to test the expectation that weak nonlinearity would lead to thermalization through energy redistribution among Fourier modes. Surprisingly, numerical simulations revealed quasi-periodic behavior: after partial energy exchange, the system returned close to its initial state, a phenomenon now known as the FPUT recurrence. Despite decades of study, the long-time behavior of the FPUT chain, especially the mechanisms governing thermalization, remains not completely explained.

In the recent twenty years the wave turbulence (WT) approach, an out-of-equilibrium statistical mechanics theory, was largely used to understand the energy transfer within the normal modes of the FPUT model in a weakly nonlinear dispersive regime. The WT approach, especially the wave kinetic equation (WKE), helps us understand the behavior of the wave spectrum in the FPUT system at long-time scales and derive the thermalization time scale.

While the WKE has been rigorously derived for the cubic nonlinear Schrödinger equation in dimensions $d \geq 2$ and for the Majda–McLaughlin–Tabak model in $d = 1$, there is still lack of rigorous justification for the β-FPUT model whose sinusoidal dispersion and unconserved frequency shift pose additional obstacles. In this thesis, we establish the WKE for a reduced evolution equation, removing the non-resonant terms, from the one-dimensional β-FPUT chain. We work in the kinetic limit $N \to \infty$ and $\beta \to 0$ under the scaling laws $\beta = N^{-\gamma}$ with $0 < \gamma < 1$. The result holds up to the sub-kinetic time scale $T = N^{-\epsilon} \min\big(N, N^{\frac{5}{4}\gamma}\big) = N^{-\epsilon} T_{\text{kin}}^{5/8}$ for $\epsilon \ll 1$, where T_{kin} represents the kinetic (thermalization) timescale. We also prove a sufficient upper bound for the nonlinearity parameter β that allows one to perform the canonical transformation on the original evolution equation. This upper bound suggests a scaling between β and N, which governs the importance of the non-resonant terms in the original equation. By applying the symplectic integrator method, we further develop numerical studies on the β-FPUT model, comparing the magnitudes of resonant and non-resonant sums across various nonlinearity strengths and particle numbers to verify the predicted β-threshold.

CHAPTER 1
Introduction

Tracing back to 1923, Fermi targeted to prove the quasi-ergodicity of general Hamiltonian systems in [1, 2]. Here the quasi-ergodicity refers to the idea that a system trajectory will be eventually dense in the phase space. Around 1954, Fermi, Pasta, Ulam, and Tsingou (FPUT) started to use a numerical approach to verify that a system with arbitrarily small nonlinearity would reach thermalization. They performed simulations for a one-dimensional chain consisting of $N = 16, 32, 64$ oscillators with fixed endpoints and initial energy concentrated on the first mode [3], for which the Hamiltonian can be given by:

$$H = \sum_{j=0}^{N-1} \left(\frac{p_j^2}{2m} + \frac{\kappa}{2}(q_{j+1} - q_j)^2 - \frac{\alpha}{3}(q_{j+1} - q_j)^3 + \frac{\beta}{4}(q_{j+1} - q_j)^4 \right). \tag{1.1}$$

where $j = 0, 1, ..., N-1$, $q_j(t)$ represents the displacement from the equilibrium position of the particle j with periodic boundary conditions: $q_0 = q_N$, and $p_j(t)$ represents the momentum of particle j. κ, α, and β are spring elastic constants. We call this system α-FPUT model if $\alpha \neq 0, \beta = 0$, β-FPUT model if $\alpha = 0, \beta \neq 0$, and $(\alpha+\beta)$-FPUT model if both $\alpha \neq 0, \beta \neq 0$.

1.1: FPUT recurrence

Fermi's expectation was to see the redistribution of the energy among the Fourier modes, due to the presence of the cubic and quartic nonlinearity in the Hamiltonian, at the thermalization. Surprisingly, the unexpected outcomes largely deviated from their original conjecture: the system presented a quasi-periodic behavior with energy almost returning to the initial condition after some energy exchange. The first quasi-period was at about 29,000 computation cycles, and the energy of the first Fourier mode returns to more than 97% of its initial energy, when $N = 32, \alpha = \frac{1}{4}$ [3]. This recurrent phenomenon, which was then called the "FPUT recurrence", indicated the failure of arguments that any nonlinearity is sufficient to guarantee ergodicity.

The FPUT experiments inspired the numerical study of microscopic dynamics, to explain

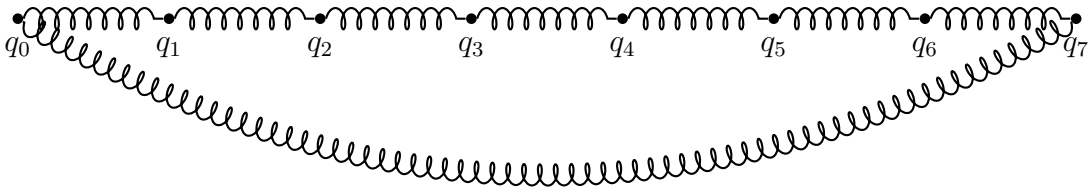


Figure 1.1: FPUT chain with periodic boundary conditions: eight masses q_j connected by nonlinear springs, with the last mass linked back to the first.

the conclusions of statistical mechanics. It was later shown that, for initial data in the long-wavelength and small-amplitude regime, the FPUT model formally reduces to the continuum Korteweg–de Vries (KdV) equation through multiple-scale expansions [4]. This connection was first demonstrated numerically by Zabusky and Kruskal in 1965, who simulated the KdV equation and uncovered the emergence of soliton solutions [5]. Their work led to two major breakthroughs in the effort to explain the "FPUT recurrence": the numerical observation of soliton interactions and the development of the inverse scattering transform, which provides exact solutions to the KdV equation [6]. Although these approximated integrable systems, whose motion is confined to invariant tori, give rise to recurrence, they cannot explain the eventual thermalization observed at longer times. Also, the approximated KdV equation conserves an $O(1)$ energy functional, whereas the discrete FPUT chain conserves a total energy that scales linearly with the number of particles, $O(N)$, in the continuum limit.

In the meantime of the FPUT experiment, Kolmogorov presented the Kolmogorov-Arnold-Moser (KAM) theorem, which illustrated a weak nonlinear perturbed integrable Hamiltonian will remain quasi-periodic if the deformed tori are under non-resonance condition. It means that the FPUT model with low enough energy would have quasi-periodic motion [7, 8]. But the big problem of the explanation was that the energy needed to be close to a minimum and the distance to the minimum had a strong dependence on the particle number N [9]. It was not until 2006, that the proof for the applicability of the KAM theorem to the FPUT model was eventually established by Rink [10]. However, the results only showed that the β-FPUT lattice with finite modes exhibits a completely integrable Birkhoff normal form, and there was no new explanation for the FPUT experiment. The results were further developed a year later for the $(\alpha + \beta)$-FPUT chain in [11].

Around the 1960s, Chirikov and Izrailev [7, 12, 13] estimated the threshold of the initial energy under which the KAM tori survive if the initial data are of long-wavelength type. They proposed, not quite rigorously, that under the presence of the nonlinearity, if the perturbation of the linear frequencies (related to the perturbation amplitude) is greater

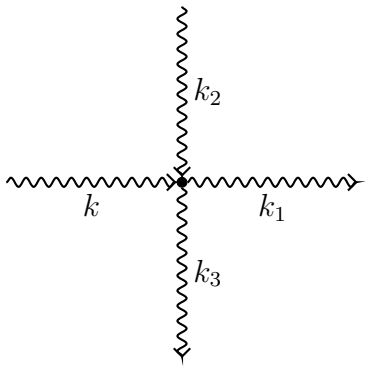
than the unperturbed frequency distance, i.e. unperturbed resonances overlap, then the deterministic trajectory may oscillate chaotically between two nonlinear resonances, which was also called the Chirikov resonance-overlap criterion. This criterion and the inspired numerical analysis showed that the FPUT chain reaches thermalization due to the overlapped nonlinear resonances when the initial energy is above a threshold. Nonetheless, it did not provide correct conclusions for the scenarios with small nonlinearity under the threshold which by the criterion may not result in resonances overlapping. Some recent numerical simulations [14, 15] showed that the α-FPUT model will reach a thermalization even with small nonlinearity and low initial energy.

Chirikov and Izrailev, along with further discussions by Ponno [16], also conjectured that in the thermodynamic limit, the FPUT recurrence would disappear, i.e. $\frac{E_c}{N} \to 0$ as $N \to \infty$, where E_c represents the critical energy threshold. However, later in 1971 Bocchieri *et al.*. [17] opposed the conjecture with numerical simulations. In 1982, a possibility for two stages of evolutions was given by Fucito *et al.* on the glasses theory [18]: the first stage, which is called the metastable state, related to the recurrence occurring at the short-time scale, and the second stage representing the thermal equilibrium state at the long-time scale. The analogy in the FPUT model below the critical energy was given recently by Carati *et al.* in [19, 20, 21]. Two years later in 2006, the metastability in the FPUT was analyzed by Bambusi and Ponno [22] using the approximation of the KdV equation [5, 6] mentioned above. The results were extended to a larger set of initial data to support the conjecture that the FPUT recurrence persists in the thermodynamic limit by [23, 24]. However, the above attempts to explain the FPUT recurrence had no progress toward obtaining the time scale for thermalization.

1.2: Wave Turbulence theory

In the recent twenty years the wave turbulence (WT) approach, an out-of-equilibrium statistical mechanics theory, was largely used to understand the energy transfer within the normal modes of the FPUT model in a weakly nonlinear dispersive regime. The WT approach, especially the wave kinetic equation, helps us understand the behavior of the wave spectrum in the FPUT system at the long-time scales and derive the thermalization time scale.

The WT theory was first introduced in 1929 by Peierls to study the phonons kinetics in anharmonic crystals [25]. It is not until the 1960s, that the WT theory, focusing on the wave kinetic equation and spectrum, was reinvestigated in the plasma physics [26] and water waves [27, 28]. The main theoretical consequences during that period were the Kolmogorov-Zakharov spectra solutions to the kinetic equation [29], discovered by Zakharov in 1965, and



$$k - k_1 + k_2 - k_3 = 0$$

Figure 1.2: Four-wave interaction satisfying the resonance condition $k - k_1 + k_2 - k_3 = 0$.

the further inspired theoretical developments were summarized by Zakharov *et al.* in [30].

The *wave kinetic equation* (WKE) occupies in wave turbulence the same position that Boltzmann's equation holds in dilute–gas theory: it furnishes an effective, statistical description of the second–moment dynamics of weakly nonlinear dispersive waves [31]. Formally the WKE is obtained in a *kinetic limit* where the domain size grows unboundedly $N \to \infty$, while the interaction strength tends to zero, $\beta \to 0$, in strict analogy with the Boltzmann–Grad scaling $N \to \infty$, $r \to 0$ and $Nr^{d-1} \sim 1$ by Lanford [32]. A precise *scaling law*—typically $\beta = N^{-\gamma}$ with $\gamma > 0$—specifies how the two parameters are tied together. Subsequent refinements [33, 34] to the Lanford's theorem extended the proof to systems with short–range potentials and to longer time intervals. In the weakly nonlinear regime ($\beta \ll 1$) these couplings accumulate slowly; the relevant time-scale is the *kinetic time* T_{kin}, when the nonlinear interactions dominate, and the spectrum $\mathbb{E}\,|a(t,k)|^2$ evolves according to the WKE collision operator.

In the recent twenty years, the rigorous justification of the WT theory via the kinetic equation has been done in dimensions $d \geq 2$. The first rigorous step towards wave-kinetic theory for the cubic nonlinear Schrödinger (NLS) equation was the derivation of the *Continuous Resonant* (CR) equation—describing the large–box limit of the deterministic dynamics—via Birkhoff normal-form reductions by Faou *et al.* [35] and independently by Buckmaster *et al.* [36, 37] in 2016. Buckmaster *et al.* then incorporated random initial data and employed Feynman diagram expansions to validate the WKE up to times $t < T_{\text{kin}}^{\frac{1}{2}}$ [38]. Shortly thereafter, Deng and Hani [39] and Collot and Germain [40, 41] extended this result—still in $d \geq 2$—to times $t \lesssim T_{\text{kin}}^{1-\epsilon}$ under scaling laws $0 < \gamma \leq 1$ and $\gamma = 1$, respectively, thus

achieving the analog of Lanford's short-time theorem for the NLS WKE. In follow-up works Deng and Hani pushed their analysis to the full kinetic time T_{kin} [42, 43] and ultimately to arbitrarily long times [44]. Remarkably, the combinatorial and renormalisation methods they introduced were then adapted to give a parallel long-time derivation of the Boltzmann equation for particle systems in [45]. In 2024, Vassilev [46] has derived the wave kinetic equations for the Majda-McLaughlin-Tabak (MMT) model at $d = 1$ of size L with the dispersion relation of $\omega(k) = |k|^{\sigma}$, and $0 < \sigma \leq 2$ and $\sigma \neq 1$ up to timescales $T \sim L^{-\epsilon} T_{\text{kin}}^{\frac{5}{8}}$. Banks et al. [47] consider finite-size systems whose dynamics arise from nonlinear interactions among six wave quintic NLS, predict that the ensemble-averaged wave dynamics in such systems are accurately described by the wave kinetic equation of wave turbulence theory, explain why the kinetic description fails outside these regimes, and validate these predictions by directly comparing ensemble averages of the full dynamical solutions with those of the kinetic equation numerically.

The key infrastructure in the above derivations, Feynman diagrams—originally introduced in 1949 for quantum-field perturbation theory—were soon adopted to depict interaction histories in both particle and wave kinetic-theory derivations. Their rigorous convergence for wave systems was first proved by Spohn in 1977 [48] and later extended to global-in-time results by Erdős–Yau [49] and Erdős–Salmhofer–Yau [50]. However, the rigorous justification above was done without the presence of the unconserved nonlinear frequency shifts as in β-FPUT model, which need to be carefully treated during the estimation and approximation processes.

1.3: The Wave Turbulence approach to the FPUT model

The early applications of WT theory to the α-FPUT model, done by Lvov *et al.* in 2002 [51, 52], analyzed the time scales of the energy spectrum approaching the equilibrium. The authors' analysis of the kinetic equation along with the previous numerical simulations, indicated that in the initial phase the energy exchanges within the low-wavenumber modes through quasi-resonant triads, and in the final phase the energy equidistributed among the modes through the quartet interactions.

In 2015, it was found that the equipartition of energy of α-FPUT model for $N = 16, 32, 64$ resulted from the six-wave interactions by Onorato *et al.* [14], which can also be applied to β-FPUT model [53], after the authors found that the exact resonant quartets are all isolated and not responsible for the energy transfer. The authors then conjectured that the time scale of the equipartition of energy due to the six-wave interaction should be of order $O(\alpha^{-8})$, which referred to the time scale for the kinetic equation of the six-wave interaction

formally derived by Nazarenko and Laurie [31, 54]. This conjecture was well supported by their numerical simulations testing the equilibrium time scale. They also assumed that the integrable part of the Hamiltonian, consisting of the isolated resonant quartets, does not contribute to the irreversible energy transfer.

However, there are several limitations in their conjecture and further discussion needed:

1. First, the evolution equation of the six-wave interactions in the FPUT model, which includes the four-wave resonances, is not the same as the evolution equation for the general six-wave interactions in [31], although they formally describe evolutions on the same time scale.
2. Second, the method of formal derivations in [31] is still far from rigorous, especially when dealing with the unconserved nonlinear frequency shifts (this part will be illustrated in detail in Section 1.6.
3. Furthermore, the canonical transformation commonly applied to remove the non-resonant parts in the evolution equation needs to be compatible with the scaling law of the rigorous derivation for the wave kinetic equation. And we will verify this carefully in the later chapters and only derive the wave kinetic equation from the reduced evolution equation in this thesis.
4. Finally, the equipartition of energy comes from the exact resonances in their regime of fixed N and $\beta \to 0$. But those exact resonances are dominated by the quasi-resonances, referring to the case $|\omega_1 - \omega_2 + \omega_3 - \omega_4| < T^{-1}$, under the scaling law when rigorously deriving the kinetic equation [39].

Bustamante *et al.* continued to analyze the exact resonances for the FPUT system in 2018 [55]. They applied a number of theoretical results to find the lowest order of resonances responsible for the irreversible energy transfer among the four-, five-, and six-wave interactions. In the same year, Lvov and Onorato find a different time scale $O(\beta^{-1})$ at equilibrium for the β-FPUT model using the Chirikov overlap criterion, when the nonlinearity β increases to the level of 0.01 [56]. They further tested the β-FPUT model under a low-temperature regime [57] so that the ratio of the anharmonic parts of the Hamiltonian is small compared to the harmonic parts. In steady state conditions, the system behaves in two components: kinetic (high-wavenumber) modes, which exhibit regular diffusive transport in agreement with Fourier's law, and scarcely interacting ballistic (low-wavenumber) modes. And the transition between the two sets of modes contributes to the divergence of the energy conductivity. Their recent work in 2022, continues to check numerically the anomalous scaling of the energy conductivity for the β-FPUT model [58]. They used a previous result

by Lukkarinen and Spohn [59], in which the authors derived the solutions to the collision integral of the β-FPUT model and reduce it to a single integral in the limiting sense. Later the next year, Onorato *et al.* published a comprehensive review [60] of one-dimensional chains—including α- and β-FPUT—highlighting both exact and quasi-resonant processes in thermalization and laying out key open problems for wave kinetic theory. In studies of the diatomic α-FPUT model [61], Pezzi *et al.* have shown that, upon diagonalizing the harmonic Hamiltonian into acoustic and optical modes via new canonical variables, isolated three-wave resonances—which only occur for mass ratios below three—fail to induce thermalization, so that on longer timescales energy transfer is governed instead by four-wave processes captured by two coupled wave-kinetic equations with corresponding equilibrium solutions.

Guasoni et al. [62] show that even in the weakly nonlinear, strongly incoherent regime, large-scale convection among random waves triggers a novel incoherent modulational instability—which suppresses Landau damping, spontaneously generates exponentially growing phase correlations, and produces FPUT-like entropy-reducing recurrences in nonintegrable wave systems while preserving time-reversal symmetry.

More recently, Ganapa [63] investigated the α-FPUT system with the modes $k = 1$ and -1 excited initially using a canonical transformation to eliminate nonresonant three-wave interactions and constructed a perturbative expansion in terms of the dimensionless parameter ε which is normalized from α. By analyzing the transformation coefficient $A^{(2)}_{1,1,2}$, they concluded that the perturbation series remains valid only when $\varepsilon A^{(2)}_{k_1,k_1,k_2} \ll 1$, leading to the condition $\varepsilon \ll O(N^{-1.5})$. To validate this estimate, the author performed direct numerical simulations of Hamilton's equations and examined the short-time behavior of the modal energy $E_k = \omega_k |a_k|^2$ for $k = 2, 3$ as a function of ε. They observed significant deviations of the modal energy E_2 and E_3 from order ε^2 and ε^4 respectively, when $\varepsilon A^{(2)}_{1,1,2} \sim 1$, indicating that the three wave resonances removed to higher orders contribute with the presence of small denominators in $A^{(2)}_{1,1,2}$. This result suggests that the canonical transformation diverges for larger N or stronger nonlinearity in α-FPUT model. And we will further investigate in this thesis on the stochastic threshold for β-FPUT model to perform the canonical transformation for initial conditions with random phase and various large N and nonlinearity β.

All of the above WT approaches to FPUT systems rely on the rigorous justification for the kinetic equations under the presence of unconserved nonlinear frequency shifts.

1.4: The FPUT model

In this thesis we derive the wave kinetic equation for β-Fermi-Pasta-Ulam-Tsingou (β-FPUT) system and at the kinetic time scale, for the partial range of scaling laws between the large box

and weak nonlinearity limits. This is the first step aiming at providing rigorous mathematical foundation for the wave turbulence theory on FPUT system. The Fermi-Pasta-Ulam-Tsingou system was first analyzed in 1955 [3] to study the thermal equipartition of crystals. The β-FPUT model has N identical masses connected by nonlinear springs with the elastic force $F = -\kappa\Delta q + \beta\Delta q^3$, where $\kappa, \beta \neq 0$ are spring elastic constants. And the equation of motion for a β-FPUT chain can be expressed as:

$$m\ddot{q}_j = \kappa\left[(q_{j+1} - q_j) - (q_j - q_{j-1})\right] + \beta\left[(q_{j+1} - q_j)^3 - (q_j - q_{j-1})^3\right], \tag{1.2}$$

where $j = 0, 1, ..., N-1$ and $q_j(t)$ represents the displacement from the equilibrium position of the particle j with periodic boundary conditions: $q_0 = q_N$ (see e.g. [3] and [55, equation (6)]). Then we can get the Hamiltonian:

$$H = \sum_{j=0}^{N-1}\left(\frac{p_j^2}{2m} + \frac{\kappa}{2}(q_{j+1} - q_j)^2 + \frac{\beta}{4}(q_{j+1} - q_j)^4\right), \tag{1.3}$$

where $p_j(t)$ represents the momentum of particle j.

1.4.1. Discrete Fourier transform. Next, we perform a Discrete Fourier transform and its inverse to the β-FPUT system as follows:

$$Q_k = \frac{1}{N}\sum_{j=0}^{N-1} q_j e^{-i2\pi kj/N}, \; q_j = \sum_{k=0}^{N-1} Q_k e^{i2\pi jk/N}; \tag{1.4}$$

$$P_k = \frac{1}{N}\sum_{j=0}^{N-1} p_j e^{-i2\pi kj/N}, \; p_j = \sum_{k=0}^{N-1} P_k e^{i2\pi jk/N}, \tag{1.5}$$

where Q_k, P_k are Fourier transforms of the displacement and momentum respectively. From the relation:

$$\dot{q}_j = \frac{\partial H}{\partial p_j} = \frac{p_j}{m},$$

we should get:

$$P_k = m\dot{Q}_k. \tag{1.6}$$

And we should also note that:

$$Q_k = Q_{N-k}^*, \; P_k = P_{N-k}^*, \text{ for } k = 0, 1, ..., N-1. \tag{1.7}$$

Plugging (1.4) and (1.5) into the equation of motion (1.2), for $j = 0, 1, ..., N-1$, we get:

$$
\begin{aligned}
m\sum_{k=0}^{N-1}\ddot{Q}_k e^{i2\pi jk/N} &= \kappa\left[\sum_{k=0}^{N-1}Q_k e^{i2\pi jk/N}\left(e^{i2\pi k/N}-2+e^{-i2\pi k/N}\right)\right] \\
&+\beta\left[\left(\sum_{k=0}^{N-1}Q_k e^{i2\pi jk/N}\left(e^{i2\pi k/N}-1\right)\right)^3-\left(\sum_{k=0}^{N-1}Q_k e^{i2\pi jk/N}\left(1-e^{-i2\pi k/N}\right)\right)^3\right], \\
&=\kappa\sum_{k=0}^{N-1}Q_k e^{i2\pi jk/N}\left(2i\sin\left(\frac{\pi k}{N}\right)\right)^2+\beta\sum_{k_2,k_3,k_4}Q_{k_2}Q_{k_3}Q_{k_4}e^{i2\pi j(k_2+k_3+k_4)/N} \\
&\times\left(\left(e^{i\pi(k_2+k_3+k_4)/N}-e^{-i\pi(k_2+k_3+k_4)/N}\right)(2i)^3\sin\left(\frac{\pi k_2}{N}\right)\sin\left(\frac{\pi k_3}{N}\right)\sin\left(\frac{\pi k_4}{N}\right)\right).
\end{aligned}
$$

Then we can get:

$$
m\left(\ddot{Q}_{k_1}+\omega_{k_1}^2 Q_{k_1}\right)=\beta\sum_{k_2+k_3+k_4=k_1}\hat{T}_{-1,2,3,4}Q_{k_2}Q_{k_3}Q_{k_4}, \tag{1.8}
$$

where the sums $\sum_{k_2+k_3+k_4=k_1}$ are taking over $\{k_2, k_3, k_4 : k_2+k_3+k_4 = k_1 \bmod N\}$, and

$$
\begin{aligned}
\omega_k &= \omega(k) = 2\sqrt{\frac{\kappa}{m}}\left|\sin\left(\frac{\pi k}{N}\right)\right|, \\
\hat{T}_{-1,2,3,4} &= 16\sin\left(\frac{\pi(k_2+k_3+k_4)}{N}\right)\sin\left(\frac{\pi k_2}{N}\right)\sin\left(\frac{\pi k_3}{N}\right)\sin\left(\frac{\pi k_4}{N}\right).
\end{aligned}
$$

1.4.2. Normal modes. We then introduce the normal modes $a_k(t)$ as:

$$
a_k=\frac{\sqrt{2}}{2}\left[(m\omega_k)^{\frac{1}{2}}Q_k+i(m\omega_k)^{-\frac{1}{2}}P_k\right],\ \text{for } k=1,...,N-1. \tag{1.9}
$$

So then if we apply the property (1.6), we will get:

$$
a_{N-k}^*=\frac{\sqrt{2}}{2}\left[(m\omega_k)^{\frac{1}{2}}Q_k-i(m\omega_k)^{-\frac{1}{2}}P_k\right]. \tag{1.10}
$$

We take the derivative of $a_k(t)$:

$$
\dot{a}_k=\frac{\sqrt{2}}{2}\left[(m\omega_k)^{\frac{1}{2}}\dot{Q}_k+i(m\omega_k)^{-\frac{1}{2}}m\ddot{Q}_k\right]. \tag{1.11}
$$

Then we can express Q_k, $\dot{Q}_k$, and $\ddot{Q}_k$ as:

$$Q_k = \frac{\sqrt{2}}{2}(m\omega_k)^{-\frac{1}{2}}(a_k + a^*_{N-k}), \tag{1.12}$$

$$\dot{Q}_k = -i\frac{\sqrt{2}}{2}\frac{(m\omega_k)^{\frac{1}{2}}}{m}(a_k - a^*_{N-k}), \tag{1.13}$$

$$\ddot{Q}_k = -i\sqrt{2}\frac{(m\omega_k)^{\frac{1}{2}}}{m}\left[\dot{a}_k + \frac{i}{2}\omega_k(a_k - a^*_{N-k})\right]. \tag{1.14}$$

Plugging (1.12) and (1.14) into (1.8), we get:

$$\begin{aligned} &m\left(-i\sqrt{2}\frac{(m\omega_{k_1})^{\frac{1}{2}}}{m}\left[\dot{a}_{k_1} + \frac{i}{2}\omega_{k_1}(a_{k_1} - a^*_{N-k_1})\right] + \omega_{k_1}^2\frac{\sqrt{2}}{2}(m\omega_{k_1})^{-\frac{1}{2}}(a_{k_1} + a^*_{N-k_1})\right) \\ =&\beta\sum_{k_2+k_3+k_4=k_1}\hat{T}_{-1,2,3,4}\frac{\sqrt{2}}{4}m^{-\frac{3}{2}}(\omega_{k_2}\omega_{k_3}\omega_{k_4})^{-\frac{1}{2}}(a_{k_2} + a^*_{N-k_2})(a_{k_3} + a^*_{N-k_3})(a_{k_4} + a^*_{N-k_4}) \end{aligned} \tag{1.15}$$

Then the evolution equation for $a_{k_1}(t)$ becomes:

$$i\dot{a}_{k_1} = \omega_{k_1}a_{k_1} + \frac{\beta}{3}\sum_{k_2+k_3+k_4=k_1}\tilde{T}_{-1,2,3,4}(a_{k_2} + a^*_{N-k_2})(a_{k_3} + a^*_{N-k_3})(a_{k_4} + a^*_{N-k_4}), \tag{1.16}$$

where

$$\tilde{T}_{-1,2,3,4} = \frac{-3\hat{T}_{-1,2,3,4}}{4m^2\sqrt{\omega_{k_1}\omega_{k_2}\omega_{k_3}\omega_{k_4}}} = -\frac{3}{4\kappa^2}\iota\left(\frac{k_2+k_3+k_4}{N}\right)\iota\left(\frac{k_2}{N}\right)\iota\left(\frac{k_3}{N}\right)\iota\left(\frac{k_4}{N}\right)\prod_{i=1}^{4}\sqrt{\omega_{k_i}}. \tag{1.17}$$

where we define $\iota(x) := \operatorname{sgn}\sin(x)$ a 2-periodic function on $\mathbb{R}$. Rewrite $k_2' = N - k_2, k_3' = N - k_3$, and $k_4' = N - k_4$, we get:

$$\begin{aligned} i\dot{a}_{k_1} =&\omega_{k_1}a_{k_1} + \frac{\beta}{3}\sum_{k_2,k_3,k_4}\Big[\tilde{T}_{-1,2,3,4}a_{k_2}a_{k_3}a_{k_4}\delta(k_1 - k_2 - k_3 - k_4) \\ &+ 3\tilde{T}_{-1,2,-3,4}a_{k_2}a^*_{k_3}a_{k_4}\delta(k_1 - k_2 + k_3 - k_4) + 3\tilde{T}_{1,2,3,-4}a^*_{k_2}a^*_{k_3}a_{k_4}\delta(k_1 + k_2 + k_3 - k_4) \\ &+ \tilde{T}_{1,2,3,4}a^*_{k_2}a^*_{k_3}a^*_{k_4}\delta(k_1 + k_2 + k_3 + k_4)\Big], \end{aligned} \tag{1.18}$$

where

$$\tilde{T}_{-1,2,3,4} = -\frac{3}{4\kappa^2}\iota\left(\frac{k_2+k_3+k_4}{N}\right)\iota\left(\frac{k_2}{N}\right)\iota\left(\frac{k_3}{N}\right)\iota\left(\frac{k_4}{N}\right)\prod_{i=1}^{4}\sqrt{\omega_{k_i}} \tag{1.19}$$

$$\tilde{T}_{-1,2,-3,4} = \frac{3}{4\kappa^2}\iota\left(\frac{k_2-k_3+k_4}{N}\right)\iota\left(\frac{k_2}{N}\right)\iota\left(\frac{k_3}{N}\right)\iota\left(\frac{k_4}{N}\right)\prod_{i=1}^{4}\sqrt{\omega_{k_i}}, \tag{1.20}$$

$$\tilde{T}_{1,2,3,-4} = \frac{3}{4\kappa^2}\iota\left(\frac{k_2+k_3-k_4}{N}\right)\iota\left(\frac{k_2}{N}\right)\iota\left(\frac{k_3}{N}\right)\iota\left(\frac{k_4}{N}\right)\prod_{i=1}^{4}\sqrt{\omega_{k_i}}, \tag{1.21}$$

$$\tilde{T}_{1,2,3,4} = -\frac{3}{4\kappa^2}\iota\left(\frac{k_2+k_3+k_4}{N}\right)\iota\left(\frac{k_2}{N}\right)\iota\left(\frac{k_3}{N}\right)\iota\left(\frac{k_4}{N}\right)\prod_{i=1}^{4}\sqrt{\omega_{k_i}}. \tag{1.22}$$

Note that due to the positivity and strict subadditivity of $\omega(k)$, we know that:

$$0 < \omega(k_1+k_2+k_3) < \omega(k_1)+\omega(k_2)+\omega(k_3), \text{ for } k_i = 1, ..., N-1. \tag{1.23}$$

This fact was well explained in [55, Theorem 3.8].

1.4.3. Covariance of normal modes. By spatial homogeneity, we may assume that

$$\langle q_j q_{j'}\rangle = f_1(j-j'), \quad \langle p_j p_{j'}\rangle = f_2(j-j'), \quad \langle q_j p_{j'}\rangle = f_3(j-j')$$

where $\langle\cdot\rangle$ averages over random initial data, and f_1, f_2 are symmetric (i.e. $f_1(j) = f_1(-j)$). This implies that $\widehat{f_1}(k) = \widehat{f_1}(-k) = \widehat{f_1}(k)^*$ (and similarly for f_2), and $\widehat{f_3}(k) = \widehat{f_3}(-k)^*$. We can calculate the covariance of a_k, $a_{k'}^*$ and $a_{k'}$:

$$\begin{aligned}\langle a_k a_{k'}^*\rangle &= \left\langle \frac{1}{m\sqrt{\omega_k\omega_{k'}}}(m\omega_k Q_k + iP_k)(m\omega_{k'}Q_{k'}^* - iP_{k'}^*)\right\rangle \\ &= \frac{1}{m\sqrt{\omega_k\omega_{k'}}}\left\langle m^2\omega_k\omega_{k'}Q_kQ_{k'}^* + im\omega_{k'}P_kQ_{k'}^* - im\omega_kP_{k'}^*Q_k + P_kP_{k'}^*\right\rangle\end{aligned} \tag{1.24}$$

for which we need:

$$\begin{aligned}\langle Q_k Q_{k'}^*\rangle &= \frac{1}{N^2}\sum_{j,j'} e^{-i2\pi kj/N}e^{i2\pi k'j'/N}\langle q_j q_{j'}\rangle \\ &= \frac{1}{N^2}\sum_{j,j'} e^{-i2\pi k(j-j')/N}e^{-i2\pi(k-k')j'/N}f_1(j-j') \\ &= \frac{1}{N^2}\sum_{j'=0}^{N-1} e^{-i2\pi(k-k')j'/N}\left(\sum_{j-j'=0}^{N-1} e^{-i2\pi k(j-j')/N}f_1(j-j')\right)\end{aligned}$$

$$= \delta(k-k')\widehat{f}_1(k). \tag{1.25}$$

Similarly, we have:

$$\langle P_k P_{k'}^* \rangle = \delta(k-k')\widehat{f}_2(k), \tag{1.26}$$
$$\langle Q_k P_{k'}^* \rangle = \delta(k-k')\widehat{f}_3(k), \tag{1.27}$$
$$\langle P_k Q_{k'}^* \rangle = \delta(k-k')\widehat{f}_3(-k), \tag{1.28}$$
$$\langle Q_k Q_{k'} \rangle = \delta(k+k')\widehat{f}_1(k), \tag{1.29}$$
$$\langle P_k P_{k'} \rangle = \delta(k+k')\widehat{f}_2(k), \tag{1.30}$$
$$\langle Q_k P_{k'} \rangle = \delta(k+k')\widehat{f}_3(k), \tag{1.31}$$
$$\langle P_k Q_{k'} \rangle = \delta(k+k')\widehat{f}_3(-k), \tag{1.32}$$

Then we can get:

$$\begin{aligned}\langle a_k a_{k'}^* \rangle &= \delta(k-k')\frac{1}{m\sqrt{\omega_k\omega_{k'}}}\left[m^2\omega_k\omega_{k'}\widehat{f}_1(k) + im\omega_{k'}\widehat{f}_3^*(k) - im\omega_k\widehat{f}_3(k) + \widehat{f}_2(k)\right] \\ &= \delta(k-k')\left[m\omega_k\widehat{f}_1(k) + 2\mathrm{Im}\widehat{f}_3(k) + \frac{1}{m\omega_k}\widehat{f}_2(k)\right] \qquad (1.33) \\ \langle a_k a_{k'} \rangle &= \delta(k+k')\frac{1}{m\sqrt{\omega_k\omega_{k'}}}\left[m^2\omega_k\omega_{k'}\widehat{f}_1(k) + im\omega_{k'}\widehat{f}_3(-k) + im\omega_k\widehat{f}_3(k) - \widehat{f}_2(k)\right] \\ &= \delta(k+k')\left[m\omega_k\widehat{f}_1(k) + 2i\mathrm{Re}\widehat{f}_3(k) - \frac{1}{m\omega_k}\widehat{f}_2(k)\right]. \qquad (1.34)\end{aligned}$$

Since $\widehat{f}_1(k)$ and $\widehat{f}_2(k)$ are real valued, this means that $\langle a_k a_{N-k}\rangle \neq 0$ unless $m^2\omega_k^2\widehat{f}_1(k) = \widehat{f}_2(k)$ and $\mathrm{Re}\widehat{f}_3(k) = 0$ or equivalently $\widehat{f}_3(-k) = -\widehat{f}_3(k)$ (i.e. $\widehat{f}_3$ is odd). It means that for the original dynamic equation (1.2), the lowest order nontrivial statistics are given by the covariances $\langle |a_k|^2\rangle$ and $\langle a_k a_{N-k}\rangle$. The latter quantity is typically assumed to vanish initially, at time $t = 0$ ([64]). For certain systems, like the reduced FPUT system introduced below, the vanishing of $\langle a_k(0)a_{N-k}(0)\rangle$ is preserved in time (see Section 1.4.5); however, in general, one can only attempt to prove that it vanishes asymptotically (i.e. upon taking the kinetic limit) for the kinetic theory to hold.

1.4.4. The reduced evolution equation. Denote $\mathbb{Z}_N := N^{-1}\mathbb{Z}$. Throughout the remainder of this section and up to Chapter 8, we adopt the lattice wave number $k \in \mathbb{Z}_N \cap (0,1)$, in place of the integer wave number in $\mathbb{Z}/N\mathbb{Z}$. Rewriting $b(t,k) = \sqrt{N}a(t,Nk)$ for $k \in \mathbb{Z}_N \cap (0,1)$, and removing the non-resonant part in (1.18), we arrive at the following reduced

evolution equation for b_k:

$$i\dot{b_k}(t) = \omega_k b_k(t) + \frac{\beta}{N} \sum_{k_1-k_2+k_3=k} T_{k,1,2,3} b_{k_1}(t) b^*_{k_2}(t) b_{k_3}(t), \tag{R-FPUT}$$

where $k, k_i \in \mathbb{Z}_N \cap (0,1)$, $\sum_{k_1-k_2+k_3=k}$ taking over $\{k_2, k_3, k_4 : k_2+k_3+k_4 = k_1 \bmod 1\}$, and we redefine:

$$\omega_k = \omega(k) := 2\sqrt{\frac{\kappa}{m}} \left|\sin(\pi k)\right|,$$
$$T_{k,1,2,3} := \frac{3}{4\kappa^2} \iota(k_1-k_2+k_3)\iota(k_1)\iota(k_2)\iota(k_3)\sqrt{\omega_k \omega_{k_1} \omega_{k_2} \omega_{k_3}}.$$

The Hamiltonian for (R-FPUT) in normal variables b_k becomes:

$$H = \sum_{k \in \mathbb{Z}_N \cap (0,1)} \omega_k |b_k|^2 + \frac{\beta}{2N} \sum_{k_1-k_2+k_3-k_4=0} T_{1,2,3,4} b^*_{k_1} b_{k_2} b^*_{k_3} b_{k_4}. \tag{1.35}$$

We will prove the WKE for (R-FPUT) instead of the full original evolution equation (1.18) in this thesis and leave the complete derivation for future work.

1.4.5. The initial data. Assuming that q_j's are of $O(1)$, it is easy to see that:

$$\|b_k\|_{\ell^2} \sim \sqrt{N} \|Q_k\|_{\ell^2} \sim O(1). \tag{1.36}$$

To apply the Wave Turbulence formalism and formally derive the kinetic equation for (R-FPUT), we need to define well-prepared initial conditions for b_k:

$$b_k(0) = \sqrt{n_{\text{in}}(k)}\eta_k(\varrho), \tag{DAT}$$

where $n_{\text{in}} \geq 0$ represents the deterministic amplitude of an $O(1)$ smooth function (or a function with sufficient regularity) defined on standard torus of size 1, namely $\mathbb{T} = [0,1]$ with periodic boundary conditions. $\eta_k(\varrho)$'s are i.i.d. mean-zero complex random variables with unit variance, which are assumed to be either standard complex Gaussian or uniform distributed on the unit circle. ϱ labels an individual random sample on which the variables η_k are evaluated. For the reduced evolution equation (R-FPUT), if we make a global phase translation $b_k \to b_k e^{i\theta}$, the initial distribution of b_k does not change, so we can get:

$$\langle b_k b_{k'} \rangle = \langle b_k e^{i\theta} b_{k'} e^{i\theta} \rangle = e^{i2\theta} \langle b_k b_{k'} \rangle \tag{1.37}$$

for any $\theta \in \mathbb{R}$, which means $\langle b_k b_{k'} \rangle \equiv 0$ for any $k, k' \in \mathbb{Z}_N \cap (0,1)$, and we only need to consider $\langle |b_k|^2 \rangle$. This is different from the original equation that we need to consider both $\langle |a_k|^2 \rangle$ and $\langle a_k a_{N-k} \rangle$ for $k \in \mathbb{Z}/N\mathbb{Z}$. We should also notice that by the standard hypercontractivity estimates as in [39, Lemma 3.1]:

$$\mathbb{P}\left(\left| \sum_{k_1 - k_2 + k_3 - k_4 = 0} T_{1,2,3,4} b_{k_2}(0) b^*_{k_3}(0) b_{k_4}(0) \right| \geq A M^{\frac{1}{2}} \right) \leq C e^{-cA^{\frac{2}{3}}}, \tag{1.38}$$

for some positive constant $A, C, c > 0$, and

$$\begin{aligned} M &= \mathbb{E} \left| \sum_{k_1 - k_2 + k_3 - k_4 = 0} T_{1,2,3,4} b_{k_2}(0) b^*_{k_3}(0) b_{k_4}(0) \right|^2 \\ &\sim \sum_{k_1 - k_2 + k_3 - k_4 = 0} |T_{1,2,3,4}|^2 \, n_{\text{in}}(k_2) \, n_{\text{in}}(k_3) \, n_{\text{in}}(k_4) \sim O(N^2). \end{aligned} \tag{1.39}$$

Here we applied the Wick's contraction theorem (see [31, Theorem 5.1]) to evaluate the expectation value. It means that with high probability:

$$\sum_{k_1 - k_2 + k_3 - k_4 = 0} T_{1,2,3,4} b_{k_2} b^*_{k_3} b_{k_4} \sim O(N), \tag{1.40}$$

which matches with the order of other terms in (R-FPUT). Similarly, in (1.35) we can get with high probability:

$$\sum_{k_1 - k_2 + k_3 - k_4 = 0} T_{1,2,3,4} b^*_{k_1} b_{k_2} b^*_{k_3} b_{k_4} \sim O(N^{\frac{3}{2}}). \tag{1.41}$$

Combining (1.36) and (1.41), we have:

$$H \sim O(N). \tag{1.42}$$

Our goal is to rigorously derive the wave kinetic equation (WKE) for the dynamic of the wave spectrum $n(t,k) = \mathbb{E}|b(t,k)|^2$, such that $n(0,k) = n_{\text{in}}(k)$.

1.4.6. The wave kinetic equation. The wave kinetic equation is given by:

$$\begin{cases} \partial_t n(t,k) = \mathcal{K}(n(t))(k), \\ n(0,k) = n_{\text{in}}(k), \end{cases} \tag{WKE}$$

where n_{in} is defined as in Section 1.4.5 for $k \in \mathbb{T}$, and the nonlinearity collision operator $\mathcal{K}$ is given by

$$\mathcal{K}(\phi)(\xi) = \int_{\substack{(\xi_1,\xi_2,\xi_3)\in\mathbb{T}^3 \\ \xi_1-\xi_2+\xi_3=\xi}} \phi_\xi\phi_{\xi_1}\phi_{\xi_2}\phi_{\xi_3}\left(\frac{1}{\phi_\xi}-\frac{1}{\phi_{\xi_1}}+\frac{1}{\phi_{\xi_2}}-\frac{1}{\phi_{\xi_3}}\right)\boldsymbol{\delta}(\omega_1-\omega_2+\omega_3-\omega)d\xi_1 d\xi_2 d\xi_3, \tag{KIN}$$

where we denote, for $i = 1, 2, 3$,

$$\begin{aligned} &\phi = \phi(t,\xi), \quad \phi_{\xi_i} = \phi(t,\xi_i), \\ &\omega = 2\sin(\pi\xi), \quad \omega_i = 2\sin(\pi\xi_i). \end{aligned}$$

Here and below $\boldsymbol{\delta}$ denotes the Dirac delta. Given any smooth initial data $n_{\text{in}}(k)$, the equation (WKE) has a unique local solution $n = n(t,k)$ on some short time interval depending on n_{in}.

1.5: Statement of the main result

The main result is stated as follows.

Theorem 1. *Fix $\gamma \in (0,1)$. Fix a smooth function $n_{\text{in}} \in C^\infty(\mathbb{T} \to [0,\infty))$, $A \geq 40$, and $\epsilon \ll 1$. Consider the equation (R-FPUT) with random initial data (DAT), and assume $\beta = N^{-\gamma}$ so that $T_{kin} = \frac{N^{2\gamma}}{4\pi}$. Fix $T = N^{-\epsilon}\min(N, N^{\frac{5}{4}\gamma})$. Then, with probability $\geq 1 - N^{-A}$, for $N^{0+} \leq t \leq T$,*

$$\mathbb{E}\,|b(t,k)|^2 = n_{\text{in}}(k) + \frac{t}{T_{\text{kin}}}\mathcal{K}(n_{\text{in}})(k) + o_{\ell^\infty_k}\left(\frac{t}{T_{\text{kin}}}\right).$$

1.6: Contributions and future directions

Although the WKE has been rigorously derived for the cubic NLS equation in dimensions $d \geq 2$ [42] and for the MMT model in $d = 1$ [46], there is still lack of rigorous justification for the β-FPUT model. We demonstrate below the main contributions of this thesis to the rigorous derivation of WKE for β-FPUT model.

Significance of unconserved frequency shift. Starting from the reduced evolution equation (R-FPUT), we would like to first make the frequency shift and remove the secular terms in the evolution equation. For other models such as NLS, the nonlinear frequency shift that enters the phase is *conserved* over time, hence its removal is trivial and requires no particular treatment. In the one-dimensional β–FPUT chain, the corresponding nonlinear

frequency shift is *not conserved*. In the previous approaches [31, 54, 53, 60], the nonlinear frequency shift is defined as:

$$\omega_k^{\mathrm{NL}} := \frac{2}{N}\sum_l T_{k,k,l,l}\,|b_l|^2$$
$$\Omega_{\mathrm{NL}} = \Omega_{k,1,2,3}^{\mathrm{NL}} := \omega_k^{\mathrm{NL}} - \omega_{k_1}^{\mathrm{NL}} + \omega_{k_2}^{\mathrm{NL}} - \omega_{k_3}^{\mathrm{NL}}.$$

To remove the nonlinear frequency shift ω_{NL}, a change of variable is needed:

$$b_k' = \exp\left(i\left(\omega_k t + \beta\int_0^t \omega_k^{\mathrm{NL}} ds\right)\right) b_k.$$

The nonlinear frequency removed above is stochastic in the phase exponent and cannot be paired using the Wick's contraction rule. In [54], the phase factor generated by $\Omega_{\mathrm{NL}}(t)$ is handled by a direct Taylor expansion,

$$\begin{aligned} e^{i\beta\int_0^t \Omega_{\mathrm{NL}}(\tau)d\tau} &= 1 + i\Big(\beta\int_0^t \Omega_{\mathrm{NL}} d\tau\Big) - \frac{1}{2}\Big(\beta\int_0^t \Omega_{\mathrm{NL}} d\tau\Big)^2 - \frac{i}{6}\Big(\beta\int_0^t \Omega_{\mathrm{NL}} d\tau\Big)^3 + \cdots \\ &\approx 1 + i\beta t\Omega_{\mathrm{NL}}^{(0)}, \qquad \text{for } \beta t\Omega_{\mathrm{NL}}^{(0)} \ll 1, \end{aligned} \tag{1.43}$$

with the expansion $\Omega_{\mathrm{NL}} := \Omega_{\mathrm{NL}}^{(0)} + \beta\Omega_{\mathrm{NL}}^{(1)} + O(\beta^2)$. This approach assumes that $\beta t\Omega_{\mathrm{NL}}^{(0)} \ll 1$, which may only work under the intermediate time scale in the author's thesis: $T \ll \beta^{-1}$.

In contrast, we want to derive the WKE up to the time scale $T = N^{-\epsilon}\beta^{-\frac{5}{4}}$ and need to choose the frequency shift carefully. We identify and make the nonlinear frequency shift $\widetilde{\omega}_k$ which satisfies the ordinary differential equation (ODE):

$$\partial_s\widetilde{\omega}_k(s) = \frac{2\beta T}{N}\sum_{k_1} T_{k,1,1,k}\mathbb{E}|c_{k_1}^{\leq n}(s)|^2. \tag{1.44}$$

Here, $c_{k_1}^{\leq n}$ represents the sum of ternary tree expansion terms up to order n. The shift itself is *deterministic* and defined implicitly as the solution of a suitable ODE such that divergent factor $2\sum_{k_1} T_{k,1,1,k}|c_{k_1}(s)|^2$ will be canceled as much as possible. Removing that shift produces an intermediate variable c whose dynamics avoid the full degenerate index pairing that would otherwise generate large secular terms into the wave kinetic equation. We further apply a bootstrap scheme developed to prove for the bound on couples and the frequency shift solution.

This carefully tailored *choice of nonlinear frequency shift* or *phase renormalization* constitutes one of the principal innovations of the thesis. After this thesis work was finalized, the recent preprint of Deng-Ionescu-Pusateri [65] appeared on arXiv, in which a similar phase

renormalization technique is also employed in the similar context of the long-time existence question for the two-dimensional gravity water waves system on large tori.

β scaling for canonical transformation. In this thesis, we prove a *sufficient upper bound* for the nonlinearity β to perform the canonical transformation, and verify this scaling with numerical studies on the β-FPUT model comparing the nonresonant sums and resonant sums in the Hamiltonian. We identify the overlap between the scalings $\beta \ll N^{-\epsilon}$ for canonical transformation, which was widely used for WKE derivation for β-FPUT model [53, 60], and $N^{-1} < \beta \ll 1$ for WKE to hold (in fact the largest range of β for the WKE to hold may be even larger than this.)

Future directions. We rigorously derived the WKE for the reduced evolution equation (R-FPUT) instead of the full evolution equation (1.18).

1. By relying on a standard normal forms argument, we hope to deal with the full FPU system (including the non-resonant interactions).
2. The general framework developed in this thesis, namely the nonlinear frequency shift, is robust, and allows for a similar derivation of the WKE to other models with various dispersion relations and unconserved frequency shifts, e.g. discrete nonlinear Klein–Gordon model and other anharmonic lattices.

CHAPTER 2
Preparations and Main Tools

The purpose of this chapter is to introduce high-level overview of the proof, the scaling law, the Feynman diagrams infrastructure, and the choice of our nonlinear frequency shift.

2.1: Overview of the proof

Before introducing the Feynman diagram formalism and carrying out the nonlinear frequency shift analysis, we first outline the main strategy and methodology used to establish the main theorem.

1. It has long been understood (see [31]) that the interactions corresponding to $k_1 = k$ or $k_3 = k$ in (R-FPUT) lead to a phase divergence in the iterates, due to the largeness of the term $2\sum_{k_1} T_{k,1,1,k}|c_{k_1}(s)|^2$. This requires a phase renormalization argument to delete those interactions as much as possible. While there have been several formal attempts at this renormalization [31, 54, 66], such formal attempts cannot be easily executed at a rigorous level since they introduce random terms to the phase factor, which spoils the pairing structure that is needed in the remainder of the proof. To remedy this, we introduce a deterministic phase renormalization in which the renormalized phase function satisfies the following ODE system:

$$\partial_s \widetilde{\omega}_k(s) = \frac{2\beta T}{N} \sum_{k_1} T_{k,1,1,k} \mathbb{E}|c_{k_1}^{\leq n}(s)|^2. \tag{2.1}$$

   Here, $c_{k_1}^{\leq n}$ represents the sum of ternary tree expansion terms up to order n, which depend themselves on $\widetilde{\omega}_k$. The shift itself is *deterministic* and defined implicitly as the solution of the above ODE. This allows for the divergent factor $2\sum_{k_1} T_{k,1,1,k}|c_{k_1}(s)|^2$ to be canceled as much as possible. It prevents further complete pairing under degenerate nodes that may cause large contribution to the main term in the kinetic equation. We will need to apply a bootstrap argument in Chapter 5 to complete the proof for the main

estimates Proposition 3.3 stated in Chapter 3. The choice of the nonlinear frequency shift and phase renormalization is one of the main novelties in this thesis.

2. As in all the typical derivations in [42, 43, 46], we write the solution c in terms of Duhamel iterates:

$$c_k = c_k^{(0)} + c_k^{(1)} + c_k^{(2)} + \ldots\ldots + c_k^{(n)} + R_k^{(n+1)} = c_k^{\leq n} + R_k^{(n+1)},$$

where n is chosen to be a sufficiently large threshold determined by the step removing the nonlinear frequency shift, $c^{(j)}$'s represent the j-th iterates, and $R^{(n+1)}$ denotes the remainder term. Similarly as in [39, 46], we choose n to be finite as we are not able to reach the kinetic time scale as $T < T_{\text{kin}}$. Instead in [42, 43], Deng and Hani set $n \sim O(\log L)$ and reach T_{kin} for NLS in $d \geq 2$.

3. We define the *ternary trees* in Section 2.2 to perform the Feynman diagram expansion so that $c^{(j)}$ is tracked by the sum of all ternary trees of order j. We keep track of the nonlinear wave interactions by the *decorations* of the wavenumbers in the ternary trees. Unlike [42, 43, 46], since we do not remove the entire nonlinear frequency shifts, we need to deal with the *degenerate nodes* (branching nodes with decorations $\{k, k_2\} = \{k_1, k_3\}$) which are still left in the ternary trees and construct an enhanced tree structure to fix specific children having the same decorations. To further analyze the correlations of the iterates, we define the *enhanced couples* of enhanced ternary trees with enhanced pairing to prevent complete pairing of the leaves originated from the children of the degenerate node with the same decoration in Section 2.7.

4. To reduce the Feynman diagram analysis to counting problems on couples, we express the couples into the form of *molecules* in Section 2.8. We adapt the cancellation process in Section 5.2 and the algorithm in Section 5.3 from [46] to incorporate the molecules involved with degenerate atoms. Repeating the definitions in [42, 46], we introduce the *irregular chains* which leads to large bad counting estimates. We could remove the irregular chains in *congruent couples* via *splicing* operations due to cancellations after we sum up those congruent couples. After the splicing operation, we need to remove the degenerate atoms in the molecule via a preprocessing step which will not result in any loss before the algorithm starts. With verification of the same structure of molecules in Proposition 5.11:

$$\#\text{ two-vector countings} \leq 3 \times (\#\text{ three-vector countings} - 1), \tag{2.2}$$

as in [46], we could use the algorithm to prove for bounds on couples. The algorithm we

adapt from [46] can only reach $T < \beta^{-\frac{5}{4}}$ instead of the kinetic time scale T_{kin} because the five-vector counting used in [42, 43] are not possible for $d = 1$ as shown in [46, Proposition 3.7].

5. Using the integral estimate Proposition 3.2 in Section 3.1 and the counting estimates we prove in Chapter 4, we are able to prove the Proposition 3.3. The main technical difficulties in the proof arise when we deal with unconserved nonlinear frequency shifts in the time integrals and the sinusoidal dispersion relation in the counting estimates. The more general version of the integral estimate Proposition 3.1 can be adapted and applied to more general models with unconserved nonlinear frequency shifts.

6. Following the same approach as in [42, 43, 46], we bound the remainder terms using a contraction mapping argument in Chapters 6 & 7 by defining the *flower trees* and *flower couples*, and applying the same preprocessing and counting process as in the proof for bounds on couples to bound and invert the linear operator $1 - \mathscr{L}$, for $\mathscr{L}$ defined in a suitable space. We express $(1 - \mathscr{L})^{-1}$ as:

$$(1 - \mathscr{L})^{-1} \;=\; (1 - \mathscr{L}^{n_h})^{-1} \left(1 + \mathscr{L} + \cdots + \mathscr{L}^{n_h - 1}\right),$$

with some large order n_h to bound the powers of $\mathscr{L}$ by Proposition 3.4 and $(1-\mathscr{L}^{n_h})^{-1}$ via Neumann series.

7. We prove the main theorem by isolating the negligible higher iterates and dealing with iterates $0, 1$, and 2. We need to prove the exact resonances to be lower order terms and quasi-resonances to be the main contribution terms. After separating the lower order terms in the time integrals, we use the fact for smooth functions f,

$$\left| t \int \left| \frac{\sin(tx/2)}{tx/2} \right|^2 f(x)dx - 2\pi f(0) \right| \lesssim C(f) t^{-\frac{1}{2}},$$

where $C(f)$ depends on the L^∞ norms of f and f' to derive the wave kinetic equation for the β-FPUT model.

8. In the last two Chapters 8 & 9, we discuss the scaling of the canonical transformations widely used by physicists [14, 55] and the overlap with the scaling law we need to rigorously derive the wave kinetic equation. We prove for a sufficient condition of the nonlinearity threshold performing the canonical transformation and present a numerical verification using simulation under the symplectic integrator method.

2.2: Ternary tree expansion

Definition 2.1. (Trees)

(i) A *ternary tree* $\mathcal{T}$ is a rooted tree where each branching node has precisely three children. Let $\mathcal{T}$ be a ternary tree, $\mathcal{N} = \mathcal{T}\backslash\mathcal{L}$ denote the set of branching nodes, and n be their number, $\mathcal{L}$ denote the set of leaves, and $l = 2n + 1$ be their number. The *scale* of a ternary tree $\mathcal{T}$ is defined as $|\mathcal{T}| = n$, i.e. the number of branching nodes.

(ii) Denote the *root* node of a ternary tree $\mathcal{T}$ as $\mathfrak{r}$ and the children subtrees of $\mathcal{T}$ as $\mathcal{T}_1, \mathcal{T}_2$ and $\mathcal{T}_3$ from left to right. Let $\mathcal{T} = \bullet$ denote a *trivial* tree with scale 0, that is, with only the root node $\mathfrak{r}$.

(iii) We assign to each ternary tree $\mathcal{T}$ a sign + or −. For any node $\mathfrak{n} \in \mathcal{N}$, let its children be $\mathfrak{n}_1, \mathfrak{n}_2, \mathfrak{n}_3$ from left to right. We assign each node the sign $\zeta_\mathfrak{n} \in \{\pm 1\}$ such that: $\zeta_\mathfrak{r} = \text{sign}(\mathcal{T})$, and $\zeta_\mathfrak{n} = \zeta_{\mathfrak{n}_1} = -\zeta_{\mathfrak{n}_2} = \zeta_{\mathfrak{n}_3}$.

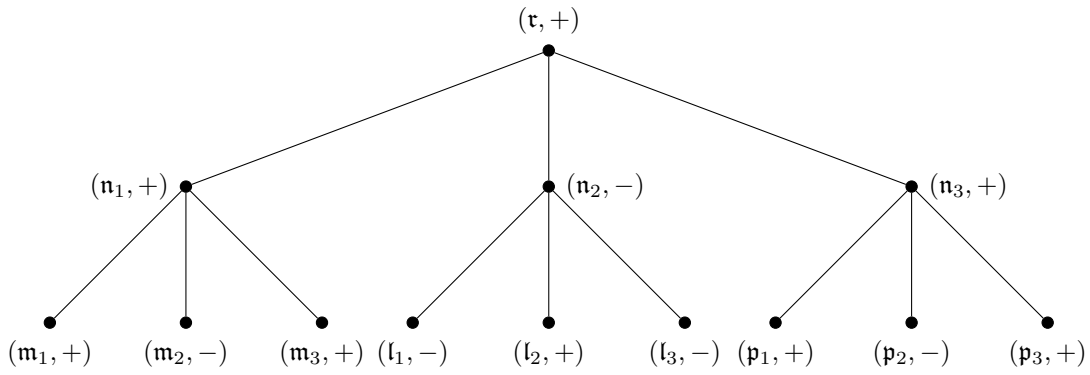


Figure 2.1: A ternary tree of scale 4 with root $(\mathfrak{r},+)$ and three branching nodes $\mathfrak{n}_i$, each with three children $\mathfrak{m}_j$, $\mathfrak{l}_j$, or $\mathfrak{p}_j$ labeled by their signs.

For each ternary tree $\mathcal{T}$, we define $b_k^\mathcal{T}(t)$'s by the following equation inductively:

$$b_k^\bullet(t) = \sqrt{n_{\text{in}}(k)}\eta_k(\varrho) \tag{2.3}$$

$$i\dot{b}_k^\mathcal{T}(t) = \frac{\beta}{N}\sum_{k_1-k_2+k_3=k} T_{k,1,2,3} b_{k_1}^{\mathcal{T}_1}(t) b_{k_2}^{\mathcal{T}_2{}^*}(t) b_{k_3}^{\mathcal{T}_3}(t) e^{i\Omega_k t}, \tag{2.4}$$

where we define:

$$\Omega_{k,1,2,3} = \Omega_k := \omega_k - \omega_{k_1} + \omega_{k_2} - \omega_{k_3},$$

And we use $\mathcal{T}_2{}^*$ to denote the transformation: $\text{sign}(\mathcal{T}_2^*) = -\text{sign}(\mathcal{T}_2)$, i.e. $\mathcal{T}_2^*$ to have opposite sign to $\mathcal{T}_2$. Note that this transformation is the same as taking complex conjugate for the

term $b_{k_2}^{\mathcal{T}_2}$. Then by induction, we can show that $b_k^{\mathcal{T}}(t)$ has the expression:

$$b_k^{\mathcal{T}}(t) = \left(\frac{\beta}{N}\right)^{|\mathcal{T}|} \sum_{\mathcal{D}} \prod_{\mathfrak{n}\in\mathcal{N}} (-i\zeta_{\mathfrak{n}} T_{\mathfrak{n},\mathfrak{l},\mathfrak{n}_2,\mathfrak{n}_3}) \mathcal{A}_{\mathcal{T}}(t,\Omega[\mathcal{N}]) \prod_{\mathfrak{l}\in\mathcal{L}} \sqrt{n_{\mathrm{in}}(k_{\mathfrak{l}})}\eta_{k_{\mathfrak{l}}}^{\zeta_{\mathfrak{l}}}(\varrho), \tag{2.5}$$

where the coefficients $\mathcal{A}_{\mathcal{T}}(t,\Omega[\mathcal{N}])$'s are defined inductively by:

$$\begin{aligned}
&\mathcal{A}_{\bullet}(t,\Omega[\mathcal{N}]) = 1,\\
&\mathcal{A}_{\mathcal{T}}(t,\Omega[\mathcal{N}]) = \int_0^t e^{\zeta i\Omega_{\mathfrak{r}} t'} \prod_{j=1}^{3} \mathcal{A}_{\mathcal{T}_j}(t',\Omega[\mathcal{N}_j])dt'.
\end{aligned}$$

Removing the linear term by substituting $b'_k(t) := e^{i\omega_k Tt} b_k(Tt)$, where $0 \le t \le 1$, we can get the evolution equation for $b'_k(t)$:

$$i\dot{b'_k}(t) = \frac{\beta T}{N} \sum_{k_1-k_2+k_3=k} T_{k,1,2,3} b'_{k_1}(t) b'^{*}_{k_2}(t) b'_{k_3}(t) e^{i\Omega_k Tt} \tag{2.6}$$

We can also express $b'_k(t)$ using the ternary tree expansion by:

$$b'_k(t) = \sum_{|\mathcal{T}^+|\le n} b_k^{\mathcal{T}^+}(t) + \mathcal{R}_k^{(n+1)}, \tag{2.7}$$

where the sum is taken over all trees with + sign and scales less than or equal to n, and $\mathcal{R}_k^{(n+1)}$ denotes the remainder term.

2.3: Nonlinear frequency shift

Suppose $c_k(t)$ is obtained from $b'_k(t)$ by removing an undetermined nonlinear frequency $\widetilde{\omega}_k(t)$ satisfying $\widetilde{\omega}_k(0) = 0$:

$$c_k(t) = b'_k(t) e^{i\widetilde{\omega}_k(t)}, \tag{2.8}$$

We define the Z norm for $\mathbf{c}(t) = (c_k(t))_{k\in\mathbb{Z}_N\cap(0,1)}$ as:

$$\|\mathbf{c}\|_Z^2 = \sup_{0\le t\le 1} \frac{1}{N} \sum_{k\in\mathbb{Z}_N\cap(0,1)} |c_k(t)|^2. \tag{2.9}$$

Then we can derive the evolution equation for $c_k(t)$ by differentiating (1.8) and separate the degenerate sums, i.e. $k \in \{k_1, k_3\}$, as follows:

$$\begin{aligned}
i\dot{c}_k(t) =& \left[i\dot{b}'_k(t) - \dot{\widetilde{\omega}}_k(t) b'_k(t) \right] e^{i\widetilde{\omega}_k(t)} \\
=& i\dot{b}'_k(t) e^{i\widetilde{\omega}_k(t)} - \dot{\widetilde{\omega}}_k(t) c_k(t) \\
=& \frac{\beta T}{N} \Bigg[\sum_{\substack{k_1 - k_2 + k_3 = k \\ k_1, k_3 \neq k_2}} T_{k,1,2,3} b'_{k_1}(t) b'^{*}_{k_2}(t) b'_{k_3}(t) e^{i(\Omega_k T t + \widetilde{\omega}_k(t))} \\
&+ \left(\sum_{k_1} T_{k,1,1,k} |b'_{k_1}(t)|^2 + \sum_{k_3} T_{k,k,3,3} |b'_{k_3}(t)|^2 - \frac{N}{\beta T} \dot{\widetilde{\omega}}_k(t) \right) c_k \Bigg] \\
=& \frac{\beta T}{N} \Bigg[\sum_{\substack{k_1 - k_2 + k_3 = k \\ k_1, k_3 \neq k_2}} T_{k,1,2,3} c_{k_1}(t) c^{*}_{k_2}(t) c_{k_3}(t) e^{i\left(\Omega_k T t + \widetilde{\omega}_k(t) - \widetilde{\omega}_{k_1}(t) + \widetilde{\omega}_{k_2}(t) - \widetilde{\omega}_{k_3}(t)\right)} \\
&+ \left(\sum_{k_1} T_{k,1,1,k} |c_{k_1}(t)|^2 + \sum_{k_3} T_{k,k,3,3} |c_{k_3}(t)|^2 - \frac{N}{\beta T} \dot{\widetilde{\omega}}_k(t) \right) c_k \Bigg]
\end{aligned} \tag{2.10}$$

Integrating both sides of (2.10), we can get:

$$\begin{aligned}
c_k(t) =& c_k(0) - i\frac{\beta T}{N} \int_0^t \Bigg[\sum_{\substack{k_1 - k_2 + k_3 = k \\ k_1, k_3 \neq k_2}} T_{k,1,2,3} c_{k_1}(s) c^{*}_{k_2}(s) c_{k_3}(s) e^{i\left(\Omega_k T s + \widetilde{\omega}_k(s) - \widetilde{\omega}_{k_1}(s) + \widetilde{\omega}_{k_2}(s) - \widetilde{\omega}_{k_3}(s)\right)} \\
&+ \left(\sum_{k_1} T_{k,1,1,k} |c_{k_1}(s)|^2 + \sum_{k_3} T_{k,k,3,3} |c_{k_3}(s)|^2 - \frac{N}{\beta T} \dot{\widetilde{\omega}}_k(s) \right) c_k \Bigg] ds
\end{aligned} \tag{2.11}$$

$$= c_k(0) + F(c) \tag{2.12}$$

2.4: The choice of frequency shift

At this point, we have not chosen what $\widetilde{\omega}_k$ is in equation (2.8). We would like to choose it to cancel as much as possible of the divergent factor $\sum_{k_1} T_{k,1,1,k} |c_{k_1}(s)|^2 + \sum_{k_3} T_{k,k,3,3} |c_{k_3}(s)|^2$ in parentheses appearing in (2.11). At the same time, we would like $\widetilde{\omega}_k$ to be deterministic (otherwise it becomes difficult to control the moments of the solution) and to have an explicit expansion in terms of the initial data. For this, we will seek a combined expansion of

$(c_k(t), \widetilde{\omega}_k)$ as follows: Similar to (2.7), we want a tree expression for $c_k(t)$ as follows:

$$c_k(t) = c_k^{\leq n}(t) + \mathcal{R}_k^{(n+1)} = \sum_{|\mathcal{T}^+| \leq n} c_k^{\mathcal{T}^+}(t) + \mathcal{R}_k^{(n+1)}, \tag{2.13}$$

where $c_k^{\mathcal{T}}(t)$ is defined inductively:

$$c_k^{\bullet}(t) = b_k^{\bullet}(t) = \sqrt{n_{\text{in}}(k)}\eta_k(\varrho) = c_k(0), \tag{2.14}$$

$$\begin{aligned} c_k^{\mathcal{T}}(t) = -i\frac{\beta T}{N}\int_0^t \Bigg[& \sum_{\substack{k_1 - k_2 + k_3 = k \\ k_1, k_3 \neq k_2}} T_{k,1,2,3} c_{k_1}^{\mathcal{T}_1}(s) c_{k_2}^{\mathcal{T}_2 *}(s) c_{k_3}^{\mathcal{T}_3}(s) e^{i\left(\Omega_k T s + \widetilde{\Omega}_k(s)\right)} \\ & + \sum_{k_1} T_{k,1,1,k} \left(c_{k_1}^{\mathcal{T}_1}(s) c_{k_1}^{\mathcal{T}_2 *}(s) - \mathbb{E}\left[c_{k_1}^{\mathcal{T}_1}(s) c_{k_1}^{\mathcal{T}_2 *}(s) \right] \right) c_k^{\mathcal{T}_3}(s) \\ & + c_k^{\mathcal{T}_1}(s) \sum_{k_3} T_{k,k,3,3} \left(c_{k_3}^{\mathcal{T}_2 *}(s) c_{k_3}^{\mathcal{T}_3}(s) - \mathbb{E}\left[c_{k_3}^{\mathcal{T}_2 *}(s) c_{k_3}^{\mathcal{T}_3}(s) \right] \right) \Bigg] ds. \end{aligned} \tag{2.15}$$

Here, $\mathcal{T}$ are ternary trees with subtrees $\mathcal{T}_1, \mathcal{T}_2$ and $\mathcal{T}_3$. The factor $\widetilde{\Omega}_k(s)$ is given by

$$\widetilde{\Omega}_k(s) := \widetilde{\omega}_k(s) - \widetilde{\omega}_{k_1}(s) + \widetilde{\omega}_{k_2}(s) - \widetilde{\omega}_{k_3}(s) \tag{2.16}$$

and $\widetilde{\omega}_k$ is chosen such that

$$\partial_s \widetilde{\omega}_k(s) = \frac{\beta T}{N} \left(\sum_{k_1} T_{k,1,1,k} \mathbb{E}|c_{k_1}^{\leq n}(s)|^2 + \sum_{k_3} T_{k,k,3,3} \mathbb{E}|c_{k_3}^{\leq n}(s)|^2 \right). \tag{2.17}$$

We use $\partial_s \widetilde{\omega}_k$ and $\dot{\widetilde{\omega}}_k$ notation interchangeably throughout the dissertation. Note that this is an ODE system for $(\widetilde{\omega}_k)_k$. However, in this particular case, and due to the definition of $T_{k,l,l,k} = \frac{3}{4\kappa^2}\omega_k \omega_l$, this ODE system reduces to a scalar ODE since

$$\begin{aligned} \partial_s \widetilde{\omega}_k(s) &= \frac{\beta T}{N} \left(\sum_{|\mathcal{T}_1|, |\mathcal{T}_2| \leq n} \sum_{k_1} T_{k,1,1,k} \mathbb{E}\left[c_{k_1}^{\mathcal{T}_1}(s) c_{k_1}^{\mathcal{T}_2 *}(s) \right] + \sum_{|\mathcal{T}_2|, |\mathcal{T}_3| \leq n} \sum_{k_3} T_{k,k,3,3} \mathbb{E}\left[c_{k_3}^{\mathcal{T}_2 *}(s) c_{k_3}^{\mathcal{T}_3}(s) \right] \right) \\ &= \frac{2\beta T}{N} \sum_{|\mathcal{T}_1|, |\mathcal{T}_2| \leq n} \sum_{l} T_{k,l,l,k} \mathbb{E}\left[c_l^{\mathcal{T}_1}(s) c_l^{\mathcal{T}_2 *}(s) \right] \qquad (2.18) \\ &= \omega_k \left[\frac{3\beta T}{2\kappa^2 N} \sum_{|\mathcal{T}_1|, |\mathcal{T}_2| \leq n} \sum_{l} \omega_l \mathbb{E}\left[c_l^{\mathcal{T}_1}(s) c_l^{\mathcal{T}_2 *}(s) \right] \right] \qquad (2.19) \end{aligned}$$

Therefore, writing

$$\widetilde{\omega}_k(s) = \omega_k A(s), \;\; A(0) = 0, \tag{2.20}$$

we obtain that

$$\widetilde{\Omega}_k = \Omega_k A(s), \tag{2.21}$$

$$\dot{A}(s) = G(s, A(s)) = \frac{3\beta T}{2\kappa^2 N} \sum_{|\mathcal{T}_1|,|\mathcal{T}_2| \le n} \sum_l \omega_l \mathbb{E}\left[c_l^{\mathcal{T}_1}(s) c_l^{\mathcal{T}_2 *}(s) \right]. \tag{2.22}$$

It is clear from (2.15) and (2.20) that $|c_l^{\mathcal{T}}|$ and hence the function $G(s, A(s))$ are bounded for almost every ϱ, and that $G(s, A(s))$ is smooth in its variables, which guarantees the global existence and uniqueness of $A(s)$ for almost all ϱ.

2.5: The remainder

It remains to write down the equation for $\mathcal{R}_k^{(n+1)}$, which will justify our choices for $c_k^{\mathcal{T}}$ and $\widetilde{\omega}_k$ above. Equating (2.12) and (2.13), we have:

$$c_k^{\le n}(t) + \mathcal{R}_k^{(n+1)} = c_k(0) + F(c^{\le n} + \mathcal{R}^{(n+1)})$$

Then we can get the expression for the remainder $\mathcal{R}_k^{(n+1)}$:

$$\mathcal{R}_k^{(n+1)} = \left[c_k(0) + F(c^{\le n}) - c_k^{\le n}(t) \right] + \left[F(c^{\le n} + \mathcal{R}^{(n+1)}) - F(c^{\le n}) \right] = I + II$$

Calculating the first term:

$$\begin{aligned} I =& c_k(0) + F(c^{\le n}) - c_k^{\le n}(t) \\ =& -i\frac{\beta T}{N} \int_0^t \Bigg\{ \Bigg[\sum_{|\mathcal{T}_1|,|\mathcal{T}_2|,|\mathcal{T}_3| \le n} \sum_{\substack{k_1 - k_2 + k_3 = k \\ k_1, k_3 \neq k_2}} T_{k,1,2,3} c_{k_1}^{\mathcal{T}_1}(s) c_{k_2}^{\mathcal{T}_2 *}(s) c_{k_3}^{\mathcal{T}_3}(s) e^{i\left(\Omega_k T s + \widetilde{\Omega}_k(s)\right)} \\ &+ \left(\sum_{|\mathcal{T}_1|,|\mathcal{T}_2| \le n} \sum_{k_1} T_{k,1,1,k} c_{k_1}^{\mathcal{T}_1}(s) c_{k_1}^{\mathcal{T}_2 *}(s) - \frac{N}{2\beta T} \dot{\widetilde{\omega}}_k(s) \right) \sum_{|\mathcal{T}_3| \le n} c_k^{\mathcal{T}_3}(s) \\ &+ \sum_{|\mathcal{T}_1| \le n} c_k^{\mathcal{T}_1}(s) \left(\sum_{|\mathcal{T}_2|,|\mathcal{T}_3| \le n} \sum_{k_3} T_{k,k,3,3} c_{k_3}^{\mathcal{T}_2 *}(s) c_{k_3}^{\mathcal{T}_3}(s) - \frac{N}{2\beta T} \dot{\widetilde{\omega}}_k(s) \right) \Bigg] \end{aligned} \tag{2.23}$$

$$
\begin{aligned}
&- \sum_{|\mathcal{T}_1|+|\mathcal{T}_2|+|\mathcal{T}_3|\leq n-1} \Bigg[\sum_{\substack{k_1-k_2+k_3=k \\ k_1,k_3\neq k_2}} T_{k,1,2,3} c_{k_1}^{\mathcal{T}_1}(s) c_{k_2}^{\mathcal{T}_2 *}(s) c_{k_3}^{\mathcal{T}_3}(s) e^{i\left(\Omega_k T s + \widetilde{\Omega}_k(s)\right)} \\
&+ \sum_{k_1} T_{k,1,1,k} \left(c_{k_1}^{\mathcal{T}_1}(s) c_{k_1}^{\mathcal{T}_2 *}(s) - \mathbb{E}\left[c_{k_1}^{\mathcal{T}_1}(s) c_{k_1}^{\mathcal{T}_2 *}(s) \right] \right) c_k^{\mathcal{T}_3}(s) \\
&+ c_k^{\mathcal{T}_1}(s) \sum_{k_3} T_{k,k,3,3} \left(c_{k_3}^{\mathcal{T}_2 *}(s) c_{k_3}^{\mathcal{T}_3}(s) - \mathbb{E}\left[c_{k_3}^{\mathcal{T}_2 *}(s) c_{k_3}^{\mathcal{T}_3}(s) \right] \right) \Bigg] \Bigg\} ds. \qquad (2.24)
\end{aligned}
$$

This expression justifies our choice of $\partial_s \widetilde{\omega}_k$ as in (2.17) and (2.18), which leads to a large of amount of cancellations in the expressions (2.23) and (2.24) above. In fact, by (2.18), we have that

$$
\begin{aligned}
I =& c_k(0) + F(c^{\leq n}) - c_k^{\leq n}(t) \\
=& -i\frac{\beta T}{N} \int_0^t \sum_{\substack{|\mathcal{T}_1|,|\mathcal{T}_2|,|\mathcal{T}_3|\leq n \\ |\mathcal{T}_1|+|\mathcal{T}_2|+|\mathcal{T}_3|\geq n}} \Bigg[\sum_{\substack{k_1-k_2+k_3=k \\ k_1,k_3\neq k_2}} T_{k,1,2,3} c_{k_1}^{\mathcal{T}_1}(s) c_{k_2}^{\mathcal{T}_2 *}(s) c_{k_3}^{\mathcal{T}_3}(s) e^{i\left(\Omega_k T s + \widetilde{\Omega}_k(s)\right)} \\
&+ \sum_{k_1} T_{k,1,1,k} \left(c_{k_1}^{\mathcal{T}_1}(s) c_{k_1}^{\mathcal{T}_2 *}(s) - \mathbb{E}\left[c_{k_1}^{\mathcal{T}_1}(s) c_{k_1}^{\mathcal{T}_2 *}(s) \right] \right) c_k^{\mathcal{T}_3}(s) \\
&+ c_k^{\mathcal{T}_1}(s) \sum_{k_3} T_{k,k,3,3} \left(c_{k_3}^{\mathcal{T}_2 *}(s) c_{k_3}^{\mathcal{T}_3}(s) - \mathbb{E}\left[c_{k_3}^{\mathcal{T}_2 *}(s) c_{k_3}^{\mathcal{T}_3}(s) \right] \right) \Bigg] ds. \qquad (2.25)
\end{aligned}
$$

Introducing the notation: $\mathbf{u} = (u_k(t))_k$, $\mathbf{v} = (v_k(t))_k$, and $\mathbf{w} = (w_k(t))_k$, we define:

$$
\mathcal{W}(\mathbf{u}, \mathbf{v}, \mathbf{w})_k(t) := -i\frac{\beta T}{N} \int_0^t \sum_{\substack{k_1-k_2+k_3=k \\ k_1,k_3\neq k_2}} T_{k,1,2,3} u_{k_1}(s) v_{k_2}^*(s) w_{k_3}(s) e^{i\left(\Omega_k T s + \widetilde{\Omega}_k(s)\right)} ds. \qquad (2.26)
$$

Then, we define:

$$
\mathscr{R}_k := I = \sum_{\substack{|\mathcal{T}_1|,|\mathcal{T}_2|,|\mathcal{T}_3|\leq n \\ |\mathcal{T}_1|+|\mathcal{T}_2|+|\mathcal{T}_3|\geq n}} \mathcal{W}(c^{\mathcal{T}_1}, c^{\mathcal{T}_2}, c^{\mathcal{T}_3})_k(t) + \mathscr{R}_D^{\mathcal{T}_1,\mathcal{T}_2,\mathcal{T}_3} \qquad (2.27)
$$

where

$$
\mathscr{R}_D^{\mathcal{T}_1,\mathcal{T}_2,\mathcal{T}_3} = -i\frac{\beta T}{N} \int_0^t \sum_{k_1} T_{k,1,1,k} \left(c_{k_1}^{\mathcal{T}_1}(s) c_{k_1}^{\mathcal{T}_2 *}(s) - \mathbb{E}\left[c_{k_1}^{\mathcal{T}_1}(s) c_{k_1}^{\mathcal{T}_2 *}(s) \right] \right) c_k^{\mathcal{T}_3}(s)
$$

$$+c_k^{\mathcal{T}_1}(s)\sum_{k_3} T_{k,k,3,3}\left(c_{k_3}^{\mathcal{T}_2 *}(s)c_{k_3}^{\mathcal{T}_3}(s)-\mathbb{E}\left[c_{k_3}^{\mathcal{T}_2 *}(s)c_{k_3}^{\mathcal{T}_3}(s)\right]\right)ds \tag{2.28}$$

Similarly, the second term can be expressed as:

$$\begin{aligned}
II &= F(c^{\leq n}+\mathcal{R}^{(n+1)})-F(c^{\leq n})\\
&= -i\frac{\beta T}{N}\int_0^t \sum_{\substack{k_1-k_2+k_3=k\\ k_1,k_3\neq k_2}} T_{k,1,2,3}\left(c_{k_1}^{\leq n}(s)+\mathcal{R}_{k_1}^{(n+1)}\right)\left(c_{k_2}^{\leq n*}(s)+\mathcal{R}_{k_2}^{(n+1)}\right)\\
&\qquad\qquad \times\left(c_{k_3}^{\leq n}(s)+\mathcal{R}_{k_3}^{(n+1)}\right)e^{i\left(\Omega_k T s+\widetilde{\Omega}_k(s)\right)}\\
&+2\sum_{k_1} T_{k,1,1,k}\left(\left|c_{k_1}^{\leq n}(s)+\mathcal{R}_{k_1}^{(n+1)}\right|^2-\mathbb{E}\left|c_{k_1}^{\leq n}(s)\right|^2\right)\left(c_k^{\leq n}(s)+\mathcal{R}_k^{(n+1)}\right)\\
&-\sum_{\substack{k_1-k_2+k_3=k\\ k_1,k_3\neq k_2}} T_{k,1,2,3}c_{k_1}^{\leq n}(s)c_{k_2}^{\leq n*}(s)c_{k_3}^{\leq n}(s)e^{i\left(\Omega_k T s+\widetilde{\Omega}_k(s)\right)}\\
&-2\sum_{k_1} T_{k,1,1,k}\left(|c_{k_1}^{\leq n}(s)|^2-\mathbb{E}|c_{k_1}^{\leq n}(s)|^2\right)c_k^{\leq n}\,ds
\end{aligned} \tag{2.29}$$

We further define:

$$\mathscr{L}_k(\mathcal{R}^{(n+1)}) := \sum_{|\mathcal{T}_1|,|\mathcal{T}_2|\leq n}^{\text{cyc}} \mathcal{W}(c^{\mathcal{T}_1},c^{\mathcal{T}_2},\mathcal{R}^{(n+1)})_k(t)+(\mathscr{L}_D)_k \tag{2.30}$$

$$\mathscr{Q}_k(\mathcal{R}^{(n+1)},\mathcal{R}^{(n+1)}) := \sum_{|\mathcal{T}_1|\leq n}^{\text{cyc}} \mathcal{W}(c^{\mathcal{T}_1},\mathcal{R}^{(n+1)},\mathcal{R}^{(n+1)})_k(t)+(\mathscr{Q}_D)_k \tag{2.31}$$

$$\mathscr{C}_k(\mathcal{R}^{(n+1)},\mathcal{R}^{(n+1)},\mathcal{R}^{(n+1)}) := \mathcal{W}(\mathcal{R}^{(n+1)},\mathcal{R}^{(n+1)},\mathcal{R}^{(n+1)})_k(t)+(\mathscr{C}_D)_k \tag{2.32}$$

where $\mathscr{L}$, $\mathscr{Q}$, and $\mathscr{C}$ are linear, bilinear, and trilinear operators respectively, and

$$\begin{aligned}
(\mathscr{L}_D)_k := -i\frac{\beta T}{N}\int_0^t 2\sum_{k_1} T_{k,1,1,k}\Big[&\left(\left|c_{k_1}^{\leq n}(s)\right|^2-\mathbb{E}\left|c_{k_1}^{\leq n}(s)\right|^2\right)\mathcal{R}_k^{(n+1)}\\
&+\left(c_{k_1}^{\leq n*}(s)\mathcal{R}_{k_1}^{(n+1)}+c_{k_1}^{\leq n}(s)\mathcal{R}_{k_1}^{(n+1)*}\right)c_k^{\leq n}(s)\Big]\,ds
\end{aligned} \tag{2.33}$$

$$\begin{aligned}
(\mathscr{Q}_D)_k := -i\frac{\beta T}{N}\int_0^t 2\sum_{k_1} T_{k,1,1,k}\Big[&\left(c_{k_1}^{\leq n*}(s)\mathcal{R}_{k_1}^{(n+1)}+c_{k_1}^{\leq n}(s)\mathcal{R}_{k_1}^{(n+1)*}\right)\mathcal{R}_k^{(n+1)}\\
&+\left|\mathcal{R}_{k_1}^{(n+1)}\right|^2 c_k^{\leq n}(s)\Big]\,ds
\end{aligned} \tag{2.34}$$

$$(\mathscr{C}_D)_k := -i\frac{\beta T}{N}\int_0^t 2\sum_{k_1} T_{k,1,1,k}\left|\mathcal{R}_{k_1}^{(n+1)}\right|^2\mathcal{R}_k^{(n+1)}ds \tag{2.35}$$

Then by calculation we can verify that:

$$II = \mathscr{L}_k(\mathcal{R}^{(n+1)}) + \mathscr{Q}_k(\mathcal{R}^{(n+1)}, \mathcal{R}^{(n+1)}) + \mathscr{C}_k(\mathcal{R}^{(n+1)}, \mathcal{R}^{(n+1)}, \mathcal{R}^{(n+1)}). \tag{2.36}$$

Therefore (2.27) and (2.36) give that

$$\mathcal{R}_k^{(n+1)} = \mathscr{R}_k + \mathscr{L}_k(\mathcal{R}^{(n+1)}) + \mathscr{Q}_k(\mathcal{R}^{(n+1)}, \mathcal{R}^{(n+1)}) + \mathscr{C}_k(\mathcal{R}^{(n+1)}, \mathcal{R}^{(n+1)}, \mathcal{R}^{(n+1)}), \tag{2.37}$$

which is equivalent to:

$$\mathcal{R} = (1 - \mathscr{L})^{-1}(\mathscr{R} + \mathscr{Q}(\mathcal{R}, \mathcal{R}) + \mathscr{C}(\mathcal{R}, \mathcal{R}, \mathcal{R})), \tag{2.38}$$

provided that $1 - \mathscr{L}$ is invertible in a suitable space.

2.6: Scaling laws

In this section, we would like to discuss the scaling law for the β-FPUT system which was not discussed in the previous literature. Similar to the expository paper [67] for NLS, we set $\beta = N^{-\gamma}$ for $\gamma \in [0, \infty]$. The endpoint $\gamma = 0$, widely used by physicists, corresponds to taking the large box limit $N \to \infty$ with β fixed, followed by the weak nonlinearity limit $\beta \to 0$, and vice versa for $\gamma = \infty$. We expand $\mathbb{E}\,|b(k,t)|^2$ to get the trivial term n_{in} with the nontrivial term:

$$\frac{\beta^2 t}{N^2} \sum_{k_1 - k_2 + k_3 = k} |T_{k,1,2,3}|^2 \phi_k \phi_{k_1} \phi_{k_2} \phi_{k_3} \left[\frac{1}{\phi_k} - \frac{1}{\phi_{k_1}} + \frac{1}{\phi_{k_2}} - \frac{1}{\phi_{k_3}}\right]$$
$$\times (t + A(t/T)) \left|\frac{\sin(\Omega(\vec{k})(t + A(t/T))/2)}{\Omega(\vec{k})(t + A(t/T))/2}\right|^2 \cdot \frac{t + A(t/T)}{t}. \tag{2.39}$$

We need to apply the approximation of identity to $(t+A(t/T)) \left|\frac{\sin(\Omega(\vec{k})(t+A(t/T))/2)}{\Omega(\vec{k})(t+A(t/T))/2}\right|^2$ as $t \to \infty$ to get the $\delta(\Omega)$ term and match the first order of (WKE). For the following discussions, we omit $A(t/T)$ for simplicity since $A(t/T)/t \sim O(N^{-\gamma})$ as we will prove in the later chapters. For this convergence to be valid, we need the *equidistribution* of Ω. Consider the *quasi-resonant* strip of width t^{-1}:

$$R_{t^{-1}} = \{(k_1, k_2, k_3) \in (\mathbb{Z}_N \cap (0,1))^3 : k_1 - k_2 + k_3 = k \bmod 1, |\Omega| \lesssim t^{-1}\},$$

Heuristically, the sufficient condition on γ that guarantees the equidistribution requires the minimum separation between values of $\omega(k)$ with nearby $\frac{k}{N}$ to be smaller than the width t^{-1}

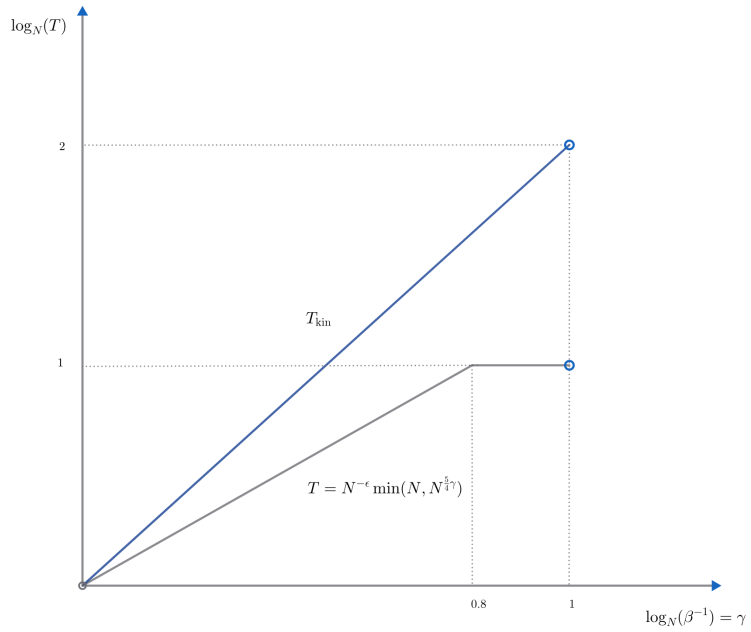


Figure 2.2: The scaling law $\beta = N^{-\gamma}$, $T = N^{-\epsilon}\min(N, N^{\frac{5}{4}\gamma})$, and $T_{\text{kin}} = \frac{N^{2\gamma}}{4\pi}$, for $\gamma \in (0,1)$, under which we derive the wave kinetic equation. In the figure we take $\epsilon = 0$ and neglecting the constant term in $\log_N(T_{\text{kin}})$ as a function of γ.

of the quasi-resonant strip $R_{t^{-1}}$. This leads to the condition [31, 68]:

$$\frac{1}{N}\left|\frac{\partial\omega}{\partial k}\right| \ll \frac{1}{t},$$

which gives the condition $t < N$. This sufficient condition aligns with our choice of timescale $T = N^{-\epsilon}\min(N, N^{\frac{5}{4}\gamma})$ in Theorem 1 for $\gamma < 1$ as shown in Figure 2.2.

On the other hand in the proof for the main theorem, we need to have the quasi-resonant terms to dominate the exact resonant terms, which requires $T \lesssim N^{1-\epsilon}$ (which is also required in the integral estimates). We would like to consider the scaling laws $\gamma < 1$ so that the kinetic time scale $T_{\text{kin}} \sim N^{2\gamma} < N^2$.

For the endpoint $\gamma = 0$, after taking the large box limit $N \to \infty$, we will get an infinite lattice β-FPUT system. The global existence and uniqueness of the solution for the infinite lattice was proved in [69] with additional requirements on the initial data. On the other hand, this endpoint will also be out of range in order to perform the canonical transformation needed for deriving the full WKE in the future work. So we will not consider $\gamma = 0$ in our derivation.

2.7: Couples and Diagrammetic expansions

Definition 2.2 (Enhanced Trees)**.** An *enhanced tree* is a ternary tree $\mathcal{T}$ (as in Definition 2.1) equipped with additional structure specified by:

(i) A designated set $\mathcal{N}_D$ of *degenerate branching nodes* within $\mathcal{T}$.

(ii) For each degenerate node $\mathfrak{n} \in \mathcal{N}_D$ with children $\{\mathfrak{n}_1, \mathfrak{n}_2, \mathfrak{n}_3\}$, we specify a choice of a distinguished child $\mathfrak{n}_c^*$ taken from $\{\mathfrak{n}_1, \mathfrak{n}_3\}$ (children with the same sign), and label the remaining child of those two as $\mathfrak{n}_c$.

Definition 2.3 (Decorations of Enhanced Trees)**.** A decoration $\mathscr{D}$ of an enhanced tree $\mathcal{T}$ is a set of vectors $\{(k_\mathfrak{n})_{\mathfrak{n}\in\mathcal{T}}\}$ such that $k_\mathfrak{n} \in \mathbb{Z}_N \cap (0,1)$. Further, if $\mathfrak{n}$ is a branching node,

$$\zeta_\mathfrak{n} k_\mathfrak{n} = \zeta_{\mathfrak{n}_1} k_{\mathfrak{n}_1} + \zeta_{\mathfrak{n}_2} k_{\mathfrak{n}_2} + \zeta_{\mathfrak{n}_3} k_{\mathfrak{n}_3},$$

where $\mathfrak{n}_1, \mathfrak{n}_2, \mathfrak{n}_3$ are the three children of $\mathfrak{n}$ labeled from left to right. We say $\mathscr{D}$ is a k-decoration if $k_\mathfrak{r} = k$. In addition, whenever $\mathfrak{n} \in \mathcal{N}_D$ is a *degenerate* branching node with children $\{\mathfrak{n}_c^*, \mathfrak{n}_2, \mathfrak{n}_c\}$, we impose the *enhanced* constraints:

$$k_{\mathfrak{n}_2} = k_{\mathfrak{n}_c^*} \quad \text{and} \quad k_\mathfrak{n} = k_{\mathfrak{n}_c},$$

following the notation in Definition 2.2. We also define

$$\epsilon_\mathscr{D} := \prod_{\mathfrak{n}\in\mathcal{N}} \epsilon_{k_{\mathfrak{n}_1} k_{\mathfrak{n}_2} k_{\mathfrak{n}_3}}. \tag{2.40}$$

where

$$\epsilon_{k_{\mathfrak{n}_1} k_{\mathfrak{n}_2} k_{\mathfrak{n}_3}} := \begin{cases} -T_{k_\mathfrak{n}, k_{\mathfrak{n}_1}, k_{\mathfrak{n}_2}, k_{\mathfrak{n}_3}} & \text{if } k_{\mathfrak{n}_1} = k_{\mathfrak{n}_2} = k_{\mathfrak{n}_3}; \\ +T_{k_\mathfrak{n}, k_{\mathfrak{n}_1}, k_{\mathfrak{n}_2}, k_{\mathfrak{n}_3}} & \text{otherwise.} \end{cases} \tag{2.41}$$

Definition 2.4. (Couples) A *couple* $\mathcal{Q}$ consists of two trees $\mathcal{T}^+$ and $\mathcal{T}^-$, each labeled with opposite signs, together with a partition $\mathscr{P}$ of the set of leaves $\mathcal{L}^+ \cup \mathcal{L}^-$ into $(n+1)$ disjoint two-element subsets, where $n = n(\mathcal{T}^+) + n(\mathcal{T}^-)$ is called the *order* of the couple. The partition $\mathscr{P}$ must satisfy the condition $\zeta_\mathfrak{l} = -\zeta_{\mathfrak{l}'}$ for every pair $\{\mathfrak{l}, \mathfrak{l}'\} \in \mathscr{P}$. For a couple $\mathcal{Q} = \{\mathcal{T}^+, \mathcal{T}^-, \mathscr{P}\}$, we denote by $\mathcal{N} = \mathcal{N}^+ \cup \mathcal{N}^-$ the branching nodes of both trees, and by $\mathcal{L} = \mathcal{L}^+ \cup \mathcal{L}^-$ their leaves. We define

$$\zeta(\mathcal{Q}) \;=\; \prod_{\mathfrak{n}\in\mathcal{N}} \big(-i\,\zeta_\mathfrak{n}\big).$$

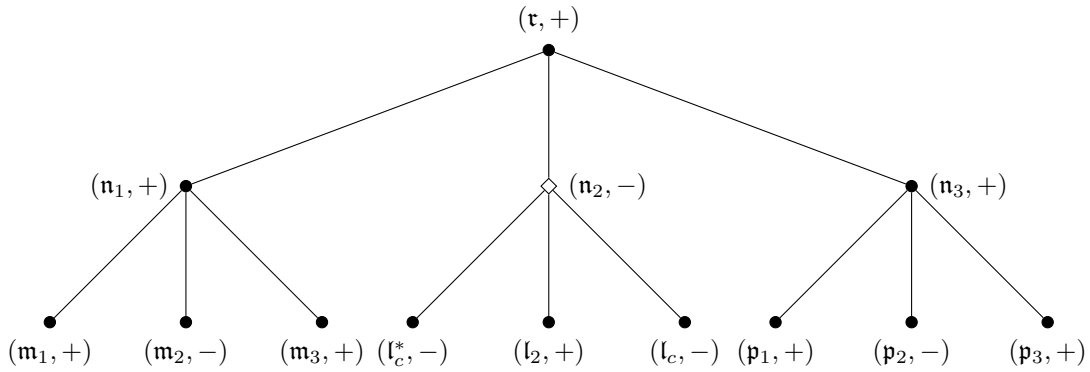


Figure 2.3: An enhanced ternary tree in which the branching node $(\mathfrak{n}_2,-)$ is a degenerate node, such that $k_{\mathfrak{l}_2} = k_{\mathfrak{l}_c^*}$ and $k_{\mathfrak{n}_2} = k_{\mathfrak{l}_c}$.

The *trivial couple* is given by two trivial trees whose roots are paired.

A *decoration* $\mathscr{E}$ of a couple $\mathcal{Q}$ is obtained by decorating each tree $\mathcal{T}^+$ and $\mathcal{T}^-$ according to $\mathscr{D}^+$ and $\mathscr{D}^-$, subject to the further requirement that $k_{\mathfrak{l}} = k_{\mathfrak{l}'}$ whenever $\{\mathfrak{l},\mathfrak{l}'\} \in \mathscr{P}$. We define

$$\epsilon_{\mathscr{E}} \;=\; \epsilon_{\mathscr{D}^+}\,\epsilon_{\mathscr{D}^-}.$$

A decoration $\mathscr{E}$ is called a *k-decoration* if $k_{\mathfrak{r}^+} = k_{\mathfrak{r}^-} = k$.

Definition 2.5. (Enhanced Couples) A couple $\mathcal{Q}$, it is called an *enhanced couple* if its partition $\mathscr{P}$ further satisfies that the leaves $\mathcal{L}(\mathfrak{n}_2,\mathfrak{n}_c^*)$ originated from $\{\mathfrak{n}_2,\mathfrak{n}_c^*\}$, children of any degenerate branching node $\mathfrak{n} \in \mathcal{N}_D$, are not completely paired together, i.e. there exist leaves $\mathfrak{l} \in \mathcal{L}(\mathfrak{n}_2,\mathfrak{n}_c^*)$ and $\mathfrak{l}' \in \mathcal{L} \setminus \mathcal{L}(\mathfrak{n}_2,\mathfrak{n}_c^*)$ such that $\{\mathfrak{l},\mathfrak{l}'\} \in \mathscr{P}$.

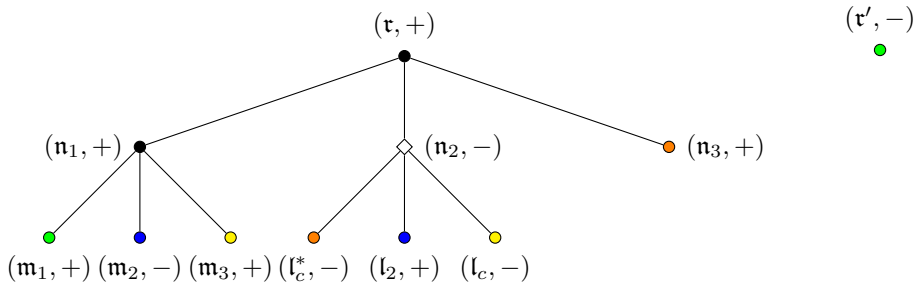


Figure 2.4: An enhanced couple with leaves paired in the same color. Note that the leaves $\mathfrak{l}_c^*$ and $\mathfrak{l}_2$ cannot be paired together by Definition 2.5.

Then we can prove the following proposition:

Proposition 2.6. *For each enhanced ternary tree $\mathcal{T}$, we have the formula:*

$$c_k^{\mathcal{T}}(t) = \left(\frac{\beta T}{N}\right)^{|\mathcal{T}|} \sum_{\mathcal{D}} \prod_{\mathfrak{n}\in\mathcal{N}} (-i\zeta_{\mathfrak{n}} T_{k_{\mathfrak{n}},k_{\mathfrak{n}_1},k_{\mathfrak{n}_2},k_{\mathfrak{n}_3}}) \mathcal{A}_{\mathcal{T}}(t,\Omega[\mathcal{N}],\widetilde{\Omega}[\mathcal{N}]) \prod_{\mathfrak{l}\in\mathcal{L}} \sqrt{n_{in}(k_{\mathfrak{l}})} \mathcal{B}_{\mathcal{T}}(\eta_{\mathcal{T}}(\varrho)) \tag{2.42}$$

where $\mathcal{D}$ denotes the decoration $(k_{\mathfrak{n}} : \mathfrak{n} \in \mathcal{T})$ such that $\mathfrak{r} = k$. $\mathcal{A}_{\mathcal{T}}(t,\Omega[\mathcal{N}],\widetilde{\Omega}[\mathcal{N}])$ and $\mathcal{B}_{\mathcal{T}}(\eta_{\mathcal{T}}(\varrho))$ are defined inductively as:

$$\mathcal{A}_{\bullet}(t,\Omega[\mathcal{N}],\widetilde{\Omega}[\mathcal{N}]) = 1, \tag{2.43}$$

$$\mathcal{A}_{\mathcal{T}}(t,\Omega[\mathcal{N}],\widetilde{\Omega}[\mathcal{N}]) = \int_0^t e^{\zeta_{\mathfrak{r}} i(\Omega_{\mathfrak{r}} T t' + \widetilde{\Omega}_{\mathfrak{r}}(t'))} \prod_{j=1}^{3} \mathcal{A}_{\mathcal{T}_j}(t',\Omega[\mathcal{N}_j],\widetilde{\Omega}[\mathcal{N}_j]) dt', \tag{2.44}$$

$$\mathcal{B}_{\bullet}(\eta_{\bullet}(\varrho)) = \eta_{\mathfrak{r}}^{\zeta_{\mathfrak{r}}}(\varrho) \tag{2.45}$$

$$\begin{aligned}\mathcal{B}_{\mathcal{T}}(\eta_{\mathcal{T}}(\varrho)) = &\prod_{j=1}^{3} \mathcal{B}_{\mathcal{T}_j}(\eta_{\mathcal{T}_j}(\varrho)) - \mathbb{1}_{\mathfrak{r}\in\mathcal{N}_D} \mathcal{B}_{\mathcal{T}_c}(\eta_{\mathcal{T}_c}(\varrho)) \\ &\times \mathbb{E}\left(\mathcal{B}_{\mathcal{T}_{c^*}}(\eta_{\mathcal{T}_{c^*}}(\varrho)) \mathcal{B}_{\mathcal{T}_2}(\eta_{\mathcal{T}_2}(\varrho))\right).\end{aligned} \tag{2.46}$$

where $\mathcal{T}_c$, $\mathcal{T}_{c^*}$, and $\mathcal{T}_2$ are trees with root node $\mathfrak{n}_c$, $\mathfrak{n}_c^*$, $\mathfrak{n}_2$ respectively, which are children of degenerate node $\mathfrak{r} \in \mathcal{N}_D$.

Proof. We now prove (2.42) inductively. From (2.14-2.15), (2.42) is true for $|\mathcal{T}| = 0, 1$. Suppose (2.42) is true for $|\mathcal{T}| \le n-1$. Then for any ternary tree $\mathcal{T}$ with scale n, its children subtrees $\mathcal{T}_1, \mathcal{T}_2$, and $\mathcal{T}_3$ with sign $(+,-,+)$ have scales of at most $(n-1)$. In this setting $\mathcal{T}_2^* = \mathcal{T}_2$ and $c_{k_2}^{\mathcal{T}_2^*}(t) = c_{k_2}^{\mathcal{T}_2}(t)$. Then for $i \in \{1,2,3\}$, we have:

$$c_{k_i}^{\mathcal{T}_i}(t) = \left(\frac{\beta T}{N}\right)^{|\mathcal{T}_i|} \sum_{\mathcal{D}_i} \prod_{\mathfrak{n}\in\mathcal{N}_i} (-i\zeta_{\mathfrak{n}} T_{k_{\mathfrak{n}},k_{\mathfrak{n}_1},k_{\mathfrak{n}_2},k_{\mathfrak{n}_3}}) \mathcal{A}_{\mathcal{T}_i}(t,\Omega[\mathcal{N}_i],\widetilde{\Omega}[\mathcal{N}_i]) \prod_{\mathfrak{l}\in\mathcal{L}_i} \sqrt{n_{\mathrm{in}}(k_{\mathfrak{l}})} \mathcal{B}_{\mathcal{T}_i}(\eta_{\mathcal{T}_i}(\varrho)), \tag{2.47}$$

where $\mathcal{N} = \cup_i \mathcal{N}_i \cup \{\mathfrak{r}\}$, $\mathcal{L} = \cup_i \mathcal{L}_i$. We also have $\mathcal{N}_D \cup \{\mathfrak{r}\} = \cup_i \mathcal{N}_D^{(i)} \cup \{\mathfrak{r}\}$, where $\mathcal{N}_D^{(i)}$ is the set of degenerate branching nodes for $\mathcal{T}_i$. Then plugging in (2.47) to (2.15), we can get:

$$\begin{aligned}c_k^{\mathcal{T}}(t) = &-i\zeta_{\mathfrak{r}} \left(\frac{\beta T}{N}\right)^{1+\sum_{i=1}^3 |\mathcal{T}_i|} \int_0^t \Bigg\{ \mathbb{1}_{\mathfrak{r}\notin\mathcal{N}_D} \sum_{\substack{k_1-k_2+k_3=k \\ k_1,k_3\neq k_2}} T_{k,1,2,3} \prod_{i=1}^{3} \Bigg[\sum_{\mathcal{D}_i} \prod_{\mathfrak{n}\in\mathcal{N}_i} (-i\zeta_{\mathfrak{n}} T_{k_{\mathfrak{n}},k_{\mathfrak{n}_1},k_{\mathfrak{n}_2},k_{\mathfrak{n}_3}}) \\ &\times \mathcal{A}_{\mathcal{T}_i}(t,\Omega[\mathcal{N}_i],\widetilde{\Omega}[\mathcal{N}_i]) \prod_{\mathfrak{l}\in\mathcal{L}_i} \sqrt{n_{\mathrm{in}}(k_{\mathfrak{l}})} \mathcal{B}_{\mathcal{T}_i}(\eta_{\mathcal{T}_i}(\varrho)) \Bigg] e^{i\left(\Omega_k T s + \widetilde{\Omega}_k(s)\right)}\end{aligned}$$

$$+ \mathbb{1}_{\mathfrak{r}\in\mathcal{N}_D} \sum_{k_2} T_{k,k,2,2} \prod_{i=1}^{3} \left[\sum_{\mathcal{D}_i} \prod_{\mathfrak{n}\in\mathcal{N}_i} (-i\zeta_{\mathfrak{n}} T_{k_{\mathfrak{n}},k_{\mathfrak{n}_1},k_{\mathfrak{n}_2},k_{\mathfrak{n}_3}}) \mathcal{A}_{\mathcal{T}_i}(t, \Omega[\mathcal{N}_i], \widetilde{\Omega}[\mathcal{N}_i]) \prod_{\mathfrak{l}\in\mathcal{L}_i} \sqrt{n_{\mathrm{in}}(k_{\mathfrak{l}})} \right]$$
$$\times \left[\prod_{j=1}^{3} \mathcal{B}_{\mathcal{T}_j}(\eta_{\mathcal{T}_j}(\varrho)) - \mathcal{B}_{\mathcal{T}_c}(\eta_{\mathcal{T}_c}(\varrho)) \mathbb{E}\left(\mathcal{B}_{\mathcal{T}_{c^*}}(\eta_{\mathcal{T}_{c^*}}(\varrho)) \mathcal{B}_{\mathcal{T}_2}(\eta_{\mathcal{T}_2}(\varrho)) \right) \right] \Bigg\} ds \tag{2.48}$$

After simplification, we find (2.48) recovers (2.42). □

Definition 2.7. For any ternary tree $\mathcal{T}$ and decoration $(k_{\mathfrak{n}} : \mathfrak{n} \in \mathcal{T})$, we fix $d_{\mathfrak{n}} \in \{0, 1\}$ for each $\mathfrak{n} \in \mathcal{N}$, and we define $q_{\mathfrak{n}}$ for each $\mathfrak{n} \in \mathcal{T}$ inductively by:

$$q_{\mathfrak{n}} = 0 \text{ if } \mathfrak{n} \in \mathcal{L};\ q_{\mathfrak{n}} = d_{\mathfrak{l}} q_{\mathfrak{l}} - d_{\mathfrak{n}_2} q_{\mathfrak{n}_2} + d_{\mathfrak{n}_3} q_{\mathfrak{n}_3} + \Omega_{\mathfrak{n}} \text{ if } \mathfrak{n} \in \mathcal{N}. \tag{2.49}$$

Remark 2.8. Note that $\Omega_{\mathfrak{n}} = \omega_{k_{\mathfrak{n}}} - \omega_{k_{\mathfrak{n}_1}} + \omega_{k_{\mathfrak{n}_2}} - \omega_{k_{\mathfrak{n}_3}}$ for each $\mathfrak{n} \in \mathcal{T}$, depending on the decoration of the tree $\mathcal{T}$.

Also, we include here the needed estimates and expansion of $A(t)$:

$$\begin{aligned}
\dot{A}(t) &= \frac{3\beta T}{2\kappa^2 N} \sum_{|\mathcal{T}_1|,|\mathcal{T}_2|\le n} \sum_{l} \omega_l \mathbb{E}\left[c_l^{\mathcal{T}_1}(t) c_l^{\mathcal{T}_2 *}(t) \right] \\
&= \frac{3\beta T}{2\kappa^2 N} \left[\sum_{\substack{|\mathcal{T}_1|=0 \\ |\mathcal{T}_2|=0}} \sum_{l} \omega_l \mathbb{E}\left[c_l^{\mathcal{T}_1}(t) c_l^{\mathcal{T}_2 *}(t) \right] + \sum_{|\mathcal{T}_1|+|\mathcal{T}_2|\ge 1} \sum_{l} \omega_l \mathbb{E}\left[c_l^{\mathcal{T}_1}(t) c_l^{\mathcal{T}_2 *}(t) \right] \right] \\
&= \frac{3\beta T}{2\kappa^2 N} \left[\sum_{l} \omega_l n_{\mathrm{in}}(l) + \sum_{|\mathcal{T}_1|+|\mathcal{T}_2|\ge 1} \sum_{l} \omega_l \mathbb{E}\left[c_l^{\mathcal{T}_1}(t) c_l^{\mathcal{T}_2 *}(t) \right] \right] \qquad (2.50) \\
&=: C_0 \beta T + \dot{A}_{\ge}(t). \qquad (2.51)
\end{aligned}$$

Then we can express $A(t)$ as: $A(t) = C_0 \beta T t + A_{\ge}(t)$.

Definition 2.9. For an enhanced couple $\mathcal{Q}$, define

$$(\mathcal{K}_{\mathcal{Q}})(t, s, k) := \left(\frac{\beta T}{N} \right)^n \zeta(\mathcal{Q}) \sum_{\mathscr{E}} \epsilon_{\mathscr{E}} \int_{\mathcal{E}} \prod_{\mathfrak{n}\in\mathcal{N}} e^{\zeta_{\mathfrak{n}} i(\Omega_{\mathfrak{n}} T t_{\mathfrak{n}} + \widetilde{\Omega}_{\mathfrak{n}}(t_{\mathfrak{n}}))} dt_{\mathfrak{n}} \prod_{\mathfrak{l}\in\mathcal{L}}^{+} n_{\mathrm{in}}(k_{\mathfrak{l}})$$
$$\times \mathbb{E}\left[\mathcal{B}_{\mathcal{T}^+}(\eta_{\mathcal{T}^+}(\varrho)) \mathcal{B}^*_{\mathcal{T}^-}(\eta_{\mathcal{T}^-}(\varrho)) \right], \tag{2.52}$$

where the sum is taken over all k-decorations $\mathscr{E}$ of $\mathcal{Q}$, the product $\prod_{\mathfrak{l}\in\mathcal{L}}^{+}$ is taken over leaves

with + signs, and

$$\mathcal{E} = \Big\{ t[\mathcal{N}] : 0 < t_{\mathfrak{n}'} < t_{\mathfrak{n}} \text{ whenever } \mathfrak{n}' \text{ is a child of } \mathfrak{n}; \quad t_{\mathfrak{n}} < t \text{ for } \mathfrak{n} \in \mathcal{N}^+, \text{ and } t_{\mathfrak{n}} < s \text{ for } \mathfrak{n} \in \mathcal{N}^- \Big\}, \tag{2.53}$$

where $t[\mathcal{N}]$ denotes the time vector $(t_{\mathfrak{n}})_{\mathfrak{n}\in\mathcal{N}}$.

Lemma 2.10. *(Complex Isserlis' Theorem) Given $k_j \in \mathbb{Z}_N \cap (0,1)$ and $\{\zeta_j\}$ for $1 \le j \le n$, then*

$$\mathbb{E}\left[\prod_{j=1}^{n} \eta_{k_j}^{\zeta_j}(\varrho)\right] = \sum_{\mathscr{P}} \prod_{\{j,j'\}\in\mathscr{P}} \mathbf{1}_{k_j = k_{j'}}. \tag{2.54}$$

where $\eta_k^+ = \eta_k$ and $\eta_k^- = \overline{\eta_k}$, and the summation is taken over all partitions $\mathscr{P}$ of $1, 2, \ldots, n$ into two-element subsets $\{j, j'\}$ such that $\zeta_j = -\zeta_{j'}$.

Proof. Here, we repeat the proof in [42]. Let $\{k^{(1)}, \ldots, k^{(r)}\}$ be the collection of distinct vectors in $\{k_j : 1 \le j \le n\}$. For every $1 \le i \le r$ and $\zeta \in \{\pm\}$ define

$$p_i^{\zeta} \;=\; \big|\{\, j : k_j = k^{(i)},\ \zeta_j = \zeta \,\}\big|.$$

With this notation we can rewrite the joint moment as

$$\mathbb{E}\left[\prod_{j=1}^{n} \eta_{k_j}^{\zeta_j}(\varrho)\right] = \mathbb{E}\left[\prod_{i=1}^{r} \eta_{k^i}^{p_i^+} \overline{\eta_{k^i}}^{p_i^-}\right] = \begin{cases} (p_1^+)! \ldots (p_r^+)! & \text{if } p_i^+ = p_i^- \text{ for all } i, \\ 0 & \text{otherwise.} \end{cases}$$

For fixed $\mathscr{P}$ in (2.54) the product is 0 or 1. If there is i such that $p_i^+ \neq p_i^-$, there is no partition $\mathscr{P}$. Otherwise, the product is 1 if and only if each pair $\{j, j'\} \in \mathscr{P}$ satisfies $\zeta_j = -\zeta_{j'}$, and $k_j = k_{j'} = k^{(i)}$ for some i. So, the number of such $\mathscr{P}$ is $(p_1^+)! \ldots (p_r^+)!$. □

Note that by Isserlis' Theorem, we have:

$$\mathbb{E}\left(c_k^{\mathcal{T}^+}(t)\overline{c_k^{\mathcal{T}^-}(s)}\right) = \sum_{\mathscr{P}} (\mathcal{K}_{\mathcal{Q}})(t, s, k). \tag{2.55}$$

2.8: Molecules

Definition 2.11 (Molecules)**.** A *molecule* $\mathbb{M}$ is a directed graph whose vertices are called *atoms* and edges are called *bonds*. Multiple bonds between the same pair of atoms and self-loops are allowed. Each atom has out-degree at most 2 and in-degree at most 2. We write

$v \in \mathbb{M}$ for an atom v in $\mathbb{M}$, and $\ell \in \mathbb{M}$ for a bond ℓ in $\mathbb{M}$. If v is an endpoint of ℓ, we write $\ell \sim v$. For each such pair (v, ℓ), define

$$\zeta_{v,\ell} = \begin{cases} 1 & \text{if } \ell \text{ is outgoing from } v, \\ -1 & \text{if } \ell \text{ is incoming to } v. \end{cases}$$

We further require that $\mathbb{M}$ does not have any connected components consisting only of atoms each having degree 4 (where the degree is considered in the undirected sense).

For a molecule $\mathbb{M}$, define the quantity

$$\chi := E - V + F,$$

where E is the number of bonds, V is the number of atoms, and F is the number of connected components.

An *atomic group* in $\mathbb{M}$ is a subset of atoms together with all bonds connecting those atoms. A single bond ℓ is called a *bridge* if removing it increases the number of connected components by one.

Definition 2.12 (Molecules of couples)**.** Let $\mathcal{Q}$ be a nontrivial couple. We define the corresponding *molecule* $\mathbb{M} = \mathbb{M}(\mathcal{Q})$ as follows. The atoms of $\mathbb{M}$ correspond to the branching nodes $\mathfrak{n} \in \mathcal{N}$ of $\mathcal{Q}$. For any two branching nodes $\mathfrak{n}_1, \mathfrak{n}_2$, we draw a bond between the corresponding atoms v_1, v_2 if:

1. One of $\mathfrak{n}_1, \mathfrak{n}_2$ is a parent of the other (Parent-Child pair), or
2. A child of $\mathfrak{n}_1$ is paired with a child of $\mathfrak{n}_2$ as leaves (Leaf Pair).

We may form a *labeled molecule* by labeling each bond. For a Parent-Child (PC) bond, we label the bond as "PC" and place a "P" at the atom corresponding to the parent branching node and a "C" at the atom corresponding to the child branching node. For a Leaf Pair (LP) bond, we label the bond as "LP".

The direction of each bond is determined as follows:

(i) For an LP bond, the bond is directed away from the atom whose corresponding child in the couple has sign "$-$" and towards the atom whose corresponding child has sign "$+$".

(ii) For a PC bond, if the child atom corresponds to a branching node with sign "$-$", then the direction goes from the "P" atom to the "C" atom. If the child atom corresponds to a branching node with sign "$+$", the direction is reversed.

For any atom $v \in \mathbb{M}(\mathcal{Q})$, let $\mathfrak{n} = \mathfrak{n}(v)$ be its corresponding branching node in $\mathcal{Q}$. For any bond $\ell \sim v$, define $\mathfrak{m} = \mathfrak{m}(v, \ell)$ by:

(i) If ℓ is PC and v is labeled C, then $\mathfrak{m} = \mathfrak{n}$.

(ii) If ℓ is PC and v is labeled P, then $\mathfrak{m}$ is the branching node corresponding to the other endpoint of ℓ.

(iii) If ℓ is LP, then $\mathfrak{m}$ is the leaf (from the leaf pair defining ℓ) that is a child of $\mathfrak{n}$.

Proposition 2.13 (Correspondence between Molecules and Couples)**.** *We summarize the relationship between nontrivial couples and molecules as follows:*

1. *For any nontrivial couple $\mathcal{Q}$ of order n, the construction in Definition 2.12 yields a connected* molecule $\mathbb{M}(\mathcal{Q})$*. This molecule $\mathbb{M}$ has exactly n atoms, $2n - 1$ bonds, and either two atoms of degree 3, or a single atom of degree 2, with all remaining atoms having degree 4.*
2. *Conversely, given any molecule $\mathbb{M}$ with n atoms (as in Definition 2.11), there are at most C^n different couples $\mathcal{Q}$ (if any) for which $\mathbb{M}(\mathcal{Q})$ is exactly $\mathbb{M}$.*

Proof. We repeat the relevant parts of the proofs of Proposition 9.2, 9.4, and 9.6 of [42] here. (a) Let $\mathcal{Q}$ be a molecule of order $n \geq 1$ and write $\mathbb{M} = \mathbb{M}(\mathcal{Q})$ for its associated molecular graph. Because each branching node of $\mathcal{Q}$ corresponds to exactly one atom of $\mathbb{M}$, the graph $\mathbb{M}$ contains n atoms. Likewise, every non-root branching node gives one bond and every paired leaf contributes one further bond, for a total of

$$2n - 1 = (n - 2) + (n + 1)$$

bonds in $\mathbb{M}$.

A priori, $\mathbb{M}$ might decompose into two connected components; each component must contain at least one atom associated with a branching *root* whose degree is strictly smaller than 4. Suppose a component contains n_1 atoms. Since the sum of degrees in any finite graph is even and each atom has degree at most 4, that sum is bounded by $4n_1$. For the whole graph $\mathbb{M}$ the degree sum equals $4n-2$. If $\mathbb{M}$ were disconnected, one component would necessarily have all of its atoms of degree 4, contradicting the preceding observation. Hence $\mathbb{M}$ is connected.

(b) A mere labeling of the atoms of $\mathbb{M}$ does not yet specify the couple $\mathcal{Q}$; one also has to record the order of the corresponding nodes. Observe that every bond $\ell \sim v$ of $\mathbb{M}$ corresponds to a unique node of $\mathcal{Q}$. We encode that correspondence by assigning to the pair (v, ℓ) a *code*

that tells where the node sits inside its atom:

$$0 \text{ for the parent}, \quad 1, 2, 3 \text{ for the left, middle, right child.}$$

For a fixed molecular graph $\mathbb{M}$ there are at most C^n distinct ways to carry out this coding, with C a universal constant.

To see that such a coding reconstructs $\mathcal{Q}$ uniquely, note first that atoms of $\mathbb{M}$ bijectively represent branching nodes of $\mathcal{Q}$. If two atoms $v_1, v_2 \in \mathbb{M}$ are joined by a bond ℓ and the codes of (v_1, ℓ) and (v_2, ℓ) are 0 and j, then v_2 is the j-th child of v_1 in the couple. Conversely, if their codes are j and k with $j, k \in \{1, 2, 3\}$, the j-th child of the node represented by v_1 is paired with the k-th child of the node represented by v_2. Hence the entire set of codes fixes all parent–child relations and all leaf pairings, and therefore determines the couple $\mathcal{Q}$ uniquely. □

Definition 2.14 (Decorations of Molecules)**.** Let $\mathbb{M}$ be a molecule. For each atom (vertex) $v \in \mathbb{M}$, we fix $k_v \in \mathbb{Z}_N \cap (0, 1)$, with the condition $k_v = 0$ if v has degree 4, and $\alpha_v \in \mathbb{R}$.

A (k_v, α_v)-*decoration* of $\mathbb{M}$ assigns an integer $k_\ell \in \mathbb{Z}_N \cap (0, 1)$ to each bond $\ell \in \mathbb{M}$, in such a way that for each atom v,

$$\sum_{\ell \sim v} \zeta_{v,\ell}\, k_\ell \;=\; k_v, \quad \text{and} \quad \big|\Gamma_v - \alpha_v\big| \;<\; T^{-1},$$

where

$$\Gamma_v = \sum_{\ell : \ell \sim v} \zeta_{v,\ell}\, \omega(k_\ell).$$

Here, the summation $\sum_{\ell \sim v}$ runs over all bonds ℓ such that $\ell \sim v$, and $\zeta_{v,\ell}$ is defined to be $+1$ whenever ℓ is outgoing from v, and -1 otherwise. $\omega(\cdot)$ is the dispersion relation taking values in $\mathbb{R}$.

***k*-Decorations.** Suppose $\mathbb{M}$ arises from a nontrivial couple $\mathcal{Q}$, and let $k \in \mathbb{Z}_N \cap (0, 1)$. A k-*decoration* of $\mathbb{M}$ is a special (k_v, α_v)-decoration where

$$k_v \;=\; \begin{cases} 0 & \text{if } v \text{ has degree 2 or 4,} \\ +k & \text{if } v \text{ has out-degree 2 and in-degree 1,} \\ -k & \text{if } v \text{ has out-degree 1 and in-degree 2.} \end{cases}$$

Given any k-decoration of $\mathcal{Q}$ in the sense of Definition 2.4, define a k-decoration of $\mathbb{M}(\mathcal{Q})$ such that $k_\ell = k_{\mathfrak{m}(v,\ell)}$ for an endpoint v of ℓ. k_ℓ is well-defined and independent of the choice of v, and gives a one-to-one correspondence between k-decorations of $\mathcal{Q}$ and k-decorations

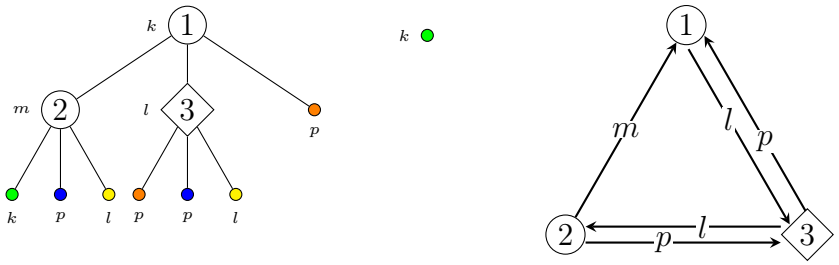


Figure 2.5: An example of an enhanced couple and its corresponding enhanced molecule.

of $\mathbb{M}(\mathcal{Q})$. Moreover, for such decorations we have

$$\Gamma_v = \begin{cases} 0 & \text{if } v \text{ has degree 2,} \\ -\zeta_{\mathfrak{n}(v)}\Omega_{\mathfrak{n}(v)} & \text{if } v \text{ has degree 4,} \\ -\zeta_{\mathfrak{n}(v)}\Omega_{\mathfrak{n}(v)} + \omega(k) & \text{if } v \text{ has out-degree 2 and in-degree 1,} \\ -\zeta_{\mathfrak{n}(v)}\Omega_{\mathfrak{n}(v)} - \omega(k) & \text{if } v \text{ has out-degree 1 and in-degree 2.} \end{cases} \tag{2.56}$$

Definition 2.15 (Enhanced Molecule of an Enhanced couple)**.** Let $\mathcal{Q}$ be an enhanced couple of order n. We construct its *enhanced molecule* $\mathbb{M}(\mathcal{Q})$ in the same manner that one constructs a molecule from a standard couple (cf. Definition 2.12), but incorporating the following *enhanced* configuration:

(i) For any degenerate branching node $\mathfrak{n} \in \mathcal{N}_D$, there exists a corresponding atom v in the enhanced molecule $\mathbb{M}(\mathcal{Q})$.

(ii) The atoms v_c^*, v_2, and v_c correspond precisely to the children $\{\mathfrak{n}_c^*, \mathfrak{n}_2, \mathfrak{n}_c\}$ of the degenerate branching node $\mathfrak{n}$ or their corresponding paired branching nodes.

(iii) Moreover, removing a single degenerate atom v together with all bonds ℓ such that $\ell \sim v$, then adding a new (PC) bond linking v_c (if it exists in the molecule) to v_p (if v has a (PC) bond ℓ_p connecting it to its parent v_p) the connectivity of $\mathbb{M}(\mathcal{Q})$ remains unchanged, i.e. $\Delta F = 0$.

Definition 2.16 (Degenerate Atoms)**.** Consider an enhanced molecule $\mathbb{M}$ equipped with a (k_v, α_v)-decoration as above. We say that an atom $v \in \mathbb{M}$ is *degenerate* if there exist two *degenerate* bonds $\ell_1, \ell_2 \sim v$, pointing in opposite directions at v, such that $k_{\ell_1} = k_{\ell_2}$. Furthermore, v is *fully degenerate* if *all* bonds $\ell \sim v$ share the same decoration k_ℓ. In particular, for each degenerate branching node in the couple $\mathcal{Q}$, there corresponds a degenerate atom in the molecule $\mathbb{M}(\mathcal{Q})$.

CHAPTER 3
Main Estimates

The purpose of this chapter is to provide the statements of the main estimates including the integral estimates and the Feynman diagram estimates.

3.1: The integral estimates

Proposition 3.1. *For any ternary tree $\mathcal{T}$, fix functions $f_{\mathfrak{n}} : [0,T] \to \mathbb{C}$ for each node $\mathfrak{n} \in \mathcal{T}$:*

$$|f_{\mathfrak{n}}(Ts)| \leq D_{\mathfrak{n}}, \tag{3.1}$$

$$\left|\frac{d}{ds} f_{\mathfrak{n}}(Ts)\right| = \left|T\dot{f}_{\mathfrak{n}}(Ts)\right| \leq D_{\mathfrak{n}}, \tag{3.2}$$

for some constants $D_{\mathfrak{n}}$. Suppose $\mathcal{T}$ has subtree children $\mathcal{T}_j$, $j = 1,2,3$ of the root $\mathfrak{r}$, and the function $\mathcal{A}^f_{\mathcal{T}}(s, \Omega[\mathcal{N}], \widetilde{\Omega}[\mathcal{N}])$ with $0 \leq s \leq 1$, is defined as:

$$\mathcal{A}^f_{\bullet}(s, \Omega[\mathcal{N}], \widetilde{\Omega}[\mathcal{N}]) = 1, \tag{3.3}$$

$$\mathcal{A}^f_{\mathcal{T}}(s, \Omega[\mathcal{N}], \widetilde{\Omega}[\mathcal{N}]) = \int_0^s e^{\zeta_{\mathfrak{r}} i(\Omega_{\mathfrak{r}} T s' + \widetilde{\Omega}_{\mathfrak{r}}(s'))} f_{\mathfrak{r}}(Ts') \prod_{j=1}^{3} \mathcal{A}^f_{\mathcal{T}_j}(s', \Omega[\mathcal{N}_j], \widetilde{\Omega}[\mathcal{N}_j]) ds' \tag{3.4}$$

$$= \int_{\mathcal{E}} \prod_{\mathfrak{n} \in \mathcal{N}} e^{\zeta_{\mathfrak{n}} i(\Omega_{\mathfrak{n}} T s_{\mathfrak{n}} + \widetilde{\Omega}_{\mathfrak{n}}(s_{\mathfrak{n}}))} f_{\mathfrak{n}}(Ts_{\mathfrak{n}}) ds_{\mathfrak{n}} \tag{3.5}$$

where $\mathcal{E} = \{s[\mathcal{N}] : 0 < s_{\mathfrak{n}'} < s_{\mathfrak{n}} < s$ whenever $\mathfrak{n}' \in \mathcal{N}$ is a child of $\mathfrak{n} \in \mathcal{N}\}$. For any node $\mathfrak{n} \in \mathcal{N}$, $\Omega_{\mathfrak{n}}$'s are constants and for some constant C_0:

$$\widetilde{\Omega}_{\mathfrak{n}}(s) := \Omega_{\mathfrak{n}} \left[C_0 \beta T s + A_{\geq}(s)\right], \tag{3.6}$$

$$\left|\dot{A}_{\geq}(s)\right| \lesssim \beta T, \tag{3.7}$$

$$\left|\ddot{A}_{\geq}(s)\right| \lesssim \beta T^{\frac{9}{5}}. \tag{3.8}$$

Then for any node $\mathfrak{n} \in \mathcal{N}$ there exist some constants $C_{\mathfrak{n}}$ such that $C_{\mathfrak{n}} \leq C_d D_{\mathfrak{n}}$ for some constant C_d, and

$$\left|\mathcal{A}^f_{\mathcal{T}}(s, \Omega[\mathcal{N}], \widetilde{\Omega}[\mathcal{N}])\right| \leq \sum_{(d_{\mathfrak{n}}:\mathfrak{n}\in\mathcal{N})} \prod_{\mathfrak{n}\in\mathcal{N}} C_{\mathfrak{n}} \langle T q_{\mathfrak{n}}\rangle^{-1}. \tag{3.9}$$

assuming $T < \beta^{-\frac{5}{4}}$.

Proof. We know that $\left|\dot{A}_{\geq}(s_{\mathfrak{n}})\right| \lesssim \beta T$, which gives that:

$$\left|\frac{T}{T + C_0\beta T + \dot{A}_{\geq}(s_{\mathfrak{n}})}\right| \lesssim 1. \tag{3.10}$$

Applying integration by parts to scale $|\mathcal{T}| = 1$ case:

$$\begin{aligned}
&\left|\int_0^s e^{\zeta_{\mathfrak{r}} i(\Omega_{\mathfrak{r}} T s' + \widetilde{\Omega}_{\mathfrak{r}}(T s'))} f_{\mathfrak{r}}(T s') ds'\right| \\
&= \frac{1}{iT\Omega_{\mathfrak{r}}}\left|\frac{e^{i\left(T\Omega_{\mathfrak{r}} s + \widetilde{\Omega}_{\mathfrak{r}}(s)\right)} T f_{\mathfrak{r}}(Ts)}{T + C_0\beta T + \dot{A}_{\geq}(s)} - \frac{f_{\mathfrak{r}}(0)}{1 + C_0\beta} + \int_0^s \frac{e^{i\left(T\Omega_{\mathfrak{r}} s' + \widetilde{\Omega}_{\mathfrak{r}}(s')\right)} T \ddot{A}_{\geq}(s') f_{\mathfrak{r}}(Ts')}{(T + C_0\beta T + \dot{A}_{\geq}(s'))^2} ds'\right. \\
&\quad \left. + \int_0^s \frac{e^{i\left(T\Omega_{\mathfrak{r}} s' + \widetilde{\Omega}_{\mathfrak{r}}(s')\right)} T^2 \dot{f}_{\mathfrak{r}}(Ts')}{T + C_0\beta T + \dot{A}_{\geq}(s')} ds'\right| \lesssim \frac{1}{\langle T\Omega_{\mathfrak{r}}\rangle} D_{\mathfrak{r}} \left(3 + \beta T^{\frac{4}{5}}\right).
\end{aligned} \tag{3.11}$$

From (3.37) and (3.11), we know (3.9) is true for $|\mathcal{T}| = 0, 1$ since $\beta T^{\frac{4}{5}} < 1$. Suppose (3.9) is true for $|\mathcal{T}| \leq n - 1$. Any ternary tree $\mathcal{T}$ with scale n can be obtained from a scale $(n-1)$ tree $\mathcal{T}' \subseteq \mathcal{T}$ by attaching a scale 1 tree $\mathcal{T}_1 \subseteq \mathcal{T}$ to one of its lowest level leaves $\mathfrak{l}$. This leaf $\mathfrak{l}$ should be chosen so that its siblings have at most scale 1. Let $\mathfrak{p}$ denote the parent of the lowest level leaf $\mathfrak{l}$ we chose, $\mathcal{T}_{\mathfrak{p}} \subseteq \mathcal{T}$ denote the subtree rooted at $\mathfrak{p}$, and $\mathcal{N}^-_{\mathfrak{p}} = \mathcal{N} \setminus \mathcal{T}_{\mathfrak{p}}$ denote the branching nodes of $\mathcal{T}$ excluding the descendants of $\mathfrak{p}$ and itself. We define:

$$\mathcal{A}(s[\mathcal{N}^-_{\mathfrak{p}}]) := \prod_{\mathfrak{n}\in\mathcal{N}^-_{\mathfrak{p}}} e^{\zeta_{\mathfrak{n}} i(\Omega_{\mathfrak{n}} T s_{\mathfrak{n}} + \widetilde{\Omega}_{\mathfrak{n}}(s_{\mathfrak{n}}))} f_{\mathfrak{n}}(T s_{\mathfrak{n}}) ds_{\mathfrak{n}}, \tag{3.12}$$

where $s[\mathcal{N}^-_{\mathfrak{p}}]$ denotes the time vector $(s_{\mathfrak{n}})_{\mathfrak{n}\in\mathcal{N}^-_{\mathfrak{p}}}$. Without loss of generality, we can assume $\zeta_{\mathfrak{p}} = \zeta_{\mathfrak{l}} = +1$. Then $\mathcal{A}^f_{\mathcal{T}'}(s, \Omega[\mathcal{N}'], \widetilde{\Omega}[\mathcal{N}'])$ and $\mathcal{A}^f_{\mathcal{T}}(s, \Omega[\mathcal{N}], \widetilde{\Omega}[\mathcal{N}])$ can also be expressed as:

$$\mathcal{A}^f_{\mathcal{T}'}(s, \Omega[\mathcal{N}'], \widetilde{\Omega}[\mathcal{N}']) = \int_{\mathcal{E}_{\mathfrak{p}}} \mathcal{A}(s[\mathcal{N}^-_{\mathfrak{p}}]) e^{i\left(T\Omega_{\mathfrak{p}} s_{\mathfrak{p}} + \widetilde{\Omega}_{\mathfrak{p}}(s_{\mathfrak{p}})\right)} f_{\mathfrak{p}}(T s_{\mathfrak{p}}) \prod_{j=2}^{3} \mathcal{A}^f_{\mathcal{T}_j}(s_{\mathfrak{p}}, \Omega[\mathcal{N}_j], \widetilde{\Omega}[\mathcal{N}_j]) ds_{\mathfrak{p}}, \tag{3.13}$$

$$\mathcal{A}^f_{\mathcal{T}}(s,\Omega[\mathcal{N}],\widetilde{\Omega}[\mathcal{N}]) = \int_{\mathcal{E}_{\mathfrak{p}}} \mathcal{A}(s[\mathcal{N}^-_{\mathfrak{p}}]) e^{i\left(T\Omega_{\mathfrak{p}} s_{\mathfrak{p}} + \widetilde{\Omega}_{\mathfrak{p}}(s_{\mathfrak{p}})\right)} f_{\mathfrak{p}}(Ts_{\mathfrak{p}})$$
$$\times \int_0^{s_{\mathfrak{p}}} e^{i\left(T\Omega_{\mathfrak{l}} s_{\mathfrak{l}} + \widetilde{\Omega}_{\mathfrak{l}}(s_{\mathfrak{l}})\right)} f_{\mathfrak{l}}(Ts_{\mathfrak{l}}) ds_{\mathfrak{l}} \prod_{j=2}^{3} \mathcal{A}^f_{\mathcal{T}_j}(s_{\mathfrak{p}},\Omega[\mathcal{N}_j],\widetilde{\Omega}[\mathcal{N}_j]) ds_{\mathfrak{p}} \tag{3.14}$$

where $\mathcal{E}_{\mathfrak{p}} = \left\{ s[\mathcal{N}^-_{\mathfrak{p}}] : 0 < s_{\mathfrak{n}'} < s_{\mathfrak{n}} < s \text{ whenever } \mathfrak{n}' \in \mathcal{N}^-_{\mathfrak{p}} \text{ is a child of } \mathfrak{n} \in \mathcal{N}^-_{\mathfrak{p}} \right\}$. Then by the hypotheses there exist constants $C_{\mathfrak{n}}$'s associated with nodes $\mathfrak{n} \in \mathcal{N}'$ such that:

$$\left| \mathcal{A}^f_{\mathcal{T}'}(s,\Omega[\mathcal{N}'],\widetilde{\Omega}[\mathcal{N}']) \right| \leq \sum_{(d_{\mathfrak{n}}:\mathfrak{n}\in\mathcal{N}')} \prod_{\mathfrak{n}\in\mathcal{N}'} C_{\mathfrak{n}} \langle T q_{\mathfrak{n}} \rangle^{-1}, \tag{3.15}$$

provided that:

$$|f_{\mathfrak{p}}(Ts)| \leq D_{\mathfrak{p}}, \tag{3.16}$$
$$\left| \frac{d}{ds} f_{\mathfrak{p}}(Ts) \right| = \left| T \dot{f}_{\mathfrak{p}}(Ts) \right| \leq D_{\mathfrak{p}}. \tag{3.17}$$

for constant $D_{\mathfrak{p}}$. Now assume:

$$|f_{\mathfrak{l}}(Ts)| \leq D_{\mathfrak{l}}, \tag{3.18}$$
$$\left| \frac{d}{ds} f_{\mathfrak{l}}(Ts) \right| = \left| T \dot{f}_{\mathfrak{l}}(Ts) \right| \leq D_{\mathfrak{l}}, \tag{3.19}$$

for constant $D_{\mathfrak{l}}$ assuming that $T < \beta^{-\frac{5}{4}}$. Then both $f_{\mathfrak{p}}$ and $f_{\mathfrak{l}}$ satisfy properties (3.1-3.2). We calculate $\mathcal{A}^f_{\mathcal{T}}(Ts,\Omega[\mathcal{N}],\widetilde{\Omega}[\mathcal{N}])$ using integration by parts from (3.11):

$$\begin{aligned}
\mathcal{A}^f_{\mathcal{T}}(Ts,\Omega[\mathcal{N}],\widetilde{\Omega}[\mathcal{N}]) =& \frac{1}{iT\Omega_{\mathfrak{l}}} \int_{\mathcal{E}_{\mathfrak{p}}} \mathcal{A}(s[\mathcal{N}^-_{\mathfrak{p}}]) e^{i\left(T\Omega_{\mathfrak{p}} s_{\mathfrak{p}} + \widetilde{\Omega}_{\mathfrak{p}}(s_{\mathfrak{p}})\right)} f_{\mathfrak{p}}(Ts_{\mathfrak{p}}) \left[\frac{e^{i\left(T\Omega_{\mathfrak{l}} s_{\mathfrak{p}} + \widetilde{\Omega}_{\mathfrak{l}}(s_{\mathfrak{p}})\right)} T f_{\mathfrak{l}}(Ts_{\mathfrak{p}})}{T + C_0\beta T + \dot{A}_{\geq}(s_{\mathfrak{p}})} \right. \\
& - \frac{f_{\mathfrak{p}}(0)}{1 + C_0\beta} + \int_0^{s_{\mathfrak{p}}} \frac{e^{i\left(T\Omega_{\mathfrak{l}} s_{\mathfrak{l}} + \widetilde{\Omega}_{\mathfrak{l}}(s_{\mathfrak{l}})\right)} T \ddot{A}_{\geq}(s_{\mathfrak{l}}) f_{\mathfrak{l}}(Ts_{\mathfrak{l}})}{(T + C_0\beta T + \dot{A}_{\geq}(s_{\mathfrak{l}}))^2} ds_{\mathfrak{l}} \\
& \left. + \int_0^{s_{\mathfrak{p}}} \frac{e^{i\left(T\Omega_{\mathfrak{l}} s_{\mathfrak{l}} + \widetilde{\Omega}_{\mathfrak{l}}(s_{\mathfrak{l}})\right)} T^2 \dot{f}_{\mathfrak{l}}(Ts_{\mathfrak{l}})}{T + C_0\beta T + \dot{A}_{\geq}(s_{\mathfrak{l}})} ds_{\mathfrak{l}} \right] \\
& \times \prod_{j=2}^{3} \mathcal{A}^f_{\mathcal{T}_j}(s_{\mathfrak{p}},\Omega[\mathcal{N}_j],\widetilde{\Omega}[\mathcal{N}_j]) ds_{\mathfrak{p}} \qquad (3.20) \\
=& I + II + III, \qquad (3.21)
\end{aligned}$$

where

$$I := \frac{1}{iT\Omega_{\mathfrak{l}}} \int_{\mathcal{E}_{\mathfrak{p}}} \mathcal{A}(s[\mathcal{N}_{\mathfrak{p}}^{-}]) e^{i\left(T(\Omega_{\mathfrak{p}}+\Omega_{\mathfrak{l}})s_{\mathfrak{p}}+(\widetilde{\Omega}_{\mathfrak{p}}+\widetilde{\Omega}_{\mathfrak{l}})(s_{\mathfrak{p}})\right)} \frac{T f_{\mathfrak{p}}(Ts_{\mathfrak{p}}) f_{\mathfrak{l}}(Ts_{\mathfrak{p}})}{T + C_0\beta T + \dot{A}_{\geq}(s_{\mathfrak{p}})} \times \prod_{j=2}^{3} \mathcal{A}^{f}_{\mathcal{T}_j}(s_{\mathfrak{p}}, \Omega[\mathcal{N}_j], \widetilde{\Omega}[\mathcal{N}_j]) ds_{\mathfrak{p}}, \tag{3.22}$$

$$II := -\frac{f_{\mathfrak{p}}(0)}{iT\Omega_{\mathfrak{l}}(1+C_0\beta)} \mathcal{A}^{f}_{\mathcal{T}'}(s, \Omega[\mathcal{N}'], \widetilde{\Omega}[\mathcal{N}']), \tag{3.23}$$

$$III := \frac{1}{iT\Omega_{\mathfrak{l}}} \int_{\mathcal{E}_{\mathfrak{p}}} \mathcal{A}(s[\mathcal{N}_{\mathfrak{p}}^{-}]) e^{i\left(T\Omega_{\mathfrak{p}}s_{\mathfrak{p}}+\widetilde{\Omega}_{\mathfrak{p}}(s_{\mathfrak{p}})\right)} f_{\mathfrak{p}}(Ts_{\mathfrak{p}}) \prod_{j=2}^{3} \mathcal{A}^{f}_{\mathcal{T}_j}(s_{\mathfrak{p}}, \Omega[\mathcal{N}_j], \widetilde{\Omega}[\mathcal{N}_j]) \times \int_{0}^{s_{\mathfrak{p}}} e^{i\left(T\Omega_{\mathfrak{l}}s_{\mathfrak{l}}+\widetilde{\Omega}_{\mathfrak{l}}(s_{\mathfrak{l}})\right)} T \left[\frac{\ddot{A}_{\geq}(s_{\mathfrak{l}}) f_{\mathfrak{l}}(Ts_{\mathfrak{l}})}{(T + C_0\beta T + \dot{A}_{\geq}(s_{\mathfrak{l}}))^2} + \frac{T\dot{f}_{\mathfrak{l}}(Ts_{\mathfrak{l}})}{T + C_0\beta T + \dot{A}_{\geq}(s_{\mathfrak{l}})} \right] ds_{\mathfrak{l}} ds_{\mathfrak{p}}. \tag{3.24}$$

Note that for I, we define:

$$f^{I}_{\mathfrak{p},\mathfrak{l}}(Ts_{\mathfrak{p}}) := \frac{T f_{\mathfrak{p}}(Ts_{\mathfrak{p}}) f_{\mathfrak{l}}(Ts_{\mathfrak{p}})}{T + C_0\beta T + \dot{A}_{\geq}(s_{\mathfrak{p}})}, \tag{3.25}$$

which gives:

$$\frac{d}{ds_{\mathfrak{p}}} f^{I}_{\mathfrak{p},\mathfrak{l}}(Ts_{\mathfrak{p}}) = \frac{T^2 \left(\dot{f}_{\mathfrak{p}}(Ts_{\mathfrak{p}}) f_{\mathfrak{l}}(Ts_{\mathfrak{p}}) + f_{\mathfrak{p}}(Ts_{\mathfrak{p}}) \dot{f}_{\mathfrak{l}}(Ts_{\mathfrak{p}}) \right)}{T + C_0\beta T + \dot{A}_{\geq}(s_{\mathfrak{p}})} - \frac{T f_{\mathfrak{p}}(Ts_{\mathfrak{p}}) f_{\mathfrak{l}}(Ts_{\mathfrak{p}}) \ddot{A}_{\geq}(s_{\mathfrak{p}})}{(T + C_0\beta T + \dot{A}_{\geq}(s_{\mathfrak{p}}))^2}. \tag{3.26}$$

Then from (3.1-3.2), (3.10), we can derive:

$$\left| f^{I}_{\mathfrak{p},\mathfrak{l}}(Ts_{\mathfrak{p}}) \right| \leq D_{\mathfrak{p}} D_{\mathfrak{l}}, \ \left| \frac{d}{ds_{\mathfrak{p}}} f^{I}_{\mathfrak{p},\mathfrak{l}}(Ts_{\mathfrak{p}}) \right| \lesssim (2 + \beta T^{\frac{4}{5}}) D_{\mathfrak{p}} D_{\mathfrak{l}}, \tag{3.27}$$

which means that the function $f^{I}_{\mathfrak{p},\mathfrak{l}}(Ts_{\mathfrak{p}})$ also satisfies properties (3.1-3.2) and I can be expressed by:

$$I = \frac{1}{iT\Omega_{\mathfrak{l}}} \int_{\mathcal{E}_{\mathfrak{p}}} \mathcal{A}(s[\mathcal{N}_{\mathfrak{p}}^{-}]) e^{i\left(T(\Omega_{\mathfrak{p}}+\Omega_{\mathfrak{l}})s_{\mathfrak{p}}+(\widetilde{\Omega}_{\mathfrak{p}}+\widetilde{\Omega}_{\mathfrak{l}})(s_{\mathfrak{p}})\right)} f^{I}_{\mathfrak{p},\mathfrak{l}}(Ts_{\mathfrak{p}}) \prod_{j=2}^{3} \mathcal{A}^{f}_{\mathcal{T}_j}(s_{\mathfrak{p}}, \Omega[\mathcal{N}_j], \widetilde{\Omega}[\mathcal{N}_j]) ds_{\mathfrak{p}}, \tag{3.28}$$

which can be derived in the form of $\mathcal{A}^{f}$ from a scale $(n-1)$ tree multiplied by a factor $\frac{1}{iT\Omega_{\mathfrak{l}}}$. Then from (3.1), (3.15), and (3.27) we know there exist constants $C_{\mathfrak{n}}$'s such that:

$$|I| \leq \frac{1}{\langle T\Omega_{\mathfrak{l}} \rangle} \sum_{(d_{\mathfrak{n}}:\mathfrak{n}\in\mathcal{N}')} \prod_{\mathfrak{n}\in\mathcal{N}'} C_{\mathfrak{n}} \langle Tq_{\mathfrak{n}} \rangle^{-1} \leq \sum_{(d_{\mathfrak{n}}:\mathfrak{n}\in\mathcal{N})} \prod_{\mathfrak{n}\in\mathcal{N}} C_{\mathfrak{n}} \langle Tq_{\mathfrak{n}} \rangle^{-1} \tag{3.29}$$

for $\rho \leq 1$. Here, $\langle Tq_{\mathfrak{n}} \rangle = \sqrt{1+(Tq_{\mathfrak{n}})^2}$ denotes the Japanese bracket. Similarly, we can bound II by the hypothesis (3.15) on $\mathcal{A}^f_{\mathcal{T}'}(s, \Omega[\mathcal{N}'], \widetilde{\Omega}[\mathcal{N}'])$ and (3.16) on $f_{\mathfrak{p}}$ respectively:

$$|II| \leq \frac{1}{\langle T\Omega_{\mathfrak{l}} \rangle} \sum_{(d_{\mathfrak{n}}:\mathfrak{n}\in\mathcal{N}')} \prod_{\mathfrak{n}\in\mathcal{N}'} C_{\mathfrak{n}} \langle Tq_{\mathfrak{n}} \rangle^{-1} \leq \sum_{(d_{\mathfrak{n}}:\mathfrak{n}\in\mathcal{N})} \prod_{\mathfrak{n}\in\mathcal{N}} C_{\mathfrak{n}} \langle Tq_{\mathfrak{n}} \rangle^{-1} \tag{3.30}$$

For III, we similarly define:

$$g_{\mathfrak{l}}(Ts_{\mathfrak{l}}) := T\left[\frac{\ddot{A}_{\geq}(s_{\mathfrak{l}}) f_{\mathfrak{l}}(Ts_{\mathfrak{l}})}{(T + C_0\beta T + \dot{A}_{\geq}(s_{\mathfrak{l}}))^2} + \frac{T\dot{f}_{\mathfrak{l}}(Ts_{\mathfrak{l}})}{T + C_0\beta T + \dot{A}_{\geq}(s_{\mathfrak{l}})}\right], \tag{3.31}$$

$$f^{III}_{\mathfrak{p},\mathfrak{l}}(Ts_{\mathfrak{p}}) := f_{\mathfrak{p}}(Ts_{\mathfrak{p}}) \int_0^{s_{\mathfrak{p}}} e^{i\left(T\Omega_{\mathfrak{l}} s_{\mathfrak{l}} + \widetilde{\Omega}_{\mathfrak{l}}(s_{\mathfrak{l}})\right)} g_{\mathfrak{l}}(Ts_{\mathfrak{l}}) ds_{\mathfrak{l}}. \tag{3.32}$$

We can easily derive from (3.1-3.2), and (3.10):

$$|g_{\mathfrak{l}}(Ts_{\mathfrak{l}})| \lesssim (1 + \beta T^{\frac{4}{5}}) D_{\mathfrak{l}}. \tag{3.33}$$

Then we can get:

$$\begin{aligned} \left|f^{III}_{\mathfrak{p},\mathfrak{l}}(Ts_{\mathfrak{p}})\right| &= \left|f_{\mathfrak{p}}(Ts_{\mathfrak{p}}) \int_0^{s_{\mathfrak{p}}} e^{i\left(T\Omega_{\mathfrak{l}} s_{\mathfrak{l}} + \widetilde{\Omega}_{\mathfrak{l}}(s_{\mathfrak{l}})\right)} g_{\mathfrak{l}}(Ts_{\mathfrak{l}}) ds_{\mathfrak{l}}\right| \\ &\leq |f_{\mathfrak{p}}(Ts_{\mathfrak{p}})| \cdot |g_{\mathfrak{l}}(Ts_{\mathfrak{p}})| \leq (1 + \beta T^{\frac{4}{5}}) D_{\mathfrak{p}} D_{\mathfrak{l}}, \end{aligned} \tag{3.34}$$

$$\begin{aligned} \left|\frac{d}{ds_{\mathfrak{p}}} f^{III}_{\mathfrak{p},\mathfrak{l}}(Ts_{\mathfrak{p}})\right| &= \left|\frac{d}{ds_{\mathfrak{p}}}\left[f_{\mathfrak{p}}(Ts_{\mathfrak{p}}) \int_0^{s_{\mathfrak{p}}} e^{i\left(T\Omega_{\mathfrak{l}} s_{\mathfrak{l}} + \widetilde{\Omega}_{\mathfrak{l}}(s_{\mathfrak{l}})\right)} g_{\mathfrak{l}}(Ts_{\mathfrak{l}}) ds_{\mathfrak{l}}\right]\right| \\ &\leq \left(\left|\frac{d}{ds_{\mathfrak{p}}} f_{\mathfrak{p}}(Ts_{\mathfrak{p}})\right| + |f_{\mathfrak{p}}(Ts_{\mathfrak{p}})|\right) \cdot |g_{\mathfrak{l}}(Ts_{\mathfrak{p}})| \\ &\lesssim 2(1 + \beta T^{\frac{4}{5}}) D_{\mathfrak{p}} D_{\mathfrak{l}} \end{aligned} \tag{3.35}$$

The function $f^{III}_{\mathfrak{p},\mathfrak{l}}(Ts_{\mathfrak{p}})$ also satisfies the property (3.1-3.2), which means III can also be derived in the form of $\mathcal{A}^f$ from a scale $(n-1)$ tree multiplied by a factor $\frac{1}{iT\Omega_{\mathfrak{l}}}$. Then there exist constants $C_{\mathfrak{n}}$'s such that:

$$\begin{aligned} |III| &= \left|\frac{1}{iT\Omega_{\mathfrak{l}}} \int_{\mathcal{E}_{\mathfrak{p}}} \mathcal{A}(s[\mathcal{N}^-_{\mathfrak{p}}]) e^{i\left(T\Omega_{\mathfrak{p}} s_{\mathfrak{p}} + \widetilde{\Omega}_{\mathfrak{p}}(s_{\mathfrak{p}})\right)} f^{III}_{\mathfrak{p},\mathfrak{l}}(Ts_{\mathfrak{p}}) \prod_{j=2}^{3} \mathcal{A}^f_{\mathcal{T}_j}(s_{\mathfrak{p}}, \Omega[\mathcal{N}_j], \widetilde{\Omega}[\mathcal{N}_j]) ds_{\mathfrak{p}}\right| \\ &\leq \frac{1}{\langle T\Omega_{\mathfrak{l}} \rangle} \sum_{(d_{\mathfrak{n}}:\mathfrak{n}\in\mathcal{N}')} \prod_{\mathfrak{n}\in\mathcal{N}'} C_{\mathfrak{n}} \langle Tq_{\mathfrak{n}} \rangle^{-1} \leq \sum_{(d_{\mathfrak{n}}:\mathfrak{n}\in\mathcal{N})} \prod_{\mathfrak{n}\in\mathcal{N}} C_{\mathfrak{n}} \langle Tq_{\mathfrak{n}} \rangle^{-1}. \end{aligned} \tag{3.36}$$

Then combining (3.29), (3.30), and (3.36), we get:

$$\left|\mathcal{A}_{\mathcal{T}}^{f}(s,\Omega[\mathcal{N}],\widetilde{\Omega}[\mathcal{N}])\right| \leq \sum_{(d_{\mathfrak{n}}:\mathfrak{n}\in\mathcal{N})}\prod_{\mathfrak{n}\in\mathcal{N}} C_{\mathfrak{n}}\langle Tq_{\mathfrak{n}}\rangle^{-1}.$$

□

Corollary 3.2. *For any ternary tree $\mathcal{T}$ with subtree children $\mathcal{T}_j$, $j=1,2,3$ of the root $\mathfrak{r}$, let the function $\mathcal{A}_{\mathcal{T}}(s,\Omega[\mathcal{N}],\widetilde{\Omega}[\mathcal{N}])$ with $0\leq s\leq 1$, be defined as:*

$$\mathcal{A}_{\bullet}(s,\Omega[\mathcal{N}],\widetilde{\Omega}[\mathcal{N}]) = 1, \tag{3.37}$$

$$\mathcal{A}_{\mathcal{T}}(s,\Omega[\mathcal{N}],\widetilde{\Omega}[\mathcal{N}]) = \int_0^s e^{\zeta_{\mathfrak{r}} i(\Omega_{\mathfrak{r}}Ts'+\widetilde{\Omega}_{\mathfrak{r}}(s'))}\prod_{j=1}^{3}\mathcal{A}_{\mathcal{T}_j}(s',\Omega[\mathcal{N}_j],\widetilde{\Omega}[\mathcal{N}_j])ds' \tag{3.38}$$

where for any node $\mathfrak{n}\in\mathcal{N}$, $\Omega_{\mathfrak{n}}$'s are constants and for some constant C_0:

$$\widetilde{\Omega}_{\mathfrak{n}}(s) = \Omega_{\mathfrak{n}}\left[(C_0\beta Ts + A_{\geq}(s)\right], \tag{3.39}$$

$$\left|\dot{A}_{\geq}(s)\right| \lesssim \beta T, \tag{3.40}$$

$$\left|\ddot{A}_{\geq}(s)\right| \lesssim \beta T^{\frac{9}{5}}. \tag{3.41}$$

Then for each node $\mathfrak{n}\in\mathcal{N}$ there exists a constant $C_{\mathfrak{n}}$, such that $\mathcal{A}_{\mathcal{T}}(s,\Omega[\mathcal{N}],\widetilde{\Omega}[\mathcal{N}])$ satisfies:

$$\left|\mathcal{A}_{\mathcal{T}}(s,\Omega[\mathcal{N}],\widetilde{\Omega}[\mathcal{N}])\right| \leq \sum_{(d_{\mathfrak{n}}:\mathfrak{n}\in\mathcal{N})}\prod_{\mathfrak{n}\in\mathcal{N}} C_{\mathfrak{n}}\langle Tq_{\mathfrak{n}}\rangle^{-1} \tag{3.42}$$

assuming $T<\beta^{-\frac{5}{4}}$.

Proof. We know that:

$$\mathcal{A}_{\mathcal{T}}(s,\Omega[\mathcal{N}],\widetilde{\Omega}[\mathcal{N}]) = \mathcal{A}_{\mathcal{T}}^{f\equiv 1}(s,\Omega[\mathcal{N}],\widetilde{\Omega}[\mathcal{N}]), \tag{3.43}$$

and (3.9) automatically yields (3.42) by taking $f_{\mathfrak{n}}\equiv 1$ for any node $\mathfrak{n}\in\mathcal{T}$. □

3.2: Bounds on Feynman diagrams

We fix a sufficiently large constant $L\ll N$.

Proposition 3.3. *(Bounds on Couples) For each $1\leq n_{\mathcal{Q}}\leq L^3$, $0\leq t\leq 1$, and enhanced*

trees $\mathcal{T}_1, \mathcal{T}_2$, the following should hold:

$$\left| \sum_{|\mathcal{T}_1|+|\mathcal{T}_2|=n_{\mathcal{Q}}} \mathbb{E}\left[c_k^{\mathcal{T}_1}(t) c_k^{\mathcal{T}_2 *}(t) \right] \right| \leq C(\log N \log T)^{n_{\mathcal{Q}}} T^{-\frac{3}{5}} \left(\beta T^{4/5}\right)^{n_{\mathcal{Q}}}, \tag{3.44}$$

$$\left| \sum_{|\mathcal{T}_1|+|\mathcal{T}_2|=n_{\mathcal{Q}}} \mathbb{E}\left[\dot{c}_k^{\mathcal{T}_1}(t) c_k^{\mathcal{T}_2 *}(t) \right] \right| \leq C(\log N \log T)^{n_{\mathcal{Q}}-1} T^{\frac{2}{5}} \left(\beta T^{4/5}\right)^{n_{\mathcal{Q}}}, \tag{3.45}$$

for some constant C.

Proposition 3.4. *(Bound on Operator $\mathscr{L}$) With probability $\geq 1 - N^{-A}$, the linear operator $\mathscr{L}$ defined in (2.30) satisfies*

$$||\mathscr{L}^n||_{Z \to Z} \lesssim \left(\beta T^{4/5}\right)^{n/2} N^{50} \tag{3.46}$$

for each $0 \leq n \leq L$ and some $A \geq 40$.

The proofs of these two propositions will be given in Chapters 5 and 6 respectively.

3.3: Plan for the rest of the thesis

In Chapter 2, we introduced the definitions of enhanced trees, enhanced couples and molecule structures, and we chose and performed the nonlinear frequency shift. In Chapter 3, we proved the integral estimates Proposition 3.1 & 3.2, and stated the bounds on couples and the operator $\mathscr{L}$.

In Chapter 4, we prove the three-vector and two-vector counting estimates and also the convergence of iterates used for the main theorem. In Chapter 5, we introduce the irregular chains and perform the splicing to remove the small-gap chains in Section 5.2. We remove the degenerate nodes by performing an additional preprocessing step before the algorithm, and prove that the molecule structure remains the same as in [46] in Section 5.3 & 5.4. We then prove Proposition 3.3 in Section 5.5 using a bootstrap argument.

In Chapter 6 we introduce the flower trees and flower couples, and prove Proposition 3.4. In Chapter 7, we bound the remainder terms using a contraction mapping argument. Finally, we prove the main Theorem 1, deriving the wave kinetic equation for the reduced evolution equation.

In Chapter 8, we prove for a sufficient threshold for the nonlinearity parameter β to perform the canonical transformation to the original evolution equation. In Chapter 9, we simulate the β-FPUT model by the symplectic integrator method and compare the sizes

of resonant sums and nonresonant sums in Hamiltonian. We plot the simulation results for different nonlinearities and number of particles to verify the nonlinearity parameter threshold for the canonical transformation.

CHAPTER 4
Counting Estimates

In this chapter, we prove the vector counting estimates and the convergence of iterates. Denote $\mathbb{Z}_N := N^{-1}\mathbb{Z}$ and $\mathcal{S}$ as the Schwartz space.

Proposition 4.1 (Three Vector Counting)**.** *Let $1 < T \leq N^{1-\epsilon}$ for $\epsilon \ll 1$. Then uniformly in $k \in \mathbb{Z}_N \cap (-1, 2) \setminus \{0, 1\}$ and $m \in \mathbb{R}$, the set:*

$$S_3 = \Big\{(x, y, z) \in \mathbb{Z}_N^3 \cap (0, 1)^3 : x - y + z = k, \\ |\sin(\pi x) - \sin(\pi y) + \sin(\pi z) - |\sin(\pi k)| - m| \leq T^{-1}\Big\} \tag{4.1}$$

satisfies the bound:

$$\sum_{(x,y,z)\in S_3} F(x, y) \lesssim N^2 T^{-1} \log T, \tag{4.2}$$

where

$$F(x, y) = |\sin(\pi x) \sin(\pi y) \sin(\pi(k - x + y))|. \tag{4.3}$$

Proof. Suppose $\Omega(x, y) = \sin(\pi x) - \sin(\pi y) + \sin(\pi(k - x + y))$, $\varphi(x, y) \in \mathcal{S}(\mathbb{R}^2)$ equal to 1 on $B(0, 1)$ and compact support on $B(0, 2)$, and $\chi \in \mathcal{S}(\mathbb{R})$ is 1 on the unit ball $B(mT, 1)$, and $\hat{\chi}$ is supported on a ball of constant radius C. Let $e(x) = \exp(2\pi i x)$. For the calculation below, we replace F with a positive Schwartz function that equals to F on S_3, and we still denote it as F without affecting any results. Applying Fourier Transform on χ and Poisson Summation on $\sum_{x,y\in\mathbb{Z}_N} F(x, y)\varphi(x, y)e(\tau\Omega(x, y))$, we get:

$$\sum_{(x,y,z)\in S_3} F(x, y) \leq \sum_{x,y\in\mathbb{Z}_N} F(x, y)\varphi(x, y)\chi(T\Omega(x, y)) \\ = \sum_{x,y\in\mathbb{Z}_N} F(x, y)\varphi(x, y) \int_{-\infty}^{\infty} \hat{\chi}(\tau)e(\tau T\Omega(x, y))\, d\tau$$

$$
\begin{aligned}
&= T^{-1} \sum_{x,y\in\mathbb{Z}_N} F(x,y)\varphi(x,y) \int_{-\infty}^{\infty} \hat{\chi}\left(\frac{\tau}{T}\right) e\left(\tau\Omega(x,y)\right) d\tau \\
&= T^{-1} \int_{-\infty}^{\infty} \hat{\chi}\left(\frac{\tau}{T}\right) \left[\sum_{x,y\in\mathbb{Z}_N} F(x,y)\varphi(x,y) e\left(\tau\Omega(x,y)\right)\right] d\tau \\
&= T^{-1} \int_{-\infty}^{\infty} \hat{\chi}\left(\frac{\tau}{T}\right) \int_{(x,y)\in\mathbb{R}^2} F\left(\frac{x}{N},\frac{y}{N}\right) \varphi\left(\frac{x}{N},\frac{y}{N}\right) e\left(\tau\Omega\left(\frac{x}{N},\frac{y}{N}\right)\right) dxdyd\tau \\
&+ T^{-1} \int_{-\infty}^{\infty} \hat{\chi}\left(\frac{\tau}{T}\right) \sum_{(c,d)\in\mathbb{Z}^2\setminus\{(0,0)\}} \int_{(x,y)\in\mathbb{R}^2} F\left(\frac{x}{N},\frac{y}{N}\right) \varphi\left(\frac{x}{N},\frac{y}{N}\right) \\
&\qquad\qquad \times e\left(\tau\Omega\left(\frac{x}{N},\frac{y}{N}\right) - cx - dy\right) dxdyd\tau \\
&= N^2T^{-1} \int_{-\infty}^{\infty} \hat{\chi}\left(\frac{\tau}{T}\right) \int_{(x,y)\in B(0,2)} F(x,y)\varphi(x,y) e\left(\tau\Omega(x,y)\right) dxdyd\tau \\
&+ N^2T^{-1} \int_{-\infty}^{\infty} \hat{\chi}\left(\frac{\tau}{T}\right) \sum_{(c,d)\in\mathbb{Z}^2\setminus\{(0,0)\}} \int_{(x,y)\in B(0,2)} F(x,y)\varphi(x,y) \\
&\qquad\qquad \times e\left(\tau\Omega(x,y) - cNx - dNy\right) dxdyd\tau \\
&= I + II
\end{aligned}
$$

For I, we can rewrite I as:

$$
\begin{aligned}
I &= N^2T^{-1} \int_{-\infty}^{\infty} \hat{\chi}\left(\frac{\tau}{T}\right) \int_{(x,y)\in B(0,2)} F(x,y)\varphi(x,y) e\left(\tau\Omega(x,y)\right) dxdyd\tau \\
&= N^2 \int_{(x,y)\in B(0,2)} F(x,y)\varphi(x,y)\chi(T\Omega(x,y)) dxdy
\end{aligned} \tag{4.4}
$$

Note that:

$$
\partial_y\Omega(x,y) = \pi[\cos(\pi y) - \cos(\pi(k-x+y))] \tag{4.5}
$$

which means $\partial_y\Omega(x,y) \neq 0$ unless $(x,y) \in \{(x,y) : x-k \in 2\mathbb{Z} \text{ or } k-x+2y \in 2\mathbb{Z}\}$. Let

$$
E := \{(x,y) : x-k \in 2\mathbb{Z} \text{ or } k-x+2y \in 2\mathbb{Z}\}, \tag{4.6}
$$

$$
E_1 := \{(x,y) \in B(0,2) : |(x,y)-E| \geq T^{-1}\}, \tag{4.7}
$$

$$
E_2 := \{(x,y) \in B(0,2) : |(x,y)-E| < T^{-1}\}. \tag{4.8}
$$

Here, $|(x,y)-E|$ denotes Euclidean distance from (x,y) to the set E. Note that due to (4.5) one can solve the equation $\Omega(x,y) = \Omega_0$ for y given x and Ω_0 on E_1. Then we can separate

I into two terms:

$$I = N^2 \int_{(x,y)\in E_1} F(x,y)\varphi(x,y)\chi(T\Omega(x,y))dxdy + N^2 \int_{(x,y)\in E_2} F(x,y)\varphi(x,y)\chi(T\Omega(x,y))dxdy \tag{4.9}$$

$$= I.1 + I.2 \tag{4.10}$$

Inside the region E_1, for any even integer p we have:

$$|x-k-p|, |k-x+2y-p| \gtrsim T^{-1}. \tag{4.11}$$

Applying substitution $y \mapsto \Omega$ and $dy = d\Omega/\partial_y\Omega$ to the region E_1 for $I.1$, we have:

$$|I.1| = \left| N^2 \int_{\mathbb{R}} \left(\int_{\substack{\Omega=s \\ (x,y(s,x))\in E_1}} \varphi(x,y(s,x)) \frac{F(x,y)}{\partial_y\Omega(x,y(s,x))} dx \right) \chi(Ts)ds \right| \tag{4.12}$$

$$\lesssim N^2 \int_{\mathbb{R}} \left(\int_{\substack{\Omega=s \\ (x,y(s,x))\in E_1}} \varphi(x,y(s,x)) \left| \frac{\sin(\pi y)\sin(\pi(k-x+y))}{\cos(\pi y) - \cos(\pi(k-x+y))} \right| dx \right) \chi(Ts)ds \tag{4.13}$$

Let $\tilde{x} = \frac{x-k}{2}$, and we can formulate the integrand as:

$$\begin{aligned}
&\left| \frac{\sin(\pi y)\sin(\pi(k-x+y))}{\cos(\pi y) - \cos(\pi(k-x+y))} \right| = \left| \frac{\sin(\pi y)\sin(\pi(y-2\tilde{x}))}{2\sin(\pi\tilde{x})\sin(\pi(y-\tilde{x}))} \right| \\
&= \left| \frac{1}{2} \cdot \frac{\sin(\pi y)\sin(\pi(y-2\tilde{x}))}{\sin(\pi\tilde{x}) - \sin(\pi(y-\tilde{x}))} \cdot \left(\frac{1}{\sin(\pi\tilde{x})} - \frac{1}{\sin(\pi(y-\tilde{x}))} \right) \right| \\
&= \left| \frac{1}{4} \cdot \frac{\sin(\pi y)\sin(\pi(y-2\tilde{x}))}{\cos(\frac{\pi y}{2})\sin(\pi(\frac{y}{2}-\tilde{x}))} \cdot \left(\frac{1}{\sin(\pi\tilde{x})} - \frac{1}{\sin(\pi(y-\tilde{x}))} \right) \right| \\
&= \left| \sin\left(\frac{\pi y}{2}\right) \cos\left(\pi\left(\frac{y}{2}-\tilde{x}\right)\right) \left(\frac{1}{\sin(\pi\tilde{x})} - \frac{1}{\sin(\pi(y-\tilde{x}))} \right) \right| \\
&\lesssim \left| \frac{1}{\sin(\pi\tilde{x})} \right| + \left| \frac{1}{\sin(\pi(y-\tilde{x}))} \right|.
\end{aligned} \tag{4.14}$$

Then we can estimate $|I.1|$ using (4.14):

$$|I.1| \lesssim N^2 \int_{\mathbb{R}} \left(\int_{\substack{\Omega=s \\ (x(\tilde{x}),y(s,x))\in E_1}} \left| \frac{1}{\sin(\pi\tilde{x})} \right| + \left| \frac{1}{\sin(\pi(y-\tilde{x}))} \right| d\tilde{x} \right) \chi(Ts)ds \tag{4.15}$$

$$\lesssim N^2 \int_{\mathbb{R}} \int_{T^{-1}}^{1} \frac{1}{\tilde{x}}\, d\tilde{x}\ \chi(Ts)\ ds = N^2 T^{-1} \log T \int_{\mathbb{R}} \chi(t)dt \lesssim N^2 T^{-1} \log T. \tag{4.16}$$

Note that the inner integral can be separated into several parts, if $y(\Omega = s)$ has more than one value, since the map $y \mapsto \Omega$ can have finitely many solutions for given fixed k and x in E_1. And inside E_1, we have $|\sin(\tilde{x})|, |\sin(\pi(y-\tilde{x})| \gtrsim T^{-1}$, which lead to counting of $\log T$. On the other hand, for $I.2$, we know that $|E_2| \lesssim T^{-1}$, and then $|I.2| \lesssim N^2T^{-1}$. For II, the phase function $\Phi(x,y) = \tau\Omega(x,y) - cNx - dNy$ satisfies:

$$|\nabla_{(x,y)}\Phi(x,y)| = |\tau\nabla_{(x,y)}\Omega(x,y) - N(c,d)| \gtrsim N|c|, \tag{4.17}$$

for $c \neq 0$ and $\tau \leq CT \lesssim N^{1-\epsilon}$. Then we can integrate by parts many times as:

$$\nabla_{(x,y)} e(\tau\Omega(x,y) - cNx - dNy) = \frac{e(\tau\Omega(x,y) - cNx - dNy)}{2\pi i \nabla_{(x,y)}\Phi(x,y)}, \tag{4.18}$$

to show that $|II| \ll N^2T^{-1}$. Hence $\sum_{(x,y,z)\in S_3} F(x,y) \lesssim N^2T^{-1}\log T$. □

Corollary 4.2. *(Convergence of Iterates) For fixed $k \in \mathbb{Z}_N \cap (-1,2)\setminus\{0,1\}$, let $F \in \mathcal{S}(\mathbb{R}^2)$, $\chi \in \mathcal{S}(\mathbb{R})$ with $\hat{\chi}$ supported in a ball of constant radius $C > 0$. Then for all $\delta > 0$ sufficiently small we have*

$$\sum_{\substack{x,y\in\mathbb{Z}_N\cap(0,1)\\ k-x+y\in(0,1)}} F(x,y)\chi(T\Omega(x,y)) = N^2 \int_{\substack{x,y\in(0,1)\\ k-x+y\in(0,1)}} F(x,y)\chi(T\Omega(x,y))dxdy + O(N^{2-\delta}T^{-1}), \tag{4.19}$$

where

$$\Omega(x,y) = \sin(\pi x) - \sin(\pi y) + \sin(\pi(k-x+y)) - |\sin(\pi k)|.$$

Proof. We choose compactly supported $\varphi \in \mathcal{S}(\mathbb{R}^2)$ to be 1 on $S = \{(x,y) \in (0,1)^2 : k-x+y \in (0,1)\}$ and nonzero on S_1 where $|S_1 \setminus S| \lesssim N^{-10\delta}T^{-1}$. Then using the result in Proposition 4.1, we get:

$$\sum_{\substack{x,y\in\mathbb{Z}_N\cap(0,1)\\ k-x+y\in(0,1)}} F(x,y)\chi(T\Omega(x,y)) = \sum_{x,y\in\mathbb{Z}_N} F(x,y)\varphi(x,y)\chi(T\Omega(x,y)) + O(N^{2-\delta}T^{-1}) \tag{4.20}$$

And similarly following the calculation in Proposition 4.1, we can write the first term in (4.20) as:

$$\sum_{x,y\in\mathbb{Z}_N} F(x,y)\varphi(x,y)\chi(T\Omega(x,y)) = N^2 \int_{(x,y)\in\mathbb{R}^2} F(x,y)\varphi(x,y)\chi(T\Omega(x,y))dxdy$$

$$+ N^2T^{-1}\int_{-\infty}^{\infty}\hat{\chi}\left(\frac{\tau}{T}\right)\sum_{(c,d)\in\mathbb{Z}^2\setminus\{(0,0)\}}\int_{\mathbb{R}^2}F(x,y)\varphi(x,y)e\left(\tau\Omega(x,y)-cNx-dNy\right)dxdyd\tau. \tag{4.21}$$

$$= N^2\int_{\substack{x,y\in(0,1)\\ k-x+y\in(0,1)}}F(x,y)\chi(T\Omega(x,y))dxdy+O(N^{2-\delta}T^{-1}).$$

Again we can use $|S_1\setminus S|\lesssim N^{-10\delta}T^{-1}$ to show that:

$$N^2\int_{(x,y)\in\mathbb{R}^2}F(x,y)|\varphi(x,y)-\mathbf{1}_S|\chi(T\Omega(x,y))dxdy\lesssim O(N^{2-\delta}T^{-1}),$$

and apply integration by parts sufficiently many times to show that (4.21)$\lesssim O(N^{2-\delta}T^{-1})$, from which (4.19) follows. □

Proposition 4.3 (Two Vector Counting)**.** *Let $1<T\leq N^{1-\epsilon}$ for $\epsilon\ll 1$. Then uniformly in $k\in\mathbb{Z}_N\cap(-1,2)$ and $m\in\mathbb{R}$, the sets:*

$$S_2^{\pm}=\Big\{(x,y)\in\mathbb{Z}_N^2\cap(0,1)^2:x\pm y=k,\\ |\sin(\pi x)\pm\sin(\pi y)-m|\leq T^{-1}\Big\}. \tag{4.22}$$

satisfy the bounds:

$$\sum_{(x,y)\in S_2^+}G(x)\lesssim NT^{-\frac{1}{2}}, \tag{4.23}$$

$$\sum_{(x,y)\in S_2^-}G(x)\lesssim\begin{cases}NT^{-\frac{1}{2}} & \text{if } |k|\gtrsim T^{-\frac{1}{2}},\\ N & \text{otherwise,}\end{cases} \tag{4.24}$$

where

$$G(x)=|\sin(\pi x)\sin(\pi(k-x))|. \tag{4.25}$$

Proof. Similarly as in Proposition 4.1, for $\sum_{(x,y)\in S_2^{\pm}}G(x)$, we define:

$$\Omega_2(x)=\sin(\pi x)+\sin(\pi(k-x)),$$

$\chi\in\mathcal{S}(\mathbb{R})$ is 1 on the unit ball $B(mT,1)$, and $\hat{\chi}$ is supported on a ball of radius constant C. Let $e(x)=\exp(2\pi ix)$, and $\psi(x)\in\mathcal{S}(\mathbb{R})$ being 1 on $(-1,1)$ and compact support on $[-2,2]$. We replace G with a positive Schwartz function that equals to G on $S_2^{\pm}$. Applying Fourier

Transform on χ and Poisson Summation again on $\sum_x G(x)\psi(x)e\left(\tau\Omega_2(x)\right)$, we get:

$$\begin{aligned}\sum_{(x,y)\in S_2^{\pm}} G(x) &\leq \sum_x G(x)\psi(x)\chi\left(T\Omega_2(x)\right)\\ &= NT^{-1}\int_{-\infty}^{\infty}\hat{\chi}\left(\frac{\tau}{T}\right)\int_{x\in(-2,2)} G(x)\psi(x)e\left(\tau\Omega_2(x)\right)dxd\tau\\ &+ NT^{-1}\int_{-\infty}^{\infty}\hat{\chi}\left(\frac{\tau}{T}\right)\sum_{c\in\mathbb{Z}\setminus\{0\}}\int_{x\in(-2,2)} G(x)\psi(x)e\left(\tau\Omega_2(x)-cNx\right)dxd\tau\\ &= III + IV\end{aligned}$$

Note that:

$$\Omega_2'(x) = \pi[\cos(\pi x) - \cos(\pi(k-x))] = 2\pi\sin\left(\frac{\pi k}{2}\right)\sin\left(\pi\left(x-\frac{k}{2}\right)\right) \tag{4.26}$$

which means $\Omega_2'(x)\neq 0$ unless $x\in\{x: 2x-k\in 2\mathbb{Z}\}$ or $k=0$. If $k=0$, the trivial countings $\sum_{(x,y)\in S_2^+} G(x)=0$ and $\sum_{(x,y)\in S_2^-} G(x)\leq N$ are true. If $|k-2|\lesssim T^{-\frac{1}{2}}$ or $|k|\lesssim T^{-\frac{1}{2}}$, then $\sum_{(x,y)\in S_2^+} G(x)\lesssim NT^{-\frac{1}{2}}$. If $k\neq 0$ and $|k-2|\gtrsim T^{-\frac{1}{2}}$, we let

$$E' = \{x: 2x-k\in 2\mathbb{Z}\}, \tag{4.27}$$

$$E_1' = \{x\in(-2,2): |x-E'|\geq T^{-\frac{1}{2}}\}, \tag{4.28}$$

$$E_2' = \{x\in(-2,2): |x-E'|< T^{-\frac{1}{2}}\}. \tag{4.29}$$

Then similarly we have:

$$III = N\int_{x\in E_1'}\psi(x)\chi(T\Omega_2(x))dx + N\int_{x\in E_2'}\psi(x,y)\chi(T\Omega_2(x))dx \tag{4.30}$$

$$= III.1 + III.2 \tag{4.31}$$

Applying substitution $dx = d\Omega_2/\Omega_2'$ to the region E_1' for $III.1$, we have:

$$|III.1| = \left|N\int_{\mathbb{R}}\left(\int_{\substack{\Omega=s\\ x\in E_1'}}\psi(x(s))\frac{G(x)}{\Omega_2'(x(s))}dx\right)\chi(Ts)ds\right| \tag{4.32}$$

$$\lesssim N\int_{x(s)\in E_1'}\psi(x(s))\left|\frac{\sin(\pi x(s))\sin(\pi(k-x(s)))}{\sin\left(\frac{\pi k}{2}\right)\sin\left(\pi\left(x(s)-\frac{k}{2}\right)\right)}\right|\chi(Ts)ds. \tag{4.33}$$

We estimate the integrand again:

$$\begin{aligned}
&\left|\frac{\sin(\pi x)\sin(\pi(k-x))}{\sin\left(\frac{\pi k}{2}\right)\sin\left(\pi\left(x-\frac{k}{2}\right)\right)}\right| = \left|\frac{\sin(\pi x)\sin(\pi(k-x))}{\sin\left(\frac{\pi k}{2}\right)-\sin\left(\pi\left(x-\frac{k}{2}\right)\right)}\cdot\left(\frac{1}{\sin\left(\frac{\pi k}{2}\right)}-\frac{1}{\sin\left(\pi\left(x-\frac{k}{2}\right)\right)}\right)\right| \\
&= \left|\frac{\sin(\pi x)\sin(\pi(k-x))}{2\cos\left(\frac{\pi x}{2}\right)\sin\left(\pi\left(\frac{k-x}{2}\right)\right)}\cdot\left(\frac{1}{\sin\left(\frac{\pi k}{2}\right)}-\frac{1}{\sin\left(\pi\left(x-\frac{k}{2}\right)\right)}\right)\right| \\
&= \left|2\sin\left(\frac{\pi x}{2}\right)\cos\left(\pi\left(\frac{k-x}{2}\right)\right)\cdot\left(\frac{1}{\sin\left(\frac{\pi k}{2}\right)}-\frac{1}{\sin\left(\pi\left(x-\frac{k}{2}\right)\right)}\right)\right| \\
&\lesssim \left|\frac{1}{\sin\left(\frac{\pi k}{2}\right)}\right| + \left|\frac{1}{\sin\left(\pi\left(x-\frac{k}{2}\right)\right)}\right|. \qquad (4.34)
\end{aligned}$$

Then similarly as in Proposition 4.1:

$$\begin{aligned}
|III.1| &\lesssim N\int_{x(s)\in E_1'}\psi(x(s))\chi(Ts)\left(\left|\frac{1}{\sin\left(\frac{\pi k}{2}\right)}\right|+\left|\frac{1}{\sin\left(\pi\left(x-\frac{k}{2}\right)\right)}\right|\right)ds \\
&\lesssim \max(NT^{-\frac{1}{2}}, NT^{-1}|k|^{-1}). \qquad (4.35)
\end{aligned}$$

On the other hand, for $III.2$, we know that $|E_2'|\lesssim T^{-\frac{1}{2}}$, and then $|III.2|\lesssim NT^{-\frac{1}{2}}$. For IV, the phase function $\Psi(x)=\tau\Omega_2(x)-cNx$ satisfies:

$$|\Psi'(x)| = |\tau\Omega_2'(x)-Nc| \gtrsim N|c|, \qquad (4.36)$$

for $c\neq 0$ and $\tau\leq CT\lesssim N^{1-\epsilon}$. Then we can integrate by parts many times as:

$$\frac{d}{dx}e\left(\tau\Omega_2(x)-cNx\right) = \frac{e\left(\tau\Omega_2(x)-cNx\right)}{2\pi i\Psi(x)}, \qquad (4.37)$$

to show that $|IV|\ll NT^{-\frac{1}{2}}$. Thus we have:

$$\sum_{(x,y)\in S_2^+} G(x) \lesssim NT^{-\frac{1}{2}}, \qquad (4.38)$$

$$\sum_{(x,y)\in S_2^-} G(x) \lesssim \begin{cases} NT^{-\frac{1}{2}} & \text{if } |k|\gtrsim T^{-\frac{1}{2}}, \\ NT^{-1}|k|^{-1} & \text{if } T^{-\frac{1}{2}}\gtrsim|k|\gtrsim T^{-1}, \\ N & \text{otherwise,} \end{cases} \qquad (4.39)$$

where we take the trivial counting N for $(x,y)\in S_2^-$ and $|k|\lesssim T^{-1}$. □

CHAPTER 5
Molecules and Couples

In this chapter, we introduce the irregular chains, the splicing process to remove the small gap irregular chains, the preprocessing steps we need to add to the algorithm from [46], and finally prove the bounds on couples using a bootstrap argument.

5.1: Double bonds and chains

In this and next sections we repeat the definitions of double bonds, chains, unit twist, congruent couples, and splicing from [42, 46].

Definition 5.1. Let $\mathcal{Q}$ be an enhanced couple such that $\mathbb{M}(\mathcal{Q})$ has two atoms, v_1 and v_2, connected by precisely two edges oriented in opposite directions (resp. same direction). Denote by $\mathfrak{n}_j = \mathfrak{n}(v_j)$ for $j = 1, 2$. Then, up to symmetry, exactly one of the following two scenarios arises by Proposition 5.1 in [46]:

(i) **Cancellation (CL) Double Bond:** There exists a child $\mathfrak{n}_{12}$ of $\mathfrak{n}_1$ which is paired with a child $\mathfrak{n}_{21}$ of $\mathfrak{n}_2$. Moreover, $\mathfrak{n}_2$ is itself a child of $\mathfrak{n}_1$ such that $\mathfrak{n}_{12}$ and $\mathfrak{n}_2$ have opposite signs (resp. same sign). All other leaf-children of $\mathfrak{n}_1$ and $\mathfrak{n}_2$ remain unpaired. In the corresponding molecular structure, this configuration represents a double bond composed of one LP bond and one PC bond.

(ii) **Connectivity (CN) Double Bond:** There are children $\mathfrak{n}_{11}, \mathfrak{n}_{12}$ of $\mathfrak{n}_1$ with opposite signs (resp. same sign), as well as children $\mathfrak{n}_{21}, \mathfrak{n}_{22}$ of $\mathfrak{n}_2$ having opposite signs (resp. same sign). These four children pair off according to their signs, leaving any remaining leaf-children of $\mathfrak{n}_1$ and $\mathfrak{n}_2$ unpaired. In addition, neither $\mathfrak{n}_1$ nor $\mathfrak{n}_2$ is a child of the other in this scenario. In the molecular structure, this corresponds to a double bond in which both bonds are LP.

Definition 5.2 (Chains)**.** Let $\mathcal{Q}$ be an enhanced couple, and let $\mathbb{M}(\mathcal{Q})$ be its corresponding molecule. A *chain* in $\mathbb{M}(\mathcal{Q})$ is a sequence of atoms (nodes) $(v_0, \ldots, v_q)$ such that each

consecutive pair v_i, v_{i+1} (for $0 \le i \le q-1$) is connected by either a CL or CN double bond. We define the following special types of chains:

(i) A *CL chain* is a chain whose double bonds are all CL.

(ii) A *negative chain* is a chain whose bonds are oriented with opposite directions.

(iii) An *irregular chain* is a negative chain that is also CL.

(iv) A *maximal chain* is a chain for which v_0 and v_q do not connect (via CL or CN double bonds) to any atoms outside the chain.

(v) A *hyperchain* is a chain where v_0 and v_q are also joined by a single bond.

(vi) A *pseudo-hyperchain* is a chain where v_0 and v_q each connect (via single bonds) to another common atom $v \notin \{v_0, \dots, v_q\}$.

(vii) A *wide ladder* is a collection of chains $(v_0^{(1)}, \dots, v_{q^{(1)}}^{(1)}), \dots, (v_0^{(m)}, \dots, v_{q^{(m)}}^{(m)})$, where each chain is referred to as a *rung*, such that or each $1 \le i \le m-1$, there is a bond connecting the vertices $v_0^{(i)}$ and $v_0^{(i+1)}$, as well as a bond connecting the vertices $v_{q^{(i)}}^{(i)}$ and $v_{q^{(i+1)}}^{(i+1)}$.

Definition 5.3 (Irregular Chains and Splicing)**.** A sequence of nodes $(\mathfrak{n}_0, \dots, \mathfrak{n}_q)$ in the couple $\mathcal{Q}$ is called a *CL chain* if, for each $0 \le j \le q-1$,

(i) $\mathfrak{n}_{j+1}$ is a child of $\mathfrak{n}_j$,

(ii) $\mathfrak{n}_j$ has a child $\mathfrak{m}_{j+1}$ paired with a child $\mathfrak{p}_{j+1}$ of $\mathfrak{n}_{j+1}$,

(iii) $\mathfrak{n}_0^1$ to be the remaining child of $\mathfrak{n}_0$,

(iv) $\mathfrak{n}_0^2$ and $\mathfrak{n}_0^3$ to be the remaining children of $\mathfrak{n}_q$.

If, in addition, each pair $(\mathfrak{n}_i, \mathfrak{m}_i)$ has opposite sign for $1 \le i \le q$, then the chain is called *irregular*. By the labeling convention relating couples to molecules, a sequence $(v_0, \dots, v_q)$ in $\mathbb{M}(\mathcal{Q})$ is a CL chain (resp. irregular chain) if and only if $(\mathfrak{n}_0, \dots, \mathfrak{n}_q)$ is.

Splicing a CL chain $(\mathfrak{n}_0, \dots, \mathfrak{n}_q)$ at $\mathfrak{n}_1, \dots, \mathfrak{n}_q$ means removing those nodes and their leaf-children $\mathfrak{n}_i, \mathfrak{m}_i, \mathfrak{p}_i$ for $(i = 1, \dots, q)$ from $\mathcal{Q}$ and redefining the children of $\mathfrak{n}_0$ accordingly. The children of $\mathfrak{n}_0$ become $\mathfrak{n}_0^1$, $\mathfrak{n}_0^2$, and $\mathfrak{n}_0^3$, with their position determined by sign or by their relative position as children of $\mathfrak{n}_q$. The resulting couple is denoted $\mathcal{Q}^{\mathrm{sp}}$, with its corresponding molecule $\mathbb{M}^{\mathrm{sp}}$.

Definition 5.4 (Gaps in Negative Chains)**.** Suppose $\mathbb{M}(\mathcal{Q})$ has a double bond whose edges point in opposite directions. For a chosen *decoration* of $\mathbb{M}(\mathcal{Q})$, let k and ℓ be the decoration values on these two edges, and define the *gap* $h := k - \ell$. The double bond is called a *large gap (LG) double bond* if $|h| \gtrsim T^{-\frac{1}{2}}$ and a *small gap (SG) double bond* if $|h| \lesssim T^{-\frac{1}{2}}$.

By [42, Proposition 8.3], all double bonds in a given chain share the same gap magnitude. Specifically, in an irregular chain $(\mathfrak{n}_0, \ldots, \mathfrak{n}_q)$, the gap can also be tracked via

$$h = k_{\mathfrak{n}_0} - k_{\mathfrak{n}_0^1} = k_{\mathfrak{n}_j} - k_{\mathfrak{m}_j} \quad (1 \le j \le q).$$

5.2: Cancellation of irregular chains

Definition 5.5 (Twist-Admissibility and Unit Twist)**.** Let $\mathcal{Q}$ be an enhanced couple with node set $\mathcal{N}$.

(i) We call a node $\mathfrak{n}_2 \in \mathcal{N}$ *twist-admissible* if it has a parent $\mathfrak{n}_1$ such that the atoms v_1, v_2 corresponding to $\mathfrak{n}_1, \mathfrak{n}_2$ in the molecule $\mathbb{M}(\mathcal{Q})$ are joined by a CL double bond and further that these two bonds have opposite orientations (i.e., the double bond is negative). Denote by $\mathfrak{n}_{12}$ and $\mathfrak{n}_{21}$ the paired children of $\mathfrak{n}_1$ and $\mathfrak{n}_2$, respectively.

(ii) A *unit twist* of $\mathcal{Q}$ at a twist-admissible node $\mathfrak{n}_2$ is performed by:

  (a) Swapping the node $\mathfrak{n}_{12}$ with $\mathfrak{n}_2$ itself,

  (b) Swapping the two children (and subtrees) of $\mathfrak{n}_2$ that are *not* $\mathfrak{n}_{21}$,

  (c) Leaving all other parent-child relationships (and their signs) unchanged.

(iii) Suppose $\mathcal{Q}$ is a *decorated* couple, where each node or leaf $\mathfrak{m}$ has a decoration $k_{\mathfrak{m}}$. A unit twist at $\mathfrak{n}_2$ induces a corresponding decoration on the new couple $\mathcal{Q}'$ by:

$$k_{\tilde{\mathfrak{m}}} = k_{\mathfrak{m}} \quad \text{for all } \mathfrak{m} \text{ except } \mathfrak{n}_2, \mathfrak{n}_{12}, \mathfrak{n}_{21},$$

and setting

$$k_{\tilde{\mathfrak{n}}_2} = k_{\mathfrak{n}_{12}} = k_{\mathfrak{n}_{21}}, \quad k_{\tilde{\mathfrak{n}}_{12}} = k_{\tilde{\mathfrak{n}}_{21}} = k_{\mathfrak{n}_2}.$$

If one splices either $\mathcal{Q}$ or $\mathcal{Q}'$ at $\mathfrak{n}_2$, the resulting couple (and its molecule) agrees in structure and decoration.

Definition 5.6 (Congruent Couples)**.** Two enhanced couples $\mathcal{Q}_1$ and $\mathcal{Q}_2$ are *congruent*, written $\mathcal{Q}_1 \sim \mathcal{Q}_2$, if one can obtain $\mathcal{Q}_2$ from $\mathcal{Q}_1$ (and vice versa) by performing any finite sequence of unit twists. If $\mathcal{Q}_1$ and $\mathcal{Q}_2$ are decorated, these decorations correspond one-to-one under the same twists. Since unit twists commute, specifying a set of twist-admissible nodes $\mathcal{M} \subset \mathcal{N}$ determines a family of congruent couples. Denote by

$$\mathfrak{Q}_{\mathcal{M}} = \{\mathcal{Q}' \mid \mathcal{Q}' \sim \mathcal{Q} \text{ via some subset of twists in } \mathcal{M}\}.$$

If $\mathcal{K}_{\mathcal{Q}}(t,s,k)$ denotes a function or weight associated to $\mathcal{Q}$, define

$$\mathcal{K}_{\mathfrak{Q}_{\mathcal{M}}}(t,s,k) \;=\; \sum_{\mathcal{Q}'\in\mathfrak{Q}_{\mathcal{M}}} \mathcal{K}_{\mathcal{Q}'}(t,s,k).$$

Lemma 5.7. *For an enhanced couple $\mathcal{Q}$ and SG irregular chain $(\mathfrak{n}_0,\dots,\mathfrak{n}_q)$ of length q,*

$$\begin{aligned}
&\mathcal{K}_{\mathfrak{Q}_{\mathcal{M}}}(t,s,k)\\
&= \left(\frac{\beta T}{N}\right)^{n_{\mathrm{sp}}} \zeta(\mathcal{Q}^{\mathrm{sp}}) \sum_{\mathscr{E}^{\mathrm{sp}}} \tilde{\epsilon}_{\mathscr{E}^{\mathrm{sp}}} \int_0^1 \int_{\mathcal{E}_\tau^{\mathrm{sp}}} P_q(\tau, t_{\mathfrak{n}_0}, k[\mathcal{N}^{\mathrm{sp}}]) \left(\prod_{\mathfrak{n}\in\mathcal{N}^{\mathrm{sp}}} e^{\zeta_{\mathfrak{n}} i(\Omega_{\mathfrak{n}} T t_{\mathfrak{n}} + \widetilde{\Omega}_{\mathfrak{n}}(t_{\mathfrak{n}}))} dt_{\mathfrak{n}}\right) d\tau \\
&\qquad\qquad \times \prod_{\mathfrak{l}\in\mathcal{L}^{\mathrm{sp}}}^{+} n_{\mathrm{in}}(k_{\mathfrak{l}}) \mathbb{E}\left[\mathcal{B}_{\mathcal{T}^+}(\eta_{\mathcal{T}^+}(\varrho))\mathcal{B}^*_{\mathcal{T}^-}(\eta_{\mathcal{T}^-}(\varrho))\right], \qquad (5.1)
\end{aligned}$$

where for some constant C_0, $\widetilde{\Omega}_{\mathfrak{n}}$ and P_q satisfies

$$\widetilde{\Omega}_{\mathfrak{n}}(s) = \Omega_{\mathfrak{n}}\left[(C_0\beta T s + A_{\geq}(s)\right], \qquad (5.2)$$

$$\left|\dot{A}_{\geq}(s)\right| \lesssim \beta T, \qquad (5.3)$$

$$\sup_{|k_{\mathfrak{n}_0} - k_{\mathfrak{n}_0^1}|\leq T^{-1/2}} ||P_q(\tau, t_0, k[\mathcal{N}^{\mathrm{sp}}])||_{\ell^\infty} \lesssim \left(\beta T^{1/2}\right)^q, \qquad (5.4)$$

$$\sup_{|k_{\mathfrak{n}_0} - k_{\mathfrak{n}_0^1}|\leq T^{-1/2}} \left|\left|\frac{d}{dt_0} P_q(\tau, t_0, k[\mathcal{N}^{\mathrm{sp}}])\right|\right|_{\ell^\infty} \lesssim \left(\beta T^{1/2}\right)^q, \qquad (5.5)$$

and

$$\mathcal{E}_\tau^{\mathrm{sp}} = \mathcal{E}^{\mathrm{sp}} \cap \{t_{\mathfrak{n}_0} \geq t_{\mathfrak{n}_0^2} + \tau, t_{\mathfrak{n}_0} \geq t_{\mathfrak{n}_0^3} + \tau\}. \qquad (5.6)$$

In the above, we let $\mathcal{Q}^{\mathrm{sp}}$ be the couple obtained from $\mathcal{Q}$ by splicing out its irregular chain, and its corresponding decorations $\mathscr{E}^{\mathrm{sp}}$, domain of integration $\mathcal{E}^{\mathrm{sp}}$ and its nodes $\mathcal{N}^{\mathrm{sp}}$ and leaves $\mathcal{L}^{\mathrm{sp}}$. The notation $k[\mathcal{N}^{\mathrm{sp}}]$ denotes the decorations on the nodes of this spliced couple, and we define $\mathcal{M} = \{\mathfrak{n}_1,\dots,\mathfrak{n}_q\}$. Furthermore, $\tilde{\epsilon}_{\mathscr{E}^{\mathrm{sp}}}$ permits degeneracies at $\mathfrak{n}_0$.

Proof. Without loss of generality, we assume that $\mathcal{Q}$ is the element of $\mathfrak{Q}_{\mathcal{M}}$ where all $\zeta_{\mathfrak{n}_j}$ $(j=0,\dots,q)$ have the same sign. Following the notation in Definition 5.3, we set $k_{\mathfrak{n}_i} = k_i$, $k_{\mathfrak{p}_i} = k_{\mathfrak{m}_i} = \ell_i$, and $t_i = t_{\mathfrak{n}_i} (0\leq i\leq q)$. In addition, we let $\ell_0 = k_{\mathfrak{n}_0^1}, k_{q+1} = k_{\mathfrak{n}_0^2}$, and $\ell_{q+1} = k_{\mathfrak{n}_0^3}$, and $t_{q+1} = \max(t_{\mathfrak{n}_0^2}, t_{\mathfrak{n}_0^3})$. We keep all $k_{\mathfrak{n}}$ and $t_{\mathfrak{n}}$ for $\mathfrak{n}\notin\{\mathfrak{n}_i,\mathfrak{p}_i,\mathfrak{m}_i\}(1\leq i\leq q)$ fixed so that the small gap is also fixed by $k_0,\ell_0,k_{q+1},\ell_{q+1}$:

$$h := k_0 - \ell_0 = k_1 - \ell_1 = \ldots = k_q - \ell_q = k_{q+1} - \ell_{q+1}.$$

As before, we define the frequency mismatch as:

$$\begin{aligned}\Omega_j &= \omega_{k_{j+1}} - \omega_{\ell_{j+1}} + \omega_{\ell_j} - \omega_{k_j} \\ &= 2(\sin(\pi k_{j+1}) - \sin(\pi \ell_{j+1}) + \sin(\pi \ell_j) - \sin(\pi k_j)) \\ &= 4\sin\left(\frac{\pi h}{2}\right)\left[\cos\left(\frac{\pi(k_{j+1}+\ell_{j+1})}{2}\right) - \cos\left(\frac{\pi(k_j+\ell_j)}{2}\right)\right].\end{aligned}$$

This sinusoidal dispersion relation gives: $|\Omega_j| \lesssim h$ for any $j = 0, \ldots, q$. Summing over the chain, we get:

$$\Omega = \sum_{j=0}^{q} \Omega_j = 2(\sin(\pi k_{q+1}) - \sin(\pi \ell_{q+1}) + \sin(\pi \ell_0) - \sin(\pi k_0)).$$

For each $\mathcal{Q}' \in \mathfrak{Q}_{\mathcal{M}}$, the difference in $\mathcal{K}_{\mathcal{Q}'}$ compared to $\mathcal{K}_{\mathcal{Q}}$ can be identified as:

$$\left(\frac{\beta T}{N}\right)^q \sum_{\substack{k_i,\ell_i \in \mathbb{Z}_N \cap (0,1) \\ k_i - \ell_i = h \\ i=1,\ldots,q}} \int_{t_{q+1}<t_q<\ldots<t_1<t_0} \left(\prod_{j=1}^{q} i\zeta_{\mathfrak{n}_j}\right)\left(\prod_{j=0}^{q} \epsilon_{k_{j+1}\ell_{j+1}m_j}\right) \times \left(\prod_{j=0}^{q} e^{\zeta_{\mathfrak{n}_j} i(\Omega_j T t_j + \widetilde{\Omega}_j(t_j))}\right)\left(\prod_{j=1}^{q} n_{\mathrm{in}}(m_j)\right) dt_1 \ldots dt_q,$$

where $m_0 = \ell_0$, and $m_j = \ell_j$ or $m_j = k_j$ for congruent couples with unit twist performed at $\mathfrak{n}_j$. A unit twist at node $\mathfrak{n}_j$ reverses the sign of $\zeta_{\mathfrak{n}_j}$ but leaves the product $\zeta_{\mathfrak{n}_j}\Omega_j$ unchanged. For congruent couples, the enhanced couple structure will not change which leaves the part $\mathbb{E}\left[\mathcal{B}_{\mathcal{T}^+}(\eta_{\mathcal{T}^+}(\varrho))\mathcal{B}^*_{\mathcal{T}^-}(\eta_{\mathcal{T}^-}(\varrho))\right]$ also unchanged. Hence, when we sum over all couples $\mathcal{Q}' \in \mathfrak{Q}_{\mathcal{M}}$, we are effectively summing over every possible choice of $\zeta_{\mathfrak{n}_j}$ for $j = 1, \ldots, q$. Note that for our FPUT model, in addition to the linear frequency shift at t_0, we also need to extract the nonlinear frequency shift at t_0 and the new coefficient $\epsilon_{k_{q+1}\ell_{q+1}\ell_0}$ after splicing. The resulting expressions are derived as follows:

$$\begin{aligned}&\left(\frac{\beta T}{N}\right)^q \sum_{\substack{k_i \in \mathbb{Z}_N \cap (0,1) \\ i=1,\ldots,q}} \int_{t_{q+1}<t_q<\ldots<t_1<t_0} \left(\prod_{j=0}^{q} \epsilon_{k_{j+1}\ell_{j+1}m_j}\right)\left(\prod_{j=0}^{q} e^{i(\Omega_j T t_j + \widetilde{\Omega}_j(t_j))}\right) \\ &\qquad \times \left(\prod_{j=1}^{q} n_{\mathrm{in}}(k_j - h) - n_{\mathrm{in}}(k_j)\right) dt_1 \ldots dt_q \\ = \epsilon_{k_{q+1}\ell_{q+1}\ell_0} \cdot e^{i(\Omega T t_0 + \widetilde{\Omega}(t_0))} &\sum_{\substack{k_i \in \mathbb{Z}_N \cap (0,1) \\ i=1,\ldots,q}} \int_{t_{q+1}<t_q<\ldots<t_1<t_0} \left(\frac{\beta T}{N}\right)^q \left(\prod_{j=1}^{q} \epsilon_{k_j \ell_j}\right)\end{aligned}$$

$$\times \left(\prod_{j=1}^{q} e^{i(\Omega_j T(t_j-t_0)+\widetilde{\Omega}_j(t_j)-\widetilde{\Omega}_j(t_0))}\right)\left(\prod_{j=1}^{q} n_{\text{in}}(k_j-h)-n_{\text{in}}(k_j)\right)dt_1\dots dt_q$$

$$= \epsilon_{k_{q+1}\ell_{q+1}\ell_0}\cdot e^{i(\Omega T t_0+\widetilde{\Omega}(t_0))}\int\limits_{0<s_1<\dots<s_q<t_0-t_{q+1}}\left(\frac{\beta T}{N}\right)^q\sum_{\substack{k_i\in\mathbb{Z}_N\cap(0,1)\\ i=1,\dots,q}}\left(\prod_{j=1}^{q}\epsilon_{k_j\ell_j}\right)$$

$$\times \left(\prod_{j=1}^{q} e^{i(\Omega_j T(s_j)+\widetilde{\Omega}_j(s_j+t_0)-\widetilde{\Omega}_j(t_0))}\right)\left(\prod_{j=1}^{q} n_{\text{in}}(k_j-h)-n_{\text{in}}(k_j)\right)dt_1\dots dt_q$$

$$= \epsilon_{k_{q+1}\ell_{q+1}\ell_0}\cdot e^{i(\Omega T t_0+\widetilde{\Omega}(t_0))}\int\limits_{\tau\in[0,t_0-t_{q+1}]}P_q(\tau,t_0,k[\mathcal{N}^{\text{sp}}])d\tau,$$

where we define:

$$\epsilon_{k_j\ell_j} := \epsilon_{k_j\ell_j m_{j-1}}\cdot\sqrt{\frac{\omega_{k_j}\omega_{\ell_j}}{\omega_{k_{j-1}}\omega_{\ell_{j-1}}}}, \tag{5.7}$$

$$P_q(\tau,t_0,k[\mathcal{N}^{\text{sp}}]) := \left(\frac{\beta T}{N}\right)^q\sum_{\substack{k_i\in\mathbb{Z}_N\cap(0,1)\\ i=1,\dots,q}}\int\limits_{0<s_1<\dots<s_{q-1}<\tau}\left(\prod_{j=1}^{q}\epsilon_{k_j\ell_j}\right)$$
$$\times\left(\prod_{j=1}^{q} e^{i(\Omega_j T(s_j)+\widetilde{\Omega}_j(s_j+t_0)-\widetilde{\Omega}_j(t_0))}\right)\left(\prod_{j=1}^{q} n_{\text{in}}(k_j-h)-n_{\text{in}}(k_j)\right)ds_1\dots ds_{q-1}. \tag{5.8}$$

Using the regularity of n_{in}, we can bound $P_q(\tau,t_0,k[\mathcal{N}^{\text{sp}}])$. Then for SG case we have:

$$\left(\frac{\beta T}{N}\right)\sum_{k\in\mathbb{Z}_N\cap(0,1)}|n_{\text{in}}(k-h)-n_{\text{in}}(k)|\lesssim\beta T h\lesssim\beta T^{\frac{1}{2}}.$$

It will then recover (5.4). Compared to the result in [46, Lemma 5.11], the expression P_q does not only depends on the time difference τ, but also depends on the initial splicing time t_0 due to the nonlinear frequency shift, which means that we are not able to isolate the integral of P_q from the multi-integral of frequency shifts. To bound the new integral as shown in (5.1), we need to apply the technique we used in Proposition 3.1 and let $f_{\mathfrak{n}_0}(Tt_0)=P_q(\tau,t_0,k[\mathcal{N}^{\text{sp}}])/\left(\beta T^{\frac{1}{2}}\right)^q$, which indicates $|f_{\mathfrak{n}_0}(Tt_0)|\lesssim 1$. Thus we further need to prove $\left|\frac{d}{dt_0}f_{\mathfrak{n}_0}(Tt_0)\right|\lesssim 1$. Similarly as above and applying the fact $|\Omega_j|\lesssim h$ for any $j=0,\dots,q$, then for $\beta T^{\frac{4}{5}}<1$ we can get (5.5):

$$\left|\frac{d}{dt_0}P_q(\tau,t_0,k[\mathcal{N}^{\text{sp}}])\right|\lesssim\left(\beta T^{\frac{1}{2}}\right)^q\max_{j=1,\dots,q}\left|\widetilde{\Omega}_j'(s_j+t_0)-\widetilde{\Omega}_j'(t_0))\right|\lesssim\left(\beta T^{\frac{1}{2}}\right)^q h\lesssim\left(\beta T^{\frac{1}{2}}\right)^q.$$

We are then able to write $\mathcal{K}_{\mathfrak{Q}_{\mathcal{M}}}(t,s,k)$ as:

$$\begin{aligned}\mathcal{K}_{\mathfrak{Q}_{\mathcal{M}}}(t,s,k) &= \left(\frac{\beta T}{N}\right)^{n_{\mathrm{sp}}} \zeta(\mathcal{Q}^{\mathrm{sp}}) \sum_{\mathscr{E}^{\mathrm{sp}}} \tilde{\epsilon}_{\mathscr{E}^{\mathrm{sp}}} \int_{\mathcal{E}^{\mathrm{sp}}} \int_{0\leq\tau\leq(t_{\mathfrak{n}_0}-\max(t_{\mathfrak{n}_0^2},t_{\mathfrak{n}_0^3}))} P_q(\tau, t_{\mathfrak{n}_0}, k[\mathcal{N}^{\mathrm{sp}}])d\tau \\ &\quad \times \left(\prod_{\mathfrak{n}\in\mathcal{N}^{\mathrm{sp}}} e^{\zeta_{\mathfrak{n}} i(\Omega_{\mathfrak{n}} T t_{\mathfrak{n}} + \widetilde{\Omega}_{\mathfrak{n}}(t_{\mathfrak{n}}))} dt_{\mathfrak{n}}\right) \prod_{\mathfrak{l}\in\mathcal{L}^{\mathrm{sp}}}^{+} n_{\mathrm{in}}(k_{\mathfrak{l}}) \mathbb{E}\left[\mathcal{B}_{\mathcal{T}^+}(\eta_{\mathcal{T}^+}(\varrho))\mathcal{B}^*_{\mathcal{T}^-}(\eta_{\mathcal{T}^-}(\varrho))\right] \\ &= \left(\frac{\beta T}{N}\right)^{n_{\mathrm{sp}}} \zeta(\mathcal{Q}^{\mathrm{sp}}) \sum_{\mathscr{E}^{\mathrm{sp}}} \tilde{\epsilon}_{\mathscr{E}^{\mathrm{sp}}} \int_0^1 \int_{\mathcal{E}^{\mathrm{sp}}_\tau} P_q(\tau, t_0, k[\mathcal{N}^{\mathrm{sp}}]) \\ &\quad \times \left(\prod_{\mathfrak{n}\in\mathcal{N}^{\mathrm{sp}}} e^{\zeta_{\mathfrak{n}} i(\Omega_{\mathfrak{n}} T t_{\mathfrak{n}} + \widetilde{\Omega}_{\mathfrak{n}}(t_{\mathfrak{n}}))} dt_{\mathfrak{n}}\right) d\tau \prod_{\mathfrak{l}\in\mathcal{L}^{\mathrm{sp}}}^{+} n_{\mathrm{in}}(k_{\mathfrak{l}}) \mathbb{E}\left[\mathcal{B}_{\mathcal{T}^+}(\eta_{\mathcal{T}^+}(\varrho))\mathcal{B}^*_{\mathcal{T}^-}(\eta_{\mathcal{T}^-}(\varrho))\right].\end{aligned}$$

□

We repeat [46, Definition 5.13] as follows:

Definition 5.8. Consider an enhanced couple $\mathcal{Q}$ and enhanced molecule $\mathbb{M}(\mathcal{Q})$. Let $\mathscr{C}$ be defined as a unique collection of disjoint atomic groups, such that each atomic group in $\mathscr{C}$ is a negative chain, negative hyperchain, or negative pseudo-hyperchain and any negative chain $\mathcal{C}$ of $\mathbb{M}$ is a subset of precisely one atomic group in $\mathscr{C}$.

Suppose also that we have chosen $\mathscr{C}_1 \subset \mathscr{C}$ of all SG negative chain-like objects. Consider the set $\mathscr{D}_{\mathscr{C}_1}$ defined as a unique collection of disjoint atomic groups, such that each atomic group in $\mathscr{D}_{\mathscr{C}_1}$ is a maximal negative wide ladder of $\mathscr{C}_1$ and each chain $\mathcal{C} \in \mathscr{C}_1$ is a subset of precisely one atomic group in $\mathscr{D}_{\mathscr{C}_1}$. Existence and uniqueness of $\mathscr{C}$ and $\mathscr{D}_{\mathscr{C}_1}$ can be found in [46, Lemma 5.12].

We define the set $\mathcal{M}_{\mathscr{C}_1}$ below. If $\mathcal{L} \in \mathscr{D}_{\mathscr{C}_1}$ consists of a single chain $\mathcal{C} = (v_0, \ldots, v_q) \in \mathscr{C}_1$:

(i) If $\mathcal{C}$ is a chain, we include all admissible $\mathfrak{n}(v_i)$ into $\mathcal{M}$.

(ii) If $\mathcal{C}$ is a hyperchain or pseudo-hyperchain with a CN double bond, we include all admissible $\mathfrak{n}(v_i)$ into $\mathcal{M}$. If there is no CN double bond, we exclude one admissible $\mathfrak{n}(v_i)$.

Otherwise, let $\mathcal{L} = \{\mathcal{C}_1, \ldots, \mathcal{C}_m\}$, where each chain $\mathcal{C}_j$ has length $q^{(j)}$. We perform the following procedure:

1. Start with $\mathcal{C}_1$ and determine which of its nodes should be added to $\mathcal{M}$ by applying the previously described procedure, treating it as a hyperchain or pseudo-hyperchain if applicable.

2. For each subsequent chain $\mathcal{C}_{j+1}$ with $j \leq m-2$, check whether all $q^{(j)}$ nodes of $\mathcal{C}_j$ are contained in $\mathcal{M}$. If so, treat $\mathcal{C}_{j+1}$ as in step (ii) above when determining which nodes to add to $\mathcal{M}$. Otherwise, treat it as in step (i).

3. For the final chain $\mathcal{C}_m$, if it is a hyperchain or pseudo-hyperchain, or if all $q^{(m-1)}$ nodes of $\mathcal{C}_{m-1}$ are in $\mathcal{M}$, then process $\mathcal{C}_m$ as in step (ii). Otherwise, treat it as in step (i).

Otherwise $\mathcal{L} = \{\mathcal{C}_1, \dots, \mathcal{C}_m\}$ with chain j having length $q^{(j)}$, perform the following:

1. Starting with $\mathcal{C}_1$ determine the nodes to be added to $\mathcal{M}$ by performing the above, considering it as a hyperchain or pseudo-hyperchain if it is.

2. For $\mathcal{C}_{j+1}$ and $j \leq m-2$, if there are $q^{(j)}$ nodes of $\mathcal{C}_j$ contained in $\mathcal{M}$, treat $\mathcal{C}_{j+1}$ as to point (2) above in determining which nodes to add to $\mathcal{M}$. Otherwise, treat it according to (1).

3. For $\mathcal{C}_m$, if it is a hyperchain or pseudo-hyperchain or there are $q^{(m-1)}$ nodes of $\mathcal{C}_{m-1}$ in $\mathcal{M}$, treat $\mathcal{C}_m$ according to (2). Otherwise, treat it according to (1).

Corollary 5.9. *For an enhanced couple $\mathcal{Q}$, and choice of SG negative chain-like objects $\mathscr{C}_1$ in $\mathbb{M}(\mathcal{Q})$, consider the resulting couple $\mathcal{Q}^{\mathrm{sp}}$ obtained by splicing $\mathcal{Q}$ at the nodes in $\mathcal{M} = \mathcal{M}_{\mathscr{C}_1}$.*

$$\mathcal{K}_{\mathfrak{Q}_{\mathcal{M}}}(t,s,k) = \left(\frac{\beta T}{N}\right)^{n_{\mathrm{sp}}} \zeta(\mathcal{Q}^{\mathrm{sp}}) \sum_{\mathscr{E}^{\mathrm{sp}}} \tilde{\epsilon}_{\mathscr{E}^{\mathrm{sp}}} \int_{[0,1]^{\mathcal{N}_0^{\mathrm{sp}}}} \int_{\mathcal{E}_{\boldsymbol{\tau}}^{\mathrm{sp}}} \prod_{\mathfrak{n}_0 \in \mathcal{N}_0^{\mathrm{sp}}} P_{q_{\mathfrak{n}_0}}(\tau_{\mathfrak{n}_0}, t_{\mathfrak{n}_0}, k[\mathcal{N}^{\mathrm{sp}}]) \\ \times \left(\prod_{\mathfrak{n} \in \mathcal{N}^{\mathrm{sp}}} e^{\zeta_{\mathfrak{n}} i(\Omega_{\mathfrak{n}} T t_{\mathfrak{n}} + \widetilde{\Omega}_{\mathfrak{n}}(t_{\mathfrak{n}}))} dt_{\mathfrak{n}} \right) d\boldsymbol{\tau} \prod_{\mathfrak{l} \in \mathcal{L}^{\mathrm{sp}}}^{+} n_{\mathrm{in}}(k_{\mathfrak{l}}) \mathbb{E}\left[\mathcal{B}_{\mathcal{T}^+}(\eta_{\mathcal{T}^+}(\varrho)) \mathcal{B}^*_{\mathcal{T}^-}(\eta_{\mathcal{T}^-}(\varrho))\right], \tag{5.9}$$

where $\mathcal{N}_0^{\mathrm{sp}}$ are the nodes at which an irregular chain was spliced out and $P_{q_{\mathfrak{n}_0}}$ is given in Lemma 5.7 and $q_{\mathfrak{n}_0}$ is the length or irregular chain spliced out below $\mathfrak{n}_0$. Additionally, $\mathcal{E}_{\boldsymbol{\tau}}^{\mathrm{sp}} = \mathcal{E} \cap \{t_{\mathfrak{n}_0} \geq t_{\mathfrak{n}_0^2} + \tau_{\mathfrak{n}_0}, t_{\mathfrak{n}_0^3} + \tau_{\mathfrak{n}_0}\}_{\mathfrak{n}_0 \in \mathcal{N}_0^{\mathrm{sp}}}$.

Proof. See [46, Proposition 5.14]. □

5.3: Pre-processing step in the algorithm

We implement the algorithm described in Section 7.2 of [46]. This algorithm enables us to bound the number of decorations of a molecule incrementally. Here, we define the number of decorations to be the sum of $\tilde{\epsilon}_{\mathscr{E}^{\mathrm{sp}}}$ over all decorations $\mathscr{E}^{\mathrm{sp}}$. Consider a molecule $\mathbb{M}^{\mathrm{pre}}$ at some stage of the algorithm, which is transformed into a molecule $\mathbb{M}^{\mathrm{post}}$ via a single operation.

Denote by $\mathfrak{D}^{\text{pre}}$ and $\mathfrak{D}^{\text{post}}$ the corresponding numbers of decorations. Let $\mathfrak{C}$ be the counting estimate for this operation. Then, we have

$$\mathfrak{D}^{\text{pre}} \leq \mathfrak{C} \cdot \mathfrak{D}^{\text{post}}. \tag{5.10}$$

To reduce our case with enhanced molecules to the molecules that satisfy modified assumptions in section 7.1 of [46]:

1. The molecule $\mathbb{M}$ has 2 degree 3 atoms, with the rest degree 4.
2. The molecule $\mathbb{M}$ contains no degenerate atoms (excluding the fully degenerate ones).

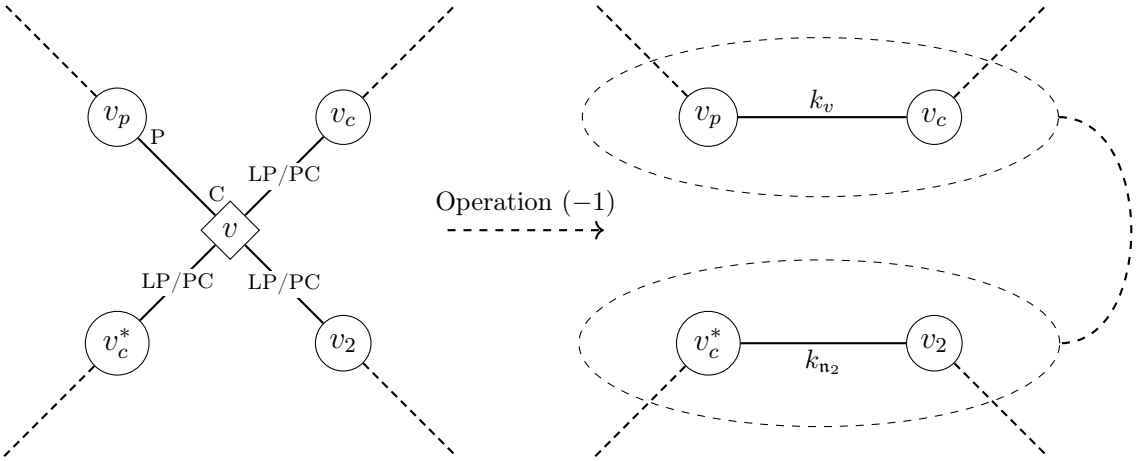


Figure 5.1: Operation (-1) on a degenerate atom v (diamond) with parent v_p and neighbors v_c^*, v_2 and v_c. Left: original configuration with PC and LP bonds; dashed stubs indicate external connections. Right: after removing the degenerate atom v and all the bonds connected, v_p joins v_c via bond with decoration k_v and v_c^* joins v_2 via bond with decoration $k_{\mathbf{n}_2}$. The resulting sub-molecules are highlighted by dashed ellipses and connected by some additional bonds represented by the curved dashed line, preserving connectivity.

We would like to perform a pre-processing step to remove all the degenerate atoms (excluding the fully degenerate ones):

Operation DEL If there is any degenerate atom v but not fully degenerate, corresponding to a degenerate node in $\mathcal{N}_D$, we remove the degenerate atom v, and also do the following (see Figure 5.1 for detailed illustration) in the order:

(a) Remove all bonds connected to it.

(b) If both of its parent atom v_p and child atom (or corresponding paired atom) v_c (recall Definition 2.15) exist in the molecule $\mathbb{M}$ and were previously connected to v via bonds with decoration k_v, we connect them via a bond with decoration k_v.

(c) If Step (a) does not create a new connected component, we also connect its child atoms (or corresponding paired atoms) v_c^* and v_2 via a bond with decoration $k_{\mathfrak{n}_2}$ (the same decoration as the bonds previously connecting them to v.) Otherwise, we do not add a new bond between v_c^* and v_2.

Start the following Operation (-1) as follows:

(i) If v is connected to another degenerate atom v' via triple bonds, of which two must have decoration $k_{\mathfrak{n}_2}$ and the remaining one must have k_v, we remove the two degenerate atoms v and v' together using Operation DEL. Go to (i).

(ii) Otherwise v is connected to another degenerate atom v' via double bonds both with decoration $k_{\mathfrak{n}_2}$, we remove the two degenerate atoms v and v' together using Operation DEL. Go to (i).

(iii) Otherwise we remove the degenerate atom v using Operation DEL. Go to (i).

There is only one way to create a new component of: after we remove two (or more) degenerate atoms v and v' with the above Operation (-1), their child atoms v_c^*, v_2 and $v_c^{*\prime}, v_2'$ are connected in a new component. According to Step (c) of removing a degenerate atom, we will not connect $v_c^{*\prime}$ and v_2', which become the two degree 3 atoms in the new connected component with all of the rest atoms degree 4. The degrees of all of the rest atoms in the molecule $\mathbb{M}$ left remain the same. Therefore, we can treat the resulting components as new molecules satisfying assumptions in section 7.1 of [46].

Remark 5.10. We always gain from the above removing degeneracy Operation (-1), as we can analyze the counting of decorations in the above operations:

- In the Operation (i) and (ii), we reduce 4 edges and 2 vertices each time removing two degenerate atoms while preserving the number of connected components. Then we have
$$\Delta\chi = \Delta E - \Delta V + \Delta F = -4 + 2 + 0 = -2,$$
with counting $\mathfrak{C} = N$ for the decoration $k_{\mathfrak{n}_2}$.
- In the Operation (iii), we either reduce 2 edges and 1 vertex each time while preserving the number of connected components, or reduce 3 edges and 1 vertex and get a new connected component, as we only allow enhanced pairings for the couples. Consequently, after two Operation (iii) we have
$$\Delta\chi = \Delta E - \Delta V + \Delta F = (-2 + 1) \times 2 + 0 = -5 + 2 + 1 = -2,$$

with counting $\mathfrak{C} = 1$ if no new component and counting $\mathfrak{C} = N$ for the decoration $k_{\mathfrak{n}_2}$ if a new component split out.

In the above scenarios, we are permitted to lose a three-vector counting $\mathfrak{C} = N^2T^{-1}\log T$ where we actually lose a counting $\mathfrak{C} \leq N < N^2T^{-1}\log T$ for $T < N$.

5.4: Operation types

We categorize the operations of the algorithm in [46] based on the corresponding values of $\mathfrak{C}$ and $\Delta\chi$ into the following types, while tracking the count of each type:

- **Bridge Operations**. These operations have $\Delta\chi = 0$ and $\mathfrak{C} = 1$, for all atoms on one side of the bridge, and every bond except the bridge appears exactly twice with opposite signs. Let m_0 denote the total number of bridge operations.
- **Sole Atom Operations**. Here, $\Delta\chi = 0$, and since no bonds are removed, $\mathfrak{C} = 1$. The total count of such operations is represented by m_1.
- **Two-Vector Counting Operations**. For this type, $\Delta\chi = -1$ and $\mathfrak{C} = N$ as given by Proposition 4.3. Let m_2 represent the count of two-vector counting operations.
- **Three-Vector Counting Operations**. These operations are characterized by $\Delta\chi = -2$ and $\mathfrak{C} = N^2T^{-1}\log T$, according to Proposition 4.1. Let m_3 denote the total number of three-vector counting operations.
- **Removing Degeneracy Operations** consist of Operation (-1). In this case $\Delta\chi = -2$ and $\mathfrak{C} \leq N$ removing every two degenerate atoms, which are gains compared with three-vector counting $\Delta\chi = -2$ and $\mathfrak{C} = N^2T^{-1}\log T$ for $T \leq N$. Let m_{-1} denote the total number of degenerate atoms removed. Let m_c denote the number of new connected components split out.

Then we can similarly prove the following proposition as in [46]:

Proposition 5.11. *For any molecule $\mathbb{M}(\mathcal{Q}) = \cup_{j=0}^{m_c}\mathbb{M}_j$ with each component $\mathbb{M}_j$ as assumed in Section 5.3, we must have:*

$$m_0 \leq m_3 - 1, \tag{5.11}$$

$$m_2 \leq 3m_3 - 3. \tag{5.12}$$

Proof. Assume that $\mathbb{M}(\mathcal{Q})$ has $n - m_{-1}$ atoms. Among these $n - m_{-1}$ atoms, $(n - m_{-1} - 2(m_c + 1))$ of them have degree 4, and the remaining $2(m_c + 1)$ atoms have degree 3.

1. **Pre-processing and edge counts.** Since each degree-4 atom contributes 4 edges and each degree-3 atom contributes 3 edges, the total number of edges is

$$\#\text{edges} = \frac{4(n - m_{-1} - 2(m_c + 1)) + 3 \cdot 2(m_c + 1)}{2} = 2n - 2m_{-1} - (m_c + 1) \quad (5.13)$$

2. **The edge and χ equations.** Recall the following "operation counts," denoting them as m_0, m_2, m_3, m_{-1}:

$$3m_3 + 2m_2 + m_0 = \#\text{edges} = 2n - 2m_{-1} - (m_c + 1), \quad (5.14)$$

and

$$\begin{aligned} 2m_3 + m_2 &= \big(\#\text{edges}\big) - \big(\#\text{atoms}\big) + \big(\#\text{components}\big) \\ &= (2n - 2m_{-1} - (m_c + 1)) - (n - m_{-1}) + (m_c + 1) = n - m_{-1}. \end{aligned} \quad (5.15)$$

From the two equations (5.14) and (5.15), we can solve for m_0 in terms of m_3 and m_{-1}:

$$m_0 = m_3 - (m_c + 1), \quad (5.16)$$

which recovers a similar statement in [46, Proposition 7.5].

3. **Deriving the inequality for m_2.** With the same proof for [46, Proposition 7.6], we have:

$$m_2 \le m_3 + 2m_0 - (m_c + 1) \le 3m_3 - 3(m_c + 1). \quad (5.17)$$

□

5.5: Bounds on couples

We record the following modified Proposition, proved in [46, Proposition 7.6].

Proposition 5.12. *Consider a labeled molecule $\mathbb{M} = \mathbb{M}(\mathcal{Q})$ of order $n \le L^3$. Suppose we fix $k \in \mathbb{Z}_N \cap (0, 1)$ and $\alpha_v \in \mathbb{R}$ for each atom v of $\mathbb{M}$. Consider all k-decorations (k_ℓ) of $\mathbb{M}$ such that*

(i) The k-decoration (k_ℓ) is inherited from a k-decoration $\mathscr{E}$ of $\mathcal{Q}$ that satisfies the SG and LG assumptions in [46, Proposition 5.14] as well as non-degeneracy conditions $\tilde{\epsilon}_{\mathscr{E}}$.

(ii) The decoration is restricted by (α_v) in the sense that $|\Omega_v - \alpha_v| \le T^{-1}$, where $T < N$.

Then, the number $\mathfrak{D}$ of such k-decorations is bounded by

$$\mathfrak{D} \leq C^n N^n T^{-\frac{n}{5}-\frac{3}{5}} (\log T)^n. \tag{5.18}$$

Proof. We have the equation for χ: $2m_3+m_2 = n-m_{-1}$ and by Proposition 5.11, $5m_3-3 \geq n-m_{-1}$. Note that we lose at most a counting of N each time we remove two (or more) degenerate atoms (whether they are connected by triple bonds, double bonds, or result in the formation of a new component). Then we have:

$$\begin{aligned}
\mathfrak{D} &\lesssim C^n (N^2 T^{-1} \log T)^{m_3} N^{m_2} N^{\frac{m_{-1}}{2}} \\
&= C^n N^{n-\frac{m_{-1}}{2}} (\log T)^{m_3} T^{-m_3} \\
&\lesssim C^n N^{n-\frac{m_{-1}}{2}} (\log T)^{m_3} T^{-\frac{n}{5}-\frac{3}{5}+\frac{m_{-1}}{5}} \\
&\lesssim C^n N^n (\log T)^n T^{-\frac{n}{5}-\frac{3}{5}},
\end{aligned}$$

for $T < N$. □

Remark 5.13. The validity of three-vector and two-vector counting requires $T < N$. On the other hand, removing degenerate atoms is advantageous when $N^{-\frac{m_{-1}}{2}} T^{\frac{m_{-1}}{5}} \leq 1$, which corresponds to $T \leq N^{\frac{5}{2}}$.

Lemma 5.14. *For enhanced trees $\mathcal{T}_1$ and $\mathcal{T}_2$,*

$$\mathbb{E}\left(\mathcal{B}_{\mathcal{T}_1}(\eta_{\mathcal{T}_1}(\varrho))\mathcal{B}^*_{\mathcal{T}_2}(\eta_{\mathcal{T}_2}(\varrho))\right) = \sum_{\substack{\mathscr{P}\text{: enhanced pairings of} \\ \mathcal{T}_1,\mathcal{T}_2}} 1. \tag{5.19}$$

Proof. We prove by induction. Suppose the formula is true for $|\mathcal{N}_D| = k-1$, then for $|\mathcal{N}_D| = k$, without loss of generality, we assume that there is one more degenerate node $\mathfrak{n}_*$ coming from $\mathcal{T}_1$. Assume that $\widetilde{\mathcal{B}}_{\mathcal{T}_1}$ represents the multiplicity (product of random phases) of the enhanced tree $\mathcal{T}_1$ with $|\mathcal{N}_{D_1}| = k_1 - 1$, that is $\mathfrak{n}_* \notin \mathcal{N}_{D_1}$, $\mathcal{T}_{1j}$'s are subtrees of degenerate node $\mathfrak{n}_*$ for $j = 1, 2, 3$, and $\widetilde{\widetilde{\mathcal{B}}}_{\mathcal{T}_1}$ represents the multiplicity of $\mathcal{T}_1$ excluding $\mathcal{T}_{11}$ and $\mathcal{T}_{12}$. Here we assume that the root $\mathfrak{n}_{11}$ of $\mathcal{T}_{11}$ is $\mathfrak{n}_{1c^*}$. Then from Proposition 2.6 we know that:

$$\mathbb{E}\left(\mathcal{B}_{\mathcal{T}_1}\mathcal{B}^*_{\mathcal{T}_2}\right) = \mathbb{E}\left(\widetilde{\mathcal{B}}_{\mathcal{T}_1}\mathcal{B}^*_{\mathcal{T}_2}\right) - \mathbb{E}\left(\mathcal{B}_{\mathcal{T}_{11}}\mathcal{B}^*_{\mathcal{T}_{12}}\right)\mathbb{E}\left(\widetilde{\widetilde{\mathcal{B}}}_{\mathcal{T}_1}\mathcal{B}^*_{\mathcal{T}_2}\right) \tag{5.20}$$

which is the number of enhanced pairing of $\mathcal{T}_1, \mathcal{T}_2$ (excluding any complete pairing from $\mathcal{T}_{11}$ and $\mathcal{T}_{12}$) and concludes the proof. □

Proof of Proposition 3.3. Recall that

$$\widetilde{\Omega}_k(t) = \Omega_k A(t),$$
$$\dot{A}(t) = G(t, A(t)) = \frac{3\beta T}{2\kappa^2 N} \sum_{|\mathcal{T}_1|,|\mathcal{T}_2|\le n} \sum_l \omega_l \mathbb{E} c_l^{\mathcal{T}_1}(t) c_l^{\mathcal{T}_2 *}(t).$$

We prove (3.44) and (3.45) using bootstrap arguments. We establish the hypotheses as:

$$\left| \sum_{|\mathcal{T}_1|+|\mathcal{T}_2|=n_{\mathcal{Q}}} \mathbb{E}\left[c_k^{\mathcal{T}_1}(t) c_k^{\mathcal{T}_2 *}(t) \right] \right| \le 2C (\log N \log T)^{n_{\mathcal{Q}}} T^{-\frac{3}{5}} \left(\beta T^{4/5}\right)^{n_{\mathcal{Q}}}, \tag{5.21}$$

$$\left| \sum_{|\mathcal{T}_1|+|\mathcal{T}_2|=n_{\mathcal{Q}}} \mathbb{E}\left[\dot{c}_k^{\mathcal{T}_1}(t) c_k^{\mathcal{T}_2 *}(t) \right] \right| \le 2C (\log N \log T)^{n_{\mathcal{Q}}-1} T^{\frac{2}{5}} \left(\beta T^{4/5}\right)^{n_{\mathcal{Q}}}, \tag{5.22}$$

for the same constant C as in (3.44, 3.45). (5.21, 5.22) give upper bound for $\dot{A}(t)$. From (2.15) and (2.20), $|c_l^{\mathcal{T}}|$ and the function $G(t, A(t))$ are bounded for almost every ϱ, and smooth in its variables, which guarantees the global existence and uniqueness of $A(t)$ for almost all ϱ. $A(t) = C_0 \beta T t + A_{\ge}(t)$, where

$$\dot{A}_{\ge}(t) = \frac{3\beta T}{2\kappa^2 N} \sum_{1\le|\mathcal{T}_1|,|\mathcal{T}_2|\le n} \sum_l \omega_l \mathbb{E}\left[c_l^{\mathcal{T}_1}(t) c_l^{\mathcal{T}_2 *}(t) \right]. \tag{5.23}$$

Then from (5.21, 5.22), we have:

$$\dot{A}_{\ge}(t) \lesssim \beta T^{1-\frac{3}{5}} \frac{\left(\beta T^{4/5}\right)^2}{1-\beta T^{4/5}} \lesssim \beta T, \tag{5.24}$$

$$\ddot{A}_{\ge}(t) \lesssim \beta T^{1+\frac{2}{5}} \frac{\left(\beta T^{4/5}\right)^2}{1-\beta T^{4/5}} \lesssim \beta T^{\frac{9}{5}}, \tag{5.25}$$

for $\beta T^{4/5} \ll 1$. Therefore we can apply proposition 3.1. Using Proposition 4.1, 3.1 and [46, Proposition 2.6], we can show bounds for couples (3.44, 3.45), which closes the bootstrap argument. Because the order of our couples is at most L^3, the total number of couples of order $n_{\mathcal{Q}}$ (independent of n_h) is on the order of $O(C^{L^3}(L^3)!)$. From Lemma 5.14, we can bound $\mathbb{E}\left(\mathcal{B}_{\mathcal{T}_1}(\eta_{\mathcal{T}_1}(\varrho))\mathcal{B}^*_{\mathcal{T}_2}(\eta_{\mathcal{T}_2}(\varrho))\right) \lesssim C^{L^3}(L^3)!$.

Similarly, given an enhanced couple $\mathcal{Q}$, there are $O(C^L)$ choices for the collection of SG negative-chain like objects $\mathscr{C}_1$ and $\mathcal{M}_{\mathscr{C}_1}$ defined in Definition 5.8. It suffices to fix an enhanced couple $\mathcal{Q}$ along with a choice $\mathscr{C}_1$ and $\mathcal{M} = \mathcal{M}_{\mathscr{C}_1}$ and bound the corresponding expression for $\mathcal{K}_{\mathfrak{Q}_{\mathcal{M}}}$ in (5.9). We could use the advantageous 2-vector counting $NT^{-\frac{1}{2}}$ for the LG irregular

chains and uni-directional S_2^+, which are as good as 3-vector counting operations and only improve the bounds.

As we have shown in the proof of Lemma 5.7, to bound the oscillatory integral after splicing in (5.9):

$$\int_{[0,1]^{\mathcal{N}_0^{\rm sp}}} \int_{\mathcal{E}_{\boldsymbol{\tau}}^{\rm sp}} \prod_{\mathfrak{n}_0\in\mathcal{N}_0^{\rm sp}} P_{q_{\mathfrak{n}_0}}(\tau_{\mathfrak{n}_0}, t_{\mathfrak{n}_0}, k[\mathcal{N}^{\rm sp}]) \left(\prod_{\mathfrak{n}\in\mathcal{N}^{\rm sp}} e^{\zeta_{\mathfrak{n}} i(\Omega_{\mathfrak{n}} T t_{\mathfrak{n}} + \widetilde{\Omega}_{\mathfrak{n}}(t_{\mathfrak{n}}))} dt_{\mathfrak{n}}\right) d\boldsymbol{\tau}, \tag{5.26}$$

we need to apply the technique we used in Proposition 3.1 and let

$$f_{\mathfrak{n}_0}(T t_{\mathfrak{n}_0}) = \left(\beta T^{\frac{1}{2}}\right)^{-q_{\mathfrak{n}_0}} P_{q_{\mathfrak{n}_0}}(\tau_{\mathfrak{n}_0}, t_{\mathfrak{n}_0}, k[\mathcal{N}^{\rm sp}]),$$

which satisfies $|f_{\mathfrak{n}_0}(T t_{\mathfrak{n}_0})| \lesssim 1$ and $\left|\frac{d}{dt_{\mathfrak{n}_0}} f_{\mathfrak{n}_0}(T t_{\mathfrak{n}_0})\right| \lesssim 1$ for each $\mathfrak{n}_0 \in \mathcal{N}_0^{\rm sp}$. Then by Corollary 5.9, we can derive:

$$\begin{aligned}
&\left|\sum_{|\mathcal{T}_1|+|\mathcal{T}_2|=n_{\mathcal{Q}}} \mathbb{E}\left[c_k^{\mathcal{T}_1}(t) c_k^{\mathcal{T}_2 *}(t)\right]\right| \\
\lesssim\ & C^{n_{\mathcal{Q}}} \left(\beta T^{1/2}\right)^{n_0} \sup_{\boldsymbol{\tau}\in[0,1]^{\mathcal{N}_0^{\rm sp}}} \sum_{\lambda[\mathcal{N}^{\rm sp}]} \left(\frac{\beta T}{N}\right)^{n_{\rm sp}} \\
&\qquad \times \sum_{\tilde{\mathscr{E}}^{\rm sp}_{\lambda[\mathcal{N}^{\rm sp}]}} \tilde{\epsilon}_{\tilde{\mathscr{E}}^{\rm sp}_{\lambda[\mathcal{N}^{\rm sp}]}} \left|\int_{\mathcal{E}_{\boldsymbol{\tau}}^{\rm sp}} \prod_{\mathfrak{n}_0\in\mathcal{N}_0^{\rm sp}} f_{\mathfrak{n}_0}(T t_{\mathfrak{n}_0}) \prod_{\mathfrak{n}\in\mathcal{N}^{\rm sp}} e^{\zeta_{\mathfrak{n}} i(\Omega_{\mathfrak{n}} T t_{\mathfrak{n}} + \widetilde{\Omega}_{\mathfrak{n}}(t_{\mathfrak{n}}))} dt_{\mathfrak{n}}\right| \\
\lesssim\ & C^{n_{\mathcal{Q}}} \left(\beta T^{1/2}\right)^{n_0} \left(\sup_{\lambda[\mathcal{N}^{\rm sp}]} \sum_{\tilde{\mathscr{E}}^{\rm sp}_{\lambda[\mathcal{N}^{\rm sp}]}} \tilde{\epsilon}_{\tilde{\mathscr{E}}^{\rm sp}_{\lambda[\mathcal{N}^{\rm sp}]}} \left(\frac{\beta T}{N}\right)^{n_{\rm sp}}\right) \\
&\qquad \times \left(\sum_{\lambda[\mathcal{N}^{\rm sp}]} \sup_{\boldsymbol{\tau}\in[0,1]^{\mathcal{N}_0^{\rm sp}}} \left|\int_{\mathcal{E}_{\boldsymbol{\tau}}^{\rm sp}} \prod_{\mathfrak{n}_0\in\mathcal{N}_0^{\rm sp}} f_{\mathfrak{n}_0}(T t_{\mathfrak{n}_0}) \prod_{\mathfrak{n}\in\mathcal{N}^{\rm sp}} e^{\zeta_{\mathfrak{n}} i\lambda_{\mathfrak{n}}(T t_{\mathfrak{n}} + A(t_{\mathfrak{n}}))} dt_{\mathfrak{n}}\right|\right),
\end{aligned} \tag{5.27}$$

where $\lambda[\mathcal{N}^{\rm sp}] \in \mathbb{Z}^{|\mathcal{N}^{\rm sp}|}$ and $\tilde{\mathscr{E}}^{\rm sp}_{\lambda[\mathcal{N}^{\rm sp}]}$ denotes decorations of the couple satisfying $|T\Omega_{\mathfrak{n}} - \lambda_{\mathfrak{n}}| \le 1$ for each $\mathfrak{n} \in \mathcal{N}^{\rm sp}$, and $C_1 > 0$ is a constant. Here, $n_0 + n_{\rm sp} = n_{\mathcal{Q}}$, where n_0 is number of nodes spliced out. We apply Proposition 3.1 to bound:

$$\sum_{\lambda[\mathcal{N}^{\rm sp}]} \sup_{\boldsymbol{\tau}\in[0,1]^{\mathcal{N}_0^{\rm sp}}} \left|\int_{\mathcal{E}_{\boldsymbol{\tau}}^{\rm sp}} \prod_{\mathfrak{n}_0\in\mathcal{N}_0^{\rm sp}} f_{\mathfrak{n}_0}(T t_{\mathfrak{n}_0}) \prod_{\mathfrak{n}\in\mathcal{N}^{\rm sp}} e^{\zeta_{\mathfrak{n}} i\lambda_{\mathfrak{n}}(T t_{\mathfrak{n}} + A(t_{\mathfrak{n}}))} dt_{\mathfrak{n}}\right|$$

$$\lesssim \sum_{\lambda[\mathcal{N}]} \sum_{d_{\mathfrak{n}}\in\{0,1\}} \frac{1}{\langle \lambda_{\mathfrak{n}} + Tq_{\mathfrak{n}}\rangle} \lesssim C^{n_{\mathcal{Q}}} (\log N)^{n_{\mathcal{Q}}}. \tag{5.28}$$

Then by Proposition 5.12, we get:

$$\begin{aligned}(5.27) &\lesssim C^{n_{\mathcal{Q}}} \left(\beta T^{1/2}\right)^{n_0} \left(\sup_{\lambda[\mathcal{N}^{\mathrm{sp}}]} \sum_{\tilde{\mathscr{E}}^{\mathrm{sp}}_{\lambda[\mathcal{N}^{\mathrm{sp}}]}} \tilde{\epsilon}_{\tilde{\mathscr{E}}^{\mathrm{sp}}_{\lambda[\mathcal{N}^{\mathrm{sp}}]}} \left(\frac{\beta T}{N}\right)^{n_{\mathrm{sp}}} \right) (\log N)^{n_{\mathcal{Q}}} \\ &< C_1 (\log N \log T)^{n_{\mathcal{Q}}} T^{-\frac{3}{5}} \left(\beta T^{4/5}\right)^{n_{\mathcal{Q}}}, \end{aligned} \tag{5.29}$$

Here we use $\beta T^{\frac{1}{2}} \ll \left(\frac{\beta T}{N}\right) N T^{-\frac{1}{5}} = \beta T^{\frac{4}{5}}$ and the size of the oscillatory integral (5.26) can be bounded by $(\log N)^{n_{\mathcal{Q}}}$. Similarly for $\mathbb{E}\left[\dot{c}_k^{\mathcal{T}_1}(t) c_k^{\mathcal{T}_2 *}(t)\right]$, we may expand $\dot{c}_k^{\mathcal{T}_1}(t)$ and get:

$$\begin{aligned} &\left| \sum_{|\mathcal{T}_1|+|\mathcal{T}_2|=n_{\mathcal{Q}}} \mathbb{E}\left[\dot{c}_k^{\mathcal{T}_1}(t) c_k^{\mathcal{T}_2 *}(t)\right] \right| \\ \lesssim\ & \frac{\beta T}{N} \max \Bigg(\sum_{\substack{k_3-k_4+k_5=k \\ k_3,k_5\neq k_4}} T_{k,3,4,5} \left| \mathbb{E}\left[c_{k_3}^{\mathcal{T}_3}(t) c_{k_4}^{\mathcal{T}_4 *}(t) c_{k_5}^{\mathcal{T}_5}(t) c_k^{\mathcal{T}_2 *}(t)\right]\right|, \\ & \sum_{k_3} T_{k,3,3,k} \Big(\left| \mathbb{E}\left[c_{k_3}^{\mathcal{T}_3}(t) c_{k_3}^{\mathcal{T}_4 *}(t) c_k^{\mathcal{T}_5}(t) c_k^{\mathcal{T}_2 *}(t)\right]\right| - \left| \mathbb{E}\left[c_{k_3}^{\mathcal{T}_3}(t) c_{k_3}^{\mathcal{T}_4 *}(t)\right]\right| \cdot \left| \mathbb{E}\left[c_k^{\mathcal{T}_5}(t) c_k^{\mathcal{T}_2 *}(t)\right]\right| \Big) \Bigg) \\ \lesssim\ & C^{n_{\mathcal{Q}}} \left(\beta T^{1/2}\right)^{n_0} \left(\sup_{\lambda[\mathcal{N}^{\mathrm{sp}}\setminus \mathfrak{r}_1]} \sum_{\tilde{\mathscr{E}}_{\lambda[\mathcal{N}^{\mathrm{sp}}\setminus \mathfrak{r}_1]}} \tilde{\epsilon}_{\tilde{\mathscr{E}}_{\lambda[\mathcal{N}^{\mathrm{sp}}\setminus \mathfrak{r}_1]}} \left(\frac{\beta T}{N}\right)^{n_{\mathrm{sp}}} \right) (\log N)^{n_{\mathcal{Q}}-1} \\ <\ & C_2 (\log N \log T)^{n_{\mathcal{Q}}-1} T^{\frac{2}{5}} \left(\beta T^{\frac{4}{5}}\right)^{n_{\mathcal{Q}}}. \end{aligned} \tag{5.30}$$

where $C_2 > 0$ is a constant. Note that for the decorations $\{(k_3, k_4, k_5) : k_3 - k_4 + k_5 = k, k_3, k_5 \neq k_4\}$ we lose a counting N^2 instead of $N^2 T^{-1} \log T$ since there is no control on the factor Ω within a T^{-1} strip. We take $C = \max(C_1, C_2)$ to complete the proof. □

CHAPTER 6
The Remainder

In this chapter, we prove Proposition 3.4.

6.1: Kernels of $\mathscr{L}$

In order to introduce the kernels of $\mathscr{L}$, we recall from [42] the following extension of trees and couples:

Definition 6.1. A *flower tree* is a tree $\mathcal{T}$ in which a particular leaf $\mathfrak{f}$ is distinguished and called the *flower*. Choosing a different leaf $\mathfrak{f}$ for the same tree $\mathcal{T}$ yields a different flower tree. The unique path connecting the root $\mathfrak{r}$ and the flower $\mathfrak{f}$ is referred to as the *stem*. A *flower couple* is a pair of flower trees whose flowers are matched in such a way that they carry opposite signs.

The *height* of a flower tree $\mathcal{T}$ is defined as the number of branching nodes along its stem. Evidently, to construct a flower tree of height n_h, one can start with a single node and successively attach two sub-trees n_h times. A flower tree is said to be *admissible* if each of the attached sub-trees has scale at most L.

We adapt the following proposition from [42, Proposition 11.2] and [46, Proposition 6.2] to our β-FPUT model:

Proposition 6.2. *Let $\mathscr{L}$ be defined as in (2.30). Note that $\mathscr{L}^{n_h}$ is an $\mathbb{R}$-linear operator for $n \geq 0$. Define its kernels $(\mathscr{L}^{n_h})^{\zeta}_{k\ell}(t,s)$ for $\zeta \in \{\pm\}$ by*

$$(\mathscr{L}^{n_h} b)_k(t) = \sum_{\zeta\in\{\pm\}} \sum_{\ell} \int_{\mathbb{R}} (\mathscr{L}^{n_h})^{\zeta}_{k\ell}(t,s) b_\ell(s)^{\zeta} ds.$$

Then, for each $1 \leq n \leq L$ and $\zeta \in \{\pm\}$, we can decompose

$$(\mathscr{L}^{n_h})^{\zeta}_{k,\ell} = \sum_{n\leq m\leq L^3} (\mathscr{L}^{n_h})^{m,\zeta}_{k,\ell}, \tag{6.1}$$

such that for any $n_h \le m \le L^3$ *and* $k, \ell \in \mathbb{Z}_N \cap (0,1)$ *and* $t, s \in (0,1)$ *with* $t > s$*, we have*

$$\mathbb{E}|(\mathscr{L}^{n_h})^{m,\zeta}_{k,\ell}(t,s)|^2 \lesssim (\beta T^{4/5})^m N^{30}. \tag{6.2}$$

Proof. We follow the proof in [42, Proposition 11.2] and [46, Proposition 6.2], for flower trees $\mathcal{T}_\mathfrak{f}$ of height n_h and scale m such that the $\zeta_\mathfrak{r} = +$ and $\zeta_\mathfrak{f} = \zeta$. Then for $t \ge s$, we similarly define as in (2.42):

$$\widetilde{c}^{\mathcal{T}_\mathfrak{f}}_{k,\ell}(t,s) = \left(\frac{\beta T}{N}\right)^m \zeta(\mathcal{T}_\mathfrak{f}) \sum_{\mathscr{D}} \epsilon_{\mathscr{D}} \boldsymbol{\delta}(t_{\mathfrak{f}^p} - s) \mathcal{A}_{\mathcal{T}_\mathfrak{f}}(t, \Omega[\mathcal{N}], \widetilde{\Omega}[\mathcal{N}]) \prod_{\mathfrak{f} \neq \mathfrak{l} \in \mathcal{L}} \sqrt{n_{\mathrm{in}}(k_\mathfrak{l})} \mathcal{B}_{\mathcal{T}_\mathfrak{f}}(\eta_{\mathcal{T}_\mathfrak{f}})(\varrho)) \mathbf{1}_{k_\mathfrak{f} = \ell}, \tag{6.3}$$

where $\mathscr{D}$ is a k-decoration of $\mathcal{T}_\mathfrak{f}$, and $\mathfrak{f}^p$ is the parent of $\mathfrak{f}$. Then for flower couples $\mathcal{Q}_\mathfrak{f} = (\mathcal{T}^+_\mathfrak{f}, \mathcal{T}^-_\mathfrak{f})$, where $\mathcal{T}^\pm_\mathfrak{f}$ has sign $\pm\zeta$, height n_h and scale m. Then for $t \ge s$, we can similarly define as in (2.52):

$$\begin{aligned}(\widetilde{\mathcal{K}}_{\mathcal{Q}_\mathfrak{f}})(t,s,k,\ell) = \left(\frac{\beta T}{N}\right)^{2m} \zeta(\mathcal{Q}) \sum_{\mathscr{E}} \epsilon_{\mathscr{E}} \int_{\mathcal{E}} \prod_{\mathfrak{n} \in \mathcal{N}} e^{\zeta_\mathfrak{n} i(\Omega_\mathfrak{n} T t_\mathfrak{n} + \widetilde{\Omega}_\mathfrak{n}(t_\mathfrak{n}))} dt_\mathfrak{n} \prod_{\mathfrak{f}} \boldsymbol{\delta}(t_{\mathfrak{f}^p} - s) \\ \times \prod_{\mathfrak{f} \neq \mathfrak{l} \in \mathcal{L}}^{+} n_{\mathrm{in}}(k_\mathfrak{l}) \mathbb{E}\left(\mathcal{B}_{\mathcal{T}_1}(\eta_{\mathcal{T}_1}(\varrho)) \mathcal{B}^*_{\mathcal{T}_2}(\eta_{\mathcal{T}_2}(\varrho))\right) \mathbf{1}_{k_\mathfrak{f} = \ell}\end{aligned} \tag{6.4}$$

where $\mathscr{E}$ is a k-decoration of $\mathcal{Q}_\mathfrak{f}$. In (6.4), the Dirac delta factor $\boldsymbol{\delta}(t_{\mathfrak{f}^p} - s)$ imposes $t_{\mathfrak{f}^p} = s$, so we skip any phase integral with respect to $t_{\mathfrak{f}^p}$ for each of the two flowers $\mathfrak{f}$. Although this alters the counting, the resulting discrepancy can be bounded by at most N^{10}. With $\widetilde{c}^{\mathcal{T}_\mathfrak{f}}_k(t)$ and $(\widetilde{\mathcal{K}}_{\mathcal{Q}_\mathfrak{f}})(t,s,k,\ell)$ we can express:

$$(\mathscr{L}^{n_h})^{m,\zeta}_{k,\ell}(t,s) = \sum_{\mathcal{T}_\mathfrak{f}} \widetilde{c}^{\mathcal{T}_\mathfrak{f}}_{k,\ell}(t,s) \tag{6.5}$$

$$\mathbb{E}\left|(\mathscr{L}^{n_h})^{m,\zeta}_{k,\ell}(t,s)\right|^2 = \sum_{\mathcal{Q}_\mathfrak{f}} \widetilde{\mathcal{K}}_{\mathcal{Q}_\mathfrak{f}}(t,s,k,\ell). \tag{6.6}$$

Suppose $\mathcal{Q}_\mathfrak{f}$ is an admissible flower couple and that $\widetilde{\mathcal{Q}_\mathfrak{f}}$ is congruent to $\mathcal{Q}_\mathfrak{f}$ in the sense of Definition 5.6. Then $\widetilde{\mathcal{Q}_\mathfrak{f}}$ is also an admissible flower couple, provided its flower is chosen as the image of the flower of $\mathcal{Q}_\mathfrak{f}$. To apply the same proof as in Proposition 3.3, we also need to first splice out the irregular chains with small gaps as we did in Lemma 5.7. Note that in our β-FPUT model, in the remainder we have extra degenerate terms as in (2.33) compared to the NLS model. The first extra term $\left(\left|c^{\le n}_{k_1}(s)\right|^2 - \mathbb{E}\left|c^{\le n}_{k_1}(s)\right|^2\right) \mathcal{R}^{(n+1)}_k$ is similar to our enhanced structure which only allow enhanced pairing under the degenerate nodes and will not cause

irregular chains stacking up. The last two terms $\left(c_{k_1}^{\leq n*}(s)\mathcal{R}_{k_1}^{(n+1)} + c_{k_1}^{\leq n}(s)\mathcal{R}_{k_1}^{(n+1)*}\right) c_k^{\leq n}(s)$ can also be handled well by the splicing process after summing up all admissible congruent flower couples. One more loss we could gain is that if the chains contain the flowers, we need to avoid splicing the flowers out which may cause a loss of N^2 with two extra double bond in the molecule. Then applying Proposition 3.3, we can recover the bound (6.2) by adding a loss of N^{30}. □

Lemma 6.3. *(Gaussian Hypercontractivity) Let $\{\eta_k\}$ be i.i.d. Gaussians or random phase. Given $\zeta_j \in \{\pm\}$ and random variable X of the form*

$$X = \sum_{k_1,\dots,k_n} a_{k_1,\dots,k_n} \prod_{j=1}^{n} \eta_{k_j}^{\zeta_j}(\omega), \tag{6.7}$$

where $a_{k_1,\dots,k_n}$ are constants. Then, for $q \geq 2$,

$$\mathbb{E}\,|X|^q \leq (q-1)^{\frac{nq}{2}} \cdot \left(\mathbb{E}|X|^2\right)^{q/2} \tag{6.8}$$

Proof. See, for instance, [70, Lemma 2.6]. □

6.2: Bound on the operator $\mathscr{L}$

Proof of Proposition 3.4. After applying Cauchy-Schwarz inequality:

$$\begin{aligned}
||\mathscr{L}^{n_h}(a)||_Z^2 &= \sup_{0\leq t\leq 1} N^{-1} \sum_{k\in\mathbb{Z}_N\cap(0,1)} |(\mathscr{L}^{n_h}a)_k(t)|^2 \\
&= \sup_{0\leq t\leq 1} N^{-1} \sum_{k\in\mathbb{Z}_N\cap(0,1)} \left| \sum_{\zeta\in\{\pm\}} \sum_{\ell\in\mathbb{Z}_N\cap(0,1)} \int_{0\leq s\leq t} \sum_{n\leq m\leq L^3} (\mathscr{L}^{n_h})_{k,\ell}^{m,\zeta} a_\ell^\zeta(s) ds \right|^2 \\
&\lesssim \sup_{0\leq s\leq t\leq 1} \sup_\zeta \sup_m N^{-1}L^3 \sum_{k\in\mathbb{Z}_N\cap(0,1)} \left| \sum_{\ell\in\mathbb{Z}_N\cap(0,1)} (\mathscr{L}^{n_h})_{k,\ell}^{m,\zeta}(t,s) a_\ell^\zeta(s) \right|^2 \\
&\lesssim ||a||_Z^2 L^3 \sup_{0\leq s\leq t\leq 1} \sup_\zeta \sup_m \sum_{k\in\mathbb{Z}_N\cap(0,1)} \sum_{\ell\in\mathbb{Z}_N\cap(0,1)} \left| (\mathscr{L}^{n_h})_{k,\ell}^{m,\zeta}(t,s) \right|^2 \\
&\lesssim ||a||_Z^2 N^2 L^3 \sup_{0\leq s\leq t\leq 1} \sup_\zeta \sup_m \sup_{k,\ell} |(\mathscr{L}^{n_h})_{k,\ell}^{m,\zeta}(t,s)|^2.
\end{aligned}$$

Let $L(t,s) = \sup_{k,\ell} \sup_{0\leq s\leq t\leq 1} |(\mathscr{L}^{n_h})_{k,\ell}^{m,\zeta}(t,s)|$, for fixed m and ζ. As taking ∂_t derivative just corresponds to omitting the $t_{\mathfrak{r}}$ integration and producing something like (5.30), then by

Proposition 6.2 and Lemma 6.3:

$$\mathbb{E}||L(t,s)||^p_{L^p_{t,s}((0,1)^2)L^p_{k,\ell}(\mathbb{Z}^2_N\cap(0,1)^2)} \lesssim p^{mp}(\beta T^{4/5})^{mp/2}N^{30p}, \tag{6.9}$$

$$\mathbb{E}||\partial_{(t,s)}L(t,s)||^p_{L^p_{t,s}((0,1)^2)L^p_{k,\ell}(\mathbb{Z}^2_N\cap(0,1)^2)} \lesssim p^{mp}(\beta T^{4/5})^{mp/2}N^{31p}. \tag{6.10}$$

By using the Gagliardo-Nirenberg inequality for $(t,s)\in(0,1)^2$, and bounding the $L^\infty_{k,\ell}$ norm by the $L^p_{k,\ell}$ norm for $k,\ell\in\mathbb{Z}_N\cap(0,1)$ with an extra loss $N^{2/p}$, we conclude that

$$\mathbb{E}||L(t,s)||^p_{L^\infty_{t,s}((0,1)^2)L^\infty_{k,\ell}(\mathbb{Z}^2_N\cap(0,1)^2)} \lesssim p^{mp}(\beta T^{4/5})^{mp/2}N^{31p+2}. \tag{6.11}$$

Thus with probability $\geq 1-N^{-p/2}$, we have

$$L(t,s)\lesssim p^m(\beta T^{4/5})^{m/2}N^{33}, \tag{6.12}$$

which implies

$$\sup_{k,\ell}\sup_{0\leq s\leq t\leq 1}|(\mathscr{L}^{n_h})^{m,\zeta}_{k,\ell}(t,s)|\lesssim(\beta T^{4/5})^{m/2}N^{35}. \tag{6.13}$$

with probability $\geq 1-N^{-A}$ by taking $p\geq 2A$. □

CHAPTER 7
Proof of the Main Theorem

Proposition 7.1. *With probability $\geq 1 - N^{-A}$, the mapping defined by the right hand side of (2.38) is a contraction mapping from the set $\{\mathcal{R} : ||\mathcal{R}||_Z \leq N^{-500}\}$ to itself.*

Proof. By Proposition 3.4, there is an exceptional event of probability at most N^{-A} on which our required estimates may fail. We exclude that event, so on the complementary event of probability at least $1 - N^{-A}$ we have, in particular,

$$\|\mathscr{R}(t)\|_Z \lesssim (\beta T^{4/5})^{n/2} N^5 \tag{7.1}$$

$$\left\| \sum_{|\mathcal{T}|=m} c_k^{\mathcal{T}}(t) \right\|_Z \lesssim (\beta T^{4/5})^{m/2} N^5. \tag{7.2}$$

We obtain the above estimates by applying Proposition 3.3 to (2.27) and arguments as in the proof of Proposition 3.4 to remove expectations. Both $\mathscr{R}$ and $\sum_{|\mathcal{T}|=m} c_k^{\mathcal{T}}(t)$ are represented by enhanced trees preserved under congruence. Next, assume $\|\mathcal{R}\|_Z \leq N^{-500}$. Observe from Section 2.5 that:

$$\|\mathscr{R}\|_Z + \|\mathscr{Q}(\mathcal{R}, \mathcal{R})\|_Z + \|\mathscr{C}(\mathcal{R}, \mathcal{R}, \mathcal{R})\|_Z \lesssim N^{-600}.$$

Here, the estimates for $\|\mathscr{Q}(\mathcal{R}, \mathcal{R})\|_Z$ and $\|\mathscr{C}(\mathcal{R}, \mathcal{R}, \mathcal{R})\|_Z$ follow from Cauchy-Schwarz that

$$\|\mathcal{W}(u, v, w)\|_Z, \|\mathscr{Q}_D(u, v, w)\|_Z, \|\mathscr{C}_D(u, v, w)\|_Z \lesssim N^3 \|u\|_Z \|v\|_Z \|w\|_Z,$$

together with the bound $\|\mathcal{R}\|_Z \leq N^{-500}$ for at least two of the factors u, v, w, and the estimate (7.2) for the remaining factor. The bound $\|\mathscr{R}\|_Z \lesssim N^{-600}$ follows from (7.1), the scaling law $\beta = N^{-\gamma}$, $T = N^{-\epsilon} \min(N, N^{\frac{5}{4}\gamma})$, and choosing $n = 10^4/\epsilon$ large enough.

We also note that $(1 - \mathscr{L})^{-1}$ maps Z to itself, since

$$(1 - \mathscr{L})^{-1} = (1 - \mathscr{L}^{n_h})^{-1} \left(1 + \mathscr{L} + \cdots + \mathscr{L}^{n_h - 1}\right),$$

and $\|\mathscr{L}^{n_h}\|_{Z\to Z} < 1$ for sufficiently large n_h. Therefore we can invert $(1-\mathscr{L}^{n_h})$ by a Neumann series, and it follows that

$$\|(1-\mathscr{L})^{-1}\|_{Z\to Z} \lesssim N^{30}.$$

Putting these facts together shows that the map given by the right-hand side of (2.38) is a self-map on the set $\{\mathcal{R} : \|\mathcal{R}\|_Z \le N^{-500}\}$, with the contraction property guaranteed by the smallness of the terms above. Consequently, by the Banach Fixed Point Theorem, there is a unique solution $\mathcal{R}$ in that ball, and this occurs with probability at least $1-N^{-A}$. □

Proof of Theorem 1. As we can derive from the initial data $\|b_k\|_{\ell^2} \sim O(1)$, and in this setting, the solution is globally well-posed for the nonlinear smooth ODE system (R-FPUT). Let E denote the complement of the union of all exceptional sets arising from Propositions 3.4 and 7.1, so that

$$\mathbb{P}(E) \ge 1 - N^{-A}.$$

Recall that $n(t,k) = \mathbb{E}|b_k(t)|^2 = \mathbb{E}|c_k(s)|^2$ where $s = \frac{t}{T}$. We decompose

$$\mathbb{E}\left(|c_k(s)|^2\right) = \mathbb{E}\left(|c_k(s)|^2 \mathbf{1}_E\right) + \mathbb{E}\left(|c_k(s)|^2 \mathbf{1}_{E^c}\right). \tag{7.3}$$

Since $\mathbb{E}\left(|c_k(s)|^2 \mathbf{1}_{E^c}\right) \lesssim N^{-A+20}$, it suffices to consider $\mathbb{E}\left(|c_k(s)|^2 \mathbf{1}_E\right)$. Then we can get:

$$\mathbb{E}\left(|c_k(s)|^2 \mathbf{1}_E\right) = \mathbb{E}\left(\left|c_k^{\le n}(s)\right|^2 \mathbf{1}_E\right) + 2\mathrm{Re}\mathbb{E}\left(c_k^{\le n}(s)\mathcal{R}_k^{(n+1)*}(s)\mathbf{1}_E\right) + \mathbb{E}\left(\left|\mathcal{R}_k^{(n+1)}(s)\right|^2 \mathbf{1}_E\right).$$

By Proposition 7.1 and (7.2), any term involving $\mathcal{R}$ can be controlled at the order N^{-500}. Consequently, our main interest is in $\left|c_k^{\le n}(s)\right|^2 = \sum_{|\mathcal{T}_1|,|\mathcal{T}_2|\le n} c_k^{\mathcal{T}_1}(s) c_k^{\mathcal{T}_2 *}(s)$ the double sum over $|\mathcal{T}_1|$ and $|\mathcal{T}_2|$. Using Cauchy-Schwarz, we observe that

$$\left|\mathbb{E}\left(\left|c_k^{\le n}(s)\right|^2 \mathbf{1}_{E^c}\right)\right| \le \left(\mathbb{E}\left|c_k^{\le n}(s)\right|^4\right)^{1/2} \left(\mathbb{P}(E^c)^{1/2}\right) \lesssim N^{-A/2+10} \tag{7.4}$$

where we have used (7.2) and Lemma 6.3. Thus, in the expectation $\mathbb{E}\left(\left|c_k^{\le n}(s)\right|^2 \mathbf{1}_E\right)$, the indicator $\mathbf{1}_E$ can effectively be replaced by 1. In that case, Proposition 3.3 shows that $\mathbb{E}\left|c_k^{\le n}(s)\right|^2$ is $o_{\ell_k^\infty}\left(\frac{t}{T_{\mathrm{kin}}}\right)$ for $T_{\mathrm{kin}} = \frac{1}{4\pi\beta^2}$ whenever $|\mathcal{T}_1| + |\mathcal{T}_2| \ge 3$. Finally, we handle the main contributing cases. If $|\mathcal{T}_1| = |\mathcal{T}_2| = 0$, the only contribution to $\mathbb{E}|b_k(t)|^2$ is $n_{\mathrm{in}}(k)$. In the case $|\mathcal{T}_1| + |\mathcal{T}_2| = 1$, we have

$$2\mathrm{Re}\left(\sum_{|\mathcal{T}_0|=0,|\mathcal{T}_1|=1} \mathbb{E}\left(c_k^{\mathcal{T}_0}(s) c_k^{\mathcal{T}_1 *}(s)\right)\right) = 0,$$

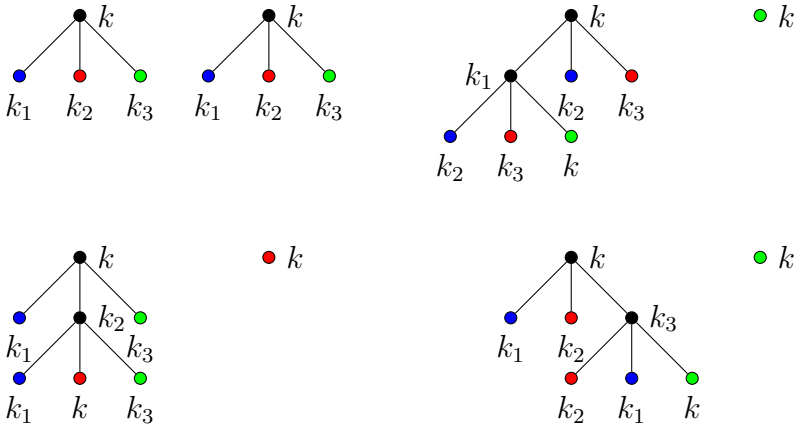


Figure 7.1: All types of couples $\mathcal{Q}$ without degenerate nodes of order $n = 2$.

since no allowed couples under enhance pairing occur there. When $|\mathcal{T}_1| + |\mathcal{T}_2| = 2$, we need to calculate the terms as shown in Figure 7.1 and its variants with degenerate nodes:

$$\mathcal{S}_k := \sum_{|\mathcal{T}_1|=1} \mathbb{E}\left|c_k^{\mathcal{T}_1}(s)\right|^2 + 2\mathrm{Re}\left(\sum_{|\mathcal{T}_0|=0,|\mathcal{T}_2|=2} \mathbb{E}\left(c_k^{\mathcal{T}_2}(s)c_k^{\mathcal{T}_0 *}(s)\right)\right)$$

as in the proof of [39, Theorem 1.3]. In the following calculations, we omit the fully degenerate cases which can be bounded by $O\left(\frac{Ts}{T_{\mathrm{kin}}}N^{-\delta}\right)$ trivially.

Since we have a nonlinear frequency shift in the phase, we need to calculate the following for $\Omega_k \neq 0$ using the fact that $A(0) = 0$:

$$\begin{aligned}
&\int_0^s e^{i\Omega_k(Ts_1+A(s_1))}ds_1 = \int_0^s \frac{d}{ds_1}\left(\int_0^{s_1} e^{i\Omega_k Ts_2}ds_2\right)e^{i\Omega_k A(s_1)}ds_1 \\
=&\left[\left(\int_0^{s_1} e^{i\Omega_k Ts_2}ds_2\right)e^{i\Omega_k A(s_1)}\right]_0^s - \int_0^s \frac{e^{i\Omega_k Ts_1}}{i\Omega_k T}i\Omega_k\dot{A}(s_1)e^{i\Omega_k A(s_1)}ds_1 \\
=&\frac{e^{i\Omega_k(Ts+A(s))}-1}{i\Omega_k T} - \int_0^s \frac{\dot{A}(s_1)}{T}e^{i\Omega_k(Ts_1+A(s_1))}ds_1. \qquad (7.5)
\end{aligned}$$

Note that the second term can be bounded by $O\left(\frac{N^{-\gamma/2}}{\langle\Omega_k T\rangle}\right)$ using $\dot{A}(s) \lesssim \beta T$, $\ddot{A}(s) \lesssim (\beta T)^3$ (using the tight bound from (5.25)) and Proposition 3.1. Then using the fact that

$$\begin{aligned}
\left|\frac{e^{i\Omega_k Ts}-1}{i\Omega_k Ts}\right|^2 &= \frac{1}{|\Omega_k Ts/2|^2}\cdot\frac{e^{i\Omega_k Ts/2}-e^{-i\Omega_k Ts/2}}{2i}\cdot\frac{e^{-i\Omega_k Ts/2}-e^{i\Omega_k Ts/2}}{-2i} \\
&= \left|\frac{\sin(\Omega_k Ts/2)}{\Omega_k Ts/2}\right|^2 = 2\mathrm{Re}\left[\frac{1-e^{i\Omega_k Ts}}{(\Omega_k Ts)^2}\right],
\end{aligned}$$

after summing all the couples with two scale 1 enhanced trees as shown in Figure 7.1 & 7.2 we can get:

$$\sum_{|\mathcal{T}_1|=1}\mathbb{E}\left|c_k^{\mathcal{T}_1}(s)\right|^2=\left(\frac{\beta Ts}{N}\right)^2\left[2\sum_{\Omega(\vec{k})\neq 0}^{\times}|T_{k,1,2,3}|^2\phi_{k_1}\phi_{k_2}\phi_{k_3}\left|\frac{\sin(\Omega(\vec{k})(Ts+A(s))/2)}{\Omega(\vec{k})Ts/2}\right|^2\right.$$
$$\left.+2\sum_{\Omega(\vec{k})=0}^{\times}|T_{k,1,2,3}|^2\phi_{k_1}\phi_{k_2}\phi_{k_3}+4\sum_{k_1\in\mathbb{Z}_N\cap(0,1)}|T_{k,1,1,k}|^2\phi_{k_1}^2\phi_k+O\left(\frac{Ts}{T_{\text{kin}}}N^{-\delta}\right)\right], \tag{7.6}$$

where $\phi_{k_i}:=n_{\text{in}}(k_i)$, $\vec{k}=(k,k_1,k_2,k_3)$, and $\times=\{(k_1,k_2,k_3)\in(\mathbb{Z}_N\cap(0,1))^3:k_1-k_2+k_3=k;k_1,k_3\neq k_2\}$. Note that the sum involved with the lower order integral in (7.5) can be bounded as:

$$\left(\frac{\beta T}{N}\right)^2\sum_{\Omega(\vec{k})\neq 0}^{\times}|T_{k,1,2,3}|^2O\left(\frac{N^{-\gamma/2}}{\langle\Omega_kT\rangle^2}\right)\lesssim\left(\frac{\beta T}{N}\right)^2N^{-\gamma/10}N^2T^{-1}\lesssim\frac{Ts}{T_{\text{kin}}}N^{-\delta}.$$

Similarly we need to calculate for $\Omega_k,\Omega_{k'}\neq 0$:

$$\begin{aligned}
&\int_0^s e^{i\Omega_k(Ts_1+A(s_1))}\int_0^{s_1}e^{i\Omega_{k'}(Ts_2+A(s_2))}ds_2ds_1\\
=&\int_0^s e^{i\Omega_k(Ts_1+A(s_1))}\left[\frac{e^{i\Omega_{k'}(Ts_1+A(s_1))}-1}{i\Omega_{k'}T}-\int_0^{s_1}\frac{\dot{A}(s_2)}{T}e^{i\Omega_{k'}(Ts_2+A(s_2))}ds_2\right]ds_1\\
=&\frac{1}{i\Omega_{k'}T}\left(\int_0^s e^{i(\Omega_k+\Omega_{k'})(Ts_1+A(s_1))}ds_1-\int_0^s e^{i\Omega_k(Ts_1+A(s_1))}ds_1\right)\\
&-\int_0^s e^{i\Omega_k(Ts_1+A(s_1))}\int_0^{s_1}\frac{\dot{A}(s_2)}{T}e^{i\Omega_{k'}(Ts_2+A(s_2))}ds_2ds_1\\
=&\frac{1}{i\Omega_{k'}T}\int_0^s e^{i(\Omega_k+\Omega_{k'})(Ts_1+A(s_1))}ds_1-\frac{e^{i\Omega_k(Ts+A(s))}-1}{(i\Omega_kT)(i\Omega_{k'}T)}+O\left(\frac{N^{-\gamma/2}}{\langle\Omega_kT\rangle\langle\Omega_{k'}T\rangle}\right)\\
=&\frac{-s}{i\Omega_kT}+\frac{1-e^{i\Omega_k(Ts+A(s))}}{(\Omega_kT)^2}+O\left(\frac{N^{-\gamma/2}}{\langle\Omega_kT\rangle^2}\right),
\end{aligned}$$

since we must have $\Omega_k+\Omega_{k'}=0$ in all cases from Figure 7.1. Summing all the couples with one scale 2 enhanced tree and one root node, we can get:

$$2\text{Re}\left(\sum_{|\mathcal{T}_0|=0,|\mathcal{T}_2|=2}\mathbb{E}\left(c_k^{\mathcal{T}_2}(s)c_k^{\mathcal{T}_0*}(s)\right)\right)$$

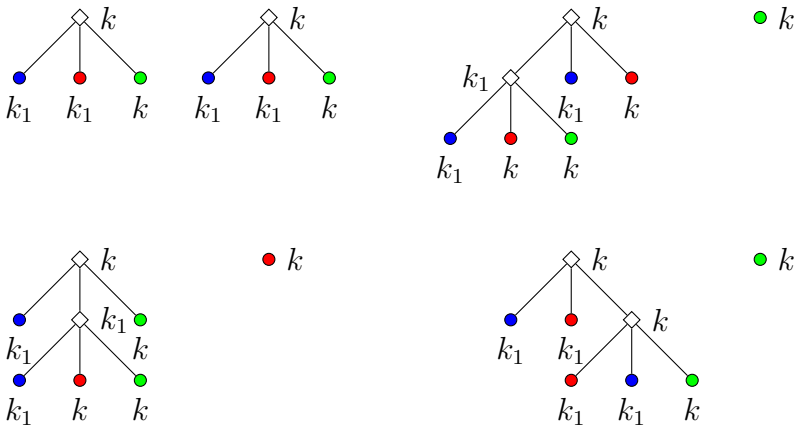


Figure 7.2: All types of enhanced couples $\mathcal{Q}$ with degenerate nodes of order $n = 2$. Note that there must be two degenerate nodes in the enhanced couple to achieve admissible pairings.

$$
\begin{aligned}
&= \left(\frac{\beta T}{N}\right)^2 \Bigg[2s^2 \sum_{\Omega(\vec{k})=0}^{\times} |T_{k,1,2,3}|^2 \left(-\phi_k\phi_{k_2}\phi_{k_3} + \phi_k\phi_{k_1}\phi_{k_3} - \phi_k\phi_{k_1}\phi_{k_2}\right) \\
&\quad + 4 \sum_{\Omega(\vec{k})\neq 0}^{\times} |T_{k,1,2,3}|^2 \mathrm{Re}\left(\frac{-s}{i\Omega_k T} + \frac{1-e^{i\Omega_k(Ts+A(s))}}{(\Omega_k T)^2}\right)\left(-\phi_k\phi_{k_2}\phi_{k_3} + \phi_k\phi_{k_1}\phi_{k_3} - \phi_k\phi_{k_1}\phi_{k_2}\right) \\
&\quad + 4s^2 \sum_{k_1\in\mathbb{Z}_N\cap(0,1)} |T_{k,1,1,k}|^2 \left(-\phi_{k_1}\phi_k^2 + \phi_{k_1}\phi_k^2 - \phi_{k_1}^2\phi_k\right) + O\left(\frac{Ts}{T_{\mathrm{kin}}}N^{-\delta}\right)\Bigg],
\end{aligned}
\tag{7.7}
$$

Then summing up (7.6) & (7.7), we can derive:

$$
\begin{aligned}
\mathcal{S}_k = \frac{\beta^2T^2s^2}{N^2}\Bigg\{ & 2\sum_{\Omega(\vec{k})\neq 0}^{\times} |T_{k,1,2,3}|^2 \phi_k\phi_{k_1}\phi_{k_2}\phi_{k_3}\left[\frac{1}{\phi_k} - \frac{1}{\phi_{k_1}} + \frac{1}{\phi_{k_2}} - \frac{1}{\phi_{k_3}}\right] \\
& \times \left|\frac{\sin(\Omega(\vec{k})(Ts+A(s))/2)}{\Omega(\vec{k})(Ts+A(s))/2}\right|^2 \cdot \left|\frac{Ts+A(s)}{Ts}\right|^2 \\
& + 2\sum_{\Omega(\vec{k})=0}^{\times} |T_{k,1,2,3}|^2 \phi_k\phi_{k_1}\phi_{k_2}\phi_{k_3}\left[\frac{1}{\phi_k} - \frac{1}{\phi_{k_1}} + \frac{1}{\phi_{k_2}} - \frac{1}{\phi_{k_3}}\right]\Bigg\} + O\left(\frac{Ts}{T_{\mathrm{kin}}}N^{-\delta}\right) \\
= \frac{2\beta^2T^2s^2}{N^2} & \sum_{\Omega(\vec{k})\neq 0}^{\times} |T_{k,1,2,3}|^2 \phi_k\phi_{k_1}\phi_{k_2}\phi_{k_3}\left[\frac{1}{\phi_k} - \frac{1}{\phi_{k_1}} + \frac{1}{\phi_{k_2}} - \frac{1}{\phi_{k_3}}\right] \\
& \times \left|\frac{\sin(\Omega(\vec{k})(Ts+A(s))/2)}{\Omega(\vec{k})(Ts+A(s))/2}\right|^2 \cdot \left|\frac{Ts+A(s)}{Ts}\right|^2 + O\left(\frac{Ts}{T_{\mathrm{kin}}}N^{-\delta}\right).
\end{aligned}
$$

For the exact resonant term, we use the bound for 3-vector countings when $\Omega = 0$ and

$\{k_1, k_3\} \neq \{k, k_2\}$, taking $m = 0$ and replacing T by TN^{δ} in the proof of Proposition 4.1. In addition we set $\delta < \frac{\epsilon}{10}$ and every step of integration by parts would gain by a factor $N^{\frac{\epsilon}{2}}$ as $T \lesssim N^{1-\epsilon}$. Applying integration by parts sufficiently many times will lead to the result $\lesssim N^{2-\delta}T^{-1}$. Using Corollary 4.2, we have that

$$\mathcal{S}_k = 2\beta^2 t \cdot \frac{t + A(t/T)}{t} \cdot (t + A(t/T)) \int_{k_i \in \mathbb{T}} \phi_k \phi_{k_1} \phi_{k_2} \phi_{k_3} \left[\frac{1}{\phi_k} - \frac{1}{\phi_{k_1}} + \frac{1}{\phi_{k_2}} - \frac{1}{\phi_{k_3}} \right] \times \left| \frac{\sin(\Omega(\vec{k})(t + A(t/T))/2)}{\Omega(\vec{k})(t + A(t/T))/2} \right|^2 dk_1 dk_2 dk_3 + O\left(\frac{t}{T_{\text{kin}}} N^{-\delta} \right).$$

Using the fact that $A(t/T)/t \sim O(N^{-\gamma})$, and for smooth functions f,

$$\left| t \int \left| \frac{\sin(tx/2)}{tx/2} \right|^2 f(x) dx - 2\pi f(0) \right| \lesssim C(f) t^{-\frac{1}{2}}, \tag{7.8}$$

where $C(f)$ depends on the L^∞ norms of f and f', we are able to get:

$$\mathcal{S}_k = \frac{t}{T_{\text{kin}}} \mathcal{K}(n_{\text{in}})(k) + o_{\ell^\infty_k}\left(\frac{t}{T_{\text{kin}}} \right), \tag{7.9}$$

which concludes the proof. □

CHAPTER 8
The Canonical Transformation

A canonical (normal-form) transformation is a symplectic change of phase-space variables [71] that cancels non-resonant or lower-order interaction terms [29]. The resulting Hamiltonian will only keep the resonant term capable of generating long-time energy transfer, yielding better asymptotics and a more transparent route to kinetic theory. In this chapter, we identify the canonical transformation removing the non-resonant interactions in the evolution equation for the action variable a_k, and find the nonlinearity threshold for β for the canonical transformation to be feasible. In this and next chapter, we will use integer wave number $k \in \mathbb{Z}/N\mathbb{Z}$ instead of the lattice wave number in $\mathbb{Z}_N \cap (0,1)$.

8.1: Choice of transformation coefficients

Recall the evolution equation from (1.18) for the normal modes a_k, which yields the following system for the normalized modes $b_k := \sqrt{N}a_k$:

$$\begin{aligned} i\dot{b}_{k_1} =&\omega_{k_1} b_{k_1} + \frac{\beta}{3N} \sum_{k_2,k_3,k_4} \Big[\tilde{T}_{-1,2,3,4} b_{k_2} b_{k_3} b_{k_4} \delta(k_1 - k_2 - k_3 - k_4) \\ &+ 3\tilde{T}_{-1,2,-3,4} b_{k_2} b^*_{k_3} b_{k_4} \delta(k_1 - k_2 + k_3 - k_4) + 3\tilde{T}_{1,2,3,-4} b^*_{k_2} b^*_{k_3} b_{k_4} \delta(k_1 + k_2 + k_3 - k_4) \\ &+ \tilde{T}_{1,2,3,4} b^*_{k_2} b^*_{k_3} b^*_{k_4} \delta(k_1 + k_2 + k_3 + k_4) \Big], \end{aligned} \tag{8.1}$$

Note that due to the positivity and strict subadditivity of $\omega(k)$, we know that:

$$0 < \omega(k_1 + k_2 + k_3) < \omega(k_1) + \omega(k_2) + \omega(k_3), \text{ for } k_i = 1, ..., N-1. \tag{8.2}$$

This fact was well explained in [55, Theorem 3.8]. So then we are able to perform a canonical transformation to remove the unwanted nonresonant interactions to higher orders terms as

in [72]:

$$b_{k_1} = c_{k_1} + \frac{\beta}{3N} \sum_{k_2,k_3,k_4} \Big[A^{(1)}_{1,2,3,4} c_{k_2} c_{k_3} c_{k_4} \delta(k_1 - k_2 - k_3 - k_4) + 3A^{(2)}_{1,2,3,4} c^*_{k_2} c^*_{k_3} c_{k_4} \delta(k_1 + k_2 + k_3 - k_4) + A^{(3)}_{1,2,3,4} c^*_{k_2} c^*_{k_3} c^*_{k_4} \delta(k_1 + k_2 + k_3 + k_4) \Big]. \quad (8.3)$$

In the following, we use the abbreviation c_i for c_{k_i}. Note that we need to use the posterior result of the evolution equation (R-FPUT) to evaluate the time derivative of the cubic terms in the transformation (8.3). Then we can get:

$$\begin{aligned} i\dot{c}_1 =& \omega_1 c_1 + \frac{\beta}{3N} \sum_{k_2,k_3,k_4} [(\tilde{T}_{-1,2,3,4} + (\omega_1 - \omega_2 - \omega_3 - \omega_4) A^{(1)}_{1,2,3,4}) c_2 c_3 c_4 \delta(k_1 - k_2 - k_3 - k_4) \\ &+ 3\tilde{T}_{-1,2,-3,4} c_2 c^*_3 c_4 \delta(k_1 - k_2 + k_3 - k_4) \\ &+ 3(\tilde{T}_{1,2,3,-4} + (\omega_1 + \omega_2 + \omega_3 - \omega_4) A^{(2)}_{1,2,3,4}) c^*_2 c^*_3 c_4 \delta(k_1 + k_2 + k_3 - k_4) \\ &+ (\tilde{T}_{1,2,3,4} + (\omega_1 + \omega_2 + \omega_3 + \omega_4) A^{(3)}_{1,2,3,4}) c^*_2 c^*_3 c^*_4 \delta(k_1 + k_2 + k_3 + k_4)] + O\left(\beta^2\right). \end{aligned} \quad (8.4)$$

So then we can choose $A^{(i)}_{1,2,3,4}$ as:

$$A^{(1)}_{1,2,3,4} = -\frac{\tilde{T}_{-1,2,3,4}}{\omega_1 - \omega_2 - \omega_3 - \omega_4}, \quad (8.5)$$

$$A^{(2)}_{1,2,3,4} = -\frac{\tilde{T}_{1,2,3,-4}}{\omega_1 + \omega_2 + \omega_3 - \omega_4}, \quad (8.6)$$

$$A^{(3)}_{1,2,3,4} = -\frac{\tilde{T}_{1,2,3,4}}{\omega_1 + \omega_2 + \omega_3 + \omega_4}, \quad (8.7)$$

to eliminate unwanted interactions. Note that this near identity transformation is canonical because it is the first–order Lie transform generated by a cubic Hamiltonian functional. The evolution equation for c_1 becomes:

$$i\dot{c}_1 = \omega_1 c_1 + \frac{\beta}{N} \sum_{k_1 - k_2 + k_3 - k_4 = 0} T_{1,2,3,4} c_2 c^*_3 c_4 + O\left(\beta^2\right). \quad (8.8)$$

where

$$T_{1,2,3,4} = \tilde{T}_{-1,2,-3,4} = \frac{3}{4\kappa^2} \iota\left(\frac{k_2 - k_3 + k_4}{N}\right) \iota\left(\frac{k_2}{N}\right) \iota\left(\frac{k_3}{N}\right) \iota\left(\frac{k_4}{N}\right) \prod_{i=1}^{4} \sqrt{\omega_{k_i}},$$

where $\iota(x) = \operatorname{sgn}\sin(\pi x)$. In the following calculation, we will only consider the size of $\left|A^{(i)}_{1,2,3,4}\right|^2$. So we can simply treat $|\tilde{T}|^2 \sim \omega_{k_1}\omega_{k_2}\omega_{k_3}\omega_{k_4}$ in (8.5), (8.6), and (8.7).

8.2: Estimates for nonresonant sums

To perform the canonical transformation (8.3), we need the validation condition:

$$\frac{\beta}{3}\sum_{k_2,k_3,k_4}\Big[A^{(1)}_{1,2,3,4}c_{k_2}c_{k_3}c_{k_4}\delta(k_1-k_2-k_3-k_4)+3A^{(2)}_{1,2,3,4}c^*_{k_2}c^*_{k_3}c_{k_4}\delta(k_1+k_2+k_3-k_4)$$
$$+A^{(3)}_{1,2,3,4}c^*_{k_2}c^*_{k_3}c^*_{k_4}\delta(k_1+k_2+k_3+k_4)\Big] \ll c_{k_1}.$$

So we want to separate the sums in the canonical transformation (8.3) into three cases with respect to the $\delta(\cdot)$ functions and find upper bounds for the sums.

Case 1: $k_1-k_2-k_3-k_4 \equiv 0 \pmod N$

1. $k_1-k_2-k_3-k_4 = 0$, then we have:

$$\begin{aligned}
&\omega_{k_1}-\omega_{k_2}-\omega_{k_3}-\omega_{k_4} = 2\left[\sin\left(\frac{\pi k_1}{N}\right)-\sin\left(\frac{\pi k_2}{N}\right)-\sin\left(\frac{\pi k_3}{N}\right)-\sin\left(\frac{\pi k_4}{N}\right)\right]\\
&= 4\left[\sin\left(\frac{\pi(k_1-k_2)}{2N}\right)\cos\left(\frac{\pi(k_1+k_2)}{2N}\right)-\sin\left(\frac{\pi(k_3+k_4)}{2N}\right)\cos\left(\frac{\pi(k_3-k_4)}{2N}\right)\right]\\
&= 4\sin\left(\frac{\pi(k_1-k_2)}{2N}\right)\left[\cos\left(\frac{\pi(k_1+k_2)}{2N}\right)-\cos\left(\frac{\pi(k_3-k_4)}{2N}\right)\right]\\
&= 8\sin\left(\frac{\pi(k_1-k_2)}{2N}\right)\sin\left(\frac{\pi(k_1+k_2+k_3-k_4)}{4N}\right)\sin\left(\frac{\pi(k_3-k_4-k_1-k_2)}{4N}\right)\\
&= 8\sin\left(\frac{\pi(k_1-k_2)}{2N}\right)\sin\left(\frac{\pi(k_1-k_4)}{2N}\right)\sin\left(\frac{\pi(k_3-k_1)}{2N}\right). \qquad (8.9)
\end{aligned}$$

We must have $k_2,k_3,k_4 < k_1$ with at least one of $k_i \sim k_1$ in the restriction of $k_1-k_2-k_3-k_4=0$. Then for fixed k_1, there are $O(k_1^2)$ choices for (k_2,k_3,k_4). We choose a constant $C=\frac{1}{3}$. Without loss of generality suppose $k_2 \geq Ck_1$, then $k_1-k_2 = k_3+k_4 \geq \max(k_3,k_4)$, $k_1-k_3 = k_2+k_4 \geq Ck_1$ and similarly $k_1-k_4 \geq Ck_1$. Then we have:

$$\left|A^{(1)}\right|^2 \lesssim \frac{\left(\frac{k_1}{N}\right)^2\left(\frac{\max(k_3,k_4)}{N}\right)^2}{\left(\frac{\max(k_3,k_4)}{N}\right)^2\left(\frac{Ck_1}{N}\right)^4} \lesssim \frac{N^2}{k_1^2}. \qquad (8.10)$$

Then we know that:

$$\sum_{k_1-k_2-k_3-k_4=0} \left|A^{(1)}\right|^2 \lesssim \frac{N^2}{k_1^2} \cdot k_1^2 = N^2 \tag{8.11}$$

2. $k_1 - k_2 - k_3 - k_4 = -2N$, then we can do a change of variable: $k_1' = N - k_1, k_2' = N - k_2, k_3' = N - k_3, k_4' = N - k_4$, we then get: $k_1' - k_2' - k_3' - k_4' = (N - k_1) - (N - k_2) - (N - k_3) - (N - k_4) = -k_1 + k_2 + k_3 + k_4 - 2N = 0$. And we still have $\sin\left(\frac{\pi k_i}{N}\right) = \sin\left(\frac{\pi k_i'}{N}\right)$. Then applying the result from the last case, we can get:

$$\sum_{k_1-k_2-k_3-k_4=-2N} \left|A^{(1)}\right|^2 \lesssim N^2 \tag{8.12}$$

3. $k_1 - k_2 - k_3 - k_4 = -N$, without loss of generality suppose $\frac{N|h|}{\pi} = |k_1 - k_4| \leq |k_1 - k_2|, |k_1 - k_3|$, $k_2 \leq k_3$, then we can write $\frac{\pi k_1}{N} = y$, $\frac{\pi k_4}{N} = y + h$, $\frac{\pi k_2}{N} = x$, $\frac{\pi k_3}{N} = \pi - x - h$, which gives:

$$\frac{\pi}{N}(k_1 - k_2 - k_3 - k_4) = y - x - (\pi - x - h) - (y + h) = -\pi$$

Then now we have:

$$\begin{aligned}
&\left|\sin\left(\frac{\pi k_1}{N}\right) - \sin\left(\frac{\pi k_2}{N}\right) - \sin\left(\frac{\pi k_3}{N}\right) - \sin\left(\frac{\pi k_4}{N}\right)\right| \\
=&|\sin(y) - \sin(y+h) - \sin(x) - \sin(\pi - x - h)| \\
\geq&\Big||\sin(y) - \sin(y+h)| - |\sin(x) + \sin(x+h)|\Big| \\
=&2\left|\left|\cos\left(y + \frac{h}{2}\right)\sin\left(\frac{h}{2}\right)\right| - \left|\sin\left(x + \frac{h}{2}\right)\cos\left(\frac{h}{2}\right)\right|\right|
\end{aligned} \tag{8.13}$$

Since we assume $k_2 \leq k_3$, we have: $x \leq \pi - x - h < \pi$, which then gives $\frac{|h|}{2} < x + \frac{h}{2} \leq \frac{\pi}{2}$. It means that:

$$\sin\left(\frac{|h|}{2}\right) < \sin\left(x + \frac{h}{2}\right).$$

On the other hand, if $y \geq \frac{\pi}{2}$, then we must have $\frac{\pi}{2} \leq y - |h| \leq \pi$ or $\frac{\pi}{2} \leq y + |h| \leq \pi$. Similarly, if $y < \frac{\pi}{2}$, then we must have $0 \leq y - |h| < \frac{\pi}{2}$ or $0 \leq y + |h| \leq \frac{\pi}{2}$. Otherwise either $k_1 > \frac{N}{2}, k_2, k_3, k_4 \leq \frac{N}{2}$ or $k_1 \leq \frac{N}{2}, k_2, k_3, k_4 > \frac{N}{2}$, which neither

give $k_1 - k_2 - k_3 - k_4 = -N$. It then means that $|h| < \frac{\pi}{2}$ and

$$0 \leq \left|\cos\left(y + \frac{h}{2}\right)\right| \leq \left|\cos\left(\frac{h}{2}\right)\right|.$$

Then we further get:

$$(8.13) \gtrsim \cos\left(\frac{h}{2}\right)\left|\sin\left(x + \frac{h}{2}\right) - \sin\left(\frac{|h|}{2}\right)\right|, \tag{8.14}$$

(i) If $h > 0$, then we have $\frac{x+h}{2} = \frac{1}{2}(x + \frac{h}{2}) + \frac{h}{4} \leq \frac{3}{8}\pi$, and:

$$(8.13) \gtrsim \cos\left(\frac{x+h}{2}\right)\sin\left(\frac{x}{2}\right) \gtrsim \sin\left(\frac{x}{2}\right),$$

then we can bound $\left|A^{(1)}\right|^2$ as:

$$\left|A^{(1)}\right|^2 \lesssim \frac{\sin(x)\sin(y)\sin(y+h)}{\sin^2\left(\frac{x}{2}\right)} \lesssim \frac{\sin(y)\sin(y+h)}{\sin\left(\frac{x}{2}\right)}. \tag{8.15}$$

In this case, since $x + \frac{h}{2} \leq \frac{\pi}{2}$, then $x < \frac{\pi}{2}$. We either have: $\pi - x - h \leq y - h$, which then gives $\frac{\pi}{2} < \pi - x \leq y$ and $\frac{\sin(y)}{\sin(\frac{x}{2})} = \frac{2\sin(y)\cos(\frac{x}{2})}{\sin(x)} \lesssim 1$, or have: $\frac{\pi}{2} > x \geq y + h$, and $\frac{\sin(y+h)}{\sin(\frac{x}{2})} = \frac{2\sin(y+h)\cos(\frac{x}{2})}{\sin(x)} \lesssim 1$. Hence we can get $\left|A^{(1)}\right|^2 \lesssim 1$ for $h > 0$.

(ii) If $h = 0$, then

$$\left|A^{(1)}\right|^2 \lesssim 1. \tag{8.16}$$

(iii) If $h < 0$, then we have $\frac{x}{2} \leq \frac{\pi}{4} + \frac{|h|}{4} \leq \frac{3}{8}\pi$, and:

$$(8.13) \gtrsim \sin\left(\frac{x+h}{2}\right)\cos\left(\frac{x}{2}\right) \gtrsim \sin\left(\frac{x+h}{2}\right),$$

then we can bound $\left|A^{(1)}\right|^2$ as:

$$\left|A^{(1)}\right|^2 \lesssim \frac{\sin(x+h)\sin(y)\sin(y+h)}{\sin^2\left(\frac{x+h}{2}\right)} \lesssim \frac{\sin(y)\sin(y+h)}{\sin\left(\frac{x+h}{2}\right)}, \tag{8.17}$$

Similarly, since $x + \frac{h}{2} \leq \frac{\pi}{2}$, then $x + h < \frac{\pi}{2}$. We either have: $\frac{\pi}{2} < \pi - x - h \leq y - |h| = y + h$, which then gives $\frac{\sin(y+h)}{\sin(\frac{x+h}{2})} \lesssim 1$, or have: $x \geq y + |h|$, i.e. $\frac{\pi}{2} > x + h \geq y$ and $\frac{\sin(y)}{\sin(\frac{x+h}{2})} \lesssim 1$. Hence we can get $\left|A^{(1)}\right|^2 \lesssim 1$ for $h < 0$.

Let $\mathbb{Z}_N := N^{-1}\mathbb{Z}$. Thus we can get the estimate for the sum:

$$\sum_{k_1-k_2-k_3-k_4=-N} \left|A^{(1)}\right|^2 \lesssim \sum_{h\in\mathbb{Z}_N\cap(0,1)} \sum_{x\in\mathbb{Z}_N\cap(0,1)} 1 \lesssim N^2. \tag{8.18}$$

From the above cases, we have:

$$\sum_{k_1-k_2-k_3-k_4\equiv 0 \pmod N} \left|A^{(1)}\right|^2 \lesssim N^2. \tag{8.19}$$

Case 2: $k_1+k_2+k_3-k_4 \equiv 0 \pmod N$

1. $k_1+k_2+k_3-k_4=0$. Similarly as Case 1.(1), we have:

$$\begin{aligned}&\omega_{k_1}+\omega_{k_2}+\omega_{k_3}-\omega_{k_4}\\ &=8\sin\left(\frac{\pi(k_4-k_2)}{2N}\right)\sin\left(\frac{\pi(k_4-k_3)}{2N}\right)\sin\left(\frac{\pi(k_4-k_1)}{2N}\right)\end{aligned} \tag{8.20}$$

And $k_1,k_2,k_3 < k_4$. Similarly we choose a constant $C<\frac{1}{3}$. Without loss of generality, suppose $k_1 \geq Ck_4$, then $k_4-k_1=k_2+k_3$, $k_4-k_2=k_1+k_3\geq k_1\geq Ck_4$, and similarly $k_4-k_3\geq Ck_4$, then we have

$$\left|A^{(2)}\right|^2 \lesssim \frac{\left(\frac{1}{N}\right)^4 k_1k_2k_3k_4}{\left(\frac{Ck_4}{N}\right)^4\left(\frac{k_2+k_3}{N}\right)^2} \lesssim \frac{N^2}{k_4^2}. \tag{8.21}$$

Then we can calculate the sum:

$$\sum_{k_1+k_2+k_3-k_4=0} \left|A^{(2)}\right|^2 \lesssim \sum_{k_4=1}^{N-1}\sum_{k_2=1}^{k_4}\frac{N^2}{k_4^2} \lesssim N^2\log N \tag{8.22}$$

2. $k_1+k_2+k_3-k_4=2N$. Then similarly as Case 1(2), we can change of variables: $k_i'=N-k_i$ for $i\in\{1,2,3,4\}$. Then we can obtain the same result as (1):

$$\sum_{k_1+k_2+k_3-k_4=2N} \left|A^{(2)}\right|^2 \lesssim N^2\log N. \tag{8.23}$$

3. $k_1+k_2+k_3-k_4=N$. We apply the same technique as in Case 1(3) and we can conclude:

$$\sum_{k_1+k_2+k_3-k_4=N} \left|A^{(2)}\right|^2 \lesssim N^2. \tag{8.24}$$

Thus we have:

$$\sum_{k_1+k_2+k_3-k_4\equiv 0 \pmod N} \left|A^{(2)}\right|^2 \lesssim N^2 \log N. \tag{8.25}$$

Case 3: $k_1+k_2+k_3+k_4 \equiv 0 \pmod N$

Let $M := \max\left(\sin\left(\frac{\pi k_1}{N}\right), \sin\left(\frac{\pi k_2}{N}\right), \sin\left(\frac{\pi k_3}{N}\right), \sin\left(\frac{\pi k_4}{N}\right)\right) \leq 1$, and

$m := \min\left(\sin\left(\frac{\pi k_1}{N}\right), \sin\left(\frac{\pi k_2}{N}\right), \sin\left(\frac{\pi k_3}{N}\right), \sin\left(\frac{\pi k_4}{N}\right)\right)$.

Then we know that:

$$\left|A^{(3)}\right|^2 \lesssim \frac{mM^3}{M^2} \lesssim 1 \tag{8.26}$$

Thus we have:

$$\sum_{k_1+k_2+k_3+k_4\equiv 0 \pmod N} \left|A^{(3)}\right|^2 \lesssim N^2. \tag{8.27}$$

Therefore we have proved the following result:

Proposition 8.1. *Let $A^{(i)}_{1,2,3,4}$, $i = 1,2,3$, be defined as in (8.5),(8.6), and (8.7), then for fixed $k_1 \in \mathbb{Z} \cap (0,N)$, we have:*

$$\begin{aligned}\sum_{\substack{k_1-k_2-k_3-k_4\equiv 0 \ (mod\ N)\\ k_2,k_3,k_4\in\mathbb{Z}\cap(0,N)}} \left|A^{(1)}_{1,2,3,4}\right|^2 + \sum_{\substack{k_1+k_2+k_3-k_4\equiv 0 \ (mod\ N)\\ k_2,k_3,k_4\in\mathbb{Z}\cap(0,N)}} \left|A^{(2)}_{1,2,3,4}\right|^2 \\ + \sum_{\substack{k_1+k_2+k_3+k_4\equiv 0 \ (mod\ N)\\ k_2,k_3,k_4\in\mathbb{Z}\cap(0,N)}} \left|A^{(3)}_{1,2,3,4}\right|^2 \lesssim N^2 \log N.\end{aligned} \tag{8.28}$$

8.3: Nonlinearity threshold

To perform the canonical transformation, we need $O(\beta)$ terms to be much less than c_{k_1} in the canonical transformation (8.3). As we defined well-prepared initial conditions for c_k:

$$c_k(0) = \sqrt{\phi_k}\eta_k(\varrho), \tag{8.29}$$

where ϕ_k's are deterministic amplitude of $O(1)$ and $\eta_k(\varrho)$'s are i.i.d. mean-zero complex random variables with unit variance, which are assumed to be either standard complex Gaussian or uniform distributed on the unit circle. We should also notice that by the

standard hypercontractivity estimates as in [39, Lemma 3.1]:

$$\mathbb{P}\left(\left|\sum_{k_1-k_2-k_3-k_4=0} A^{(1)}_{1,2,3,4} c_{k_2}(0)c_{k_3}(0)c_{k_4}(0)\right| \geq AM^{\frac{1}{2}}\right) \leq Ce^{-cA^{\frac{2}{3}}}, \tag{8.30}$$

for some positive constants $A, C, c > 0$, and

$$M = \mathbb{E}\left|\sum_{k_1-k_2-k_3-k_4=0} A^{(1)}_{1,2,3,4} c_{k_2}(0)c_{k_3}(0)c_{k_4}(0)\right|^2 \sim \sum_{k_1-k_2-k_3-k_4=0} \left|A^{(1)}_{1,2,3,4}\right|^2 \phi_2\phi_3\phi_4 \lesssim N^2 \log N. \tag{8.31}$$

Here we applied the Wick contraction theorem (see [31, Theorem 5.1]) to evaluate the expectation value. It means that with high probability for arbitrarily small $\epsilon > 0$:

$$\left|\sum_{k_1-k_2-k_3-k_4=0} A^{(1)}_{1,2,3,4} c_{k_2}(0)c_{k_3}(0)c_{k_4}(0)\right| \lesssim N^{1+\epsilon}, \tag{8.32}$$

Thus to meet the following requirement:

$$\frac{\beta}{3N}\left|\sum_{k_2,k_3,k_4} A^{(1)}_{1,2,3,4} c_{k_2}c_{k_3}c_{k_4}\delta(k_1-k_2-k_3-k_4)\right| \ll |c_{k_1}| \tag{8.33}$$

we may need a sufficient condition on the nonlinearity β:

$$\beta \ll \frac{1}{N^{\epsilon}}. \tag{8.34}$$

This is a scaling that overlaps with our scaling required in the derivation for the wave kinetic equation. In Theorem 1 we require $\beta = N^{-\gamma}$ for $\gamma \in (0,1)$, which indicates $N^{-1} < \beta < 1$ and overlaps with the nonlinearity threshold for the canonical transformation $\beta \ll N^{-\epsilon}$. However, in this thesis we only prove for the reduced evolution equation (R-FPUT) but not the original evolution equation (8.1). It remains to bound the lower order non-resonant interactions after canonical transformation in the evolution equation for future work.

CHAPTER 9
The Numerical Verification

In the last chapter, we established a sufficient upper bound for the scaling of nonlinearity β that guarantees the canonical transformation remains well defined and keeps the non-resonant contributions under control. To test the validity of this theoretical bound, we now turn to direct simulations of the β-FPUT chain. By varying β and N and measuring the size of the resulting non-resonant sums, we can verify whether the predicted scaling indeed makes the magnitude of the non-resonant sums remarkably small compared to the resonant sums. This numerical check provides an essential bridge between the theoretical upper bound and the practical dynamics of the lattice.

9.1: Rescaled nonlinearity

Throughout this chapter we replace the original nonlinearity by a rescaled one defined as:

$$\widetilde{\beta} := \frac{\beta}{N}.$$

We use $\widetilde{\beta}$ instead of β for the following reasons:

1. **Direct comparison with the theoretical bound.** In Chapter 8 we proved the sufficient upper bound:
$$\beta \ll N^{-\epsilon} \quad (\epsilon \ll 1).$$
Rewriting this upper bound with the new nonlinearity gives
$$\widetilde{\beta} \ \ll \ N^{-(1+\epsilon)},$$
so the decay rate in N appears explicitly. Monitoring $\widetilde{\beta}$ as N grows therefore tells us immediately whether the hypothesis is satisfied.
2. **Practical convenience in simulations.** Numerical experiments often obscure what "$O(1)$" means, because the implied constant depends on normalisation choices, grid

resolution and accumulated error. By contrast, the dependence of $\widetilde{\beta}$ on N can be read off directly from the data; empirical checks of the bound thus become unambiguous.

Recall the evolution equations (1.18) for the action variable from the equations of motion. We perform a change of variable $b_k = \sqrt{N}a_k$ to get:

$$\begin{aligned} i\dot{b}_{k_1} =&\omega_{k_1} b_{k_1} + \frac{\widetilde{\beta}}{3}\sum_{k_2,k_3,k_4}\Big[\tilde{T}_{-1,2,3,4}b_{k_2}b_{k_3}b_{k_4}\delta(k_1-k_2-k_3-k_4) \\ &+ 3\tilde{T}_{-1,2,-3,4}b_{k_2}b^*_{k_3}b_{k_4}\delta(k_1-k_2+k_3-k_4) + 3\tilde{T}_{1,2,3,-4}b^*_{k_2}b^*_{k_3}b_{k_4}\delta(k_1+k_2+k_3-k_4) \\ &+ \tilde{T}_{1,2,3,4}b^*_{k_2}b^*_{k_3}b^*_{k_4}\delta(k_1+k_2+k_3+k_4)\Big] \end{aligned} \tag{9.1}$$

We use $\widetilde{\beta}$ instead of β because we want to verify the sufficient upper bound $\beta \ll N^{-\epsilon}$ we derived in the last chapter. It will be more straightforward to test how $\widetilde{\beta}$ is related to N than how β is related to $O(1)$ values. After the canonical transformation, we get (R-FPUT):

$$i\dot{b_{k_1}}(t) = \omega_{k_1}b_{k_1}(t) + \widetilde{\beta}\sum_{k_1-k_2+k_3-k_4=0} T_{k,1,2,3}b_{k_2}(t)b^*_{k_3}(t)b_{k_4}(t).$$

Reconstruct the Fourier transform of position and momentum from b_k:

$$Q_k = (2\omega_k)^{-\frac{1}{2}}(b_k + b^*_{N-k}),\ P_k = -i(2\omega_k)^{-\frac{1}{2}}(b_k - b^*_{N-k}). \tag{9.2}$$

We still use the (forward) inverse Fourier Transform to get the position and momentum:

$$q_j = \sum_{k=0}^{N-1} Q_k e^{i2\pi jk/N},\ p_j = \sum_{k=0}^{N-1} P_k e^{i2\pi jk/N}. \tag{9.3}$$

Then we can get the canonical equations of motion:

$$\dot{q_j} = \frac{\partial H}{\partial p_j} = \frac{p_j}{m} \tag{9.4}$$

$$\dot{p_j} = -\frac{\partial H}{\partial q_j} = \kappa(q_{j-1} - 2q_j + q_{j+1}) + \widetilde{\beta}\left[(q_{j+1}-q_j)^3 - (q_{j-1}-q_j)^3\right], \tag{9.5}$$

for $j \in \mathbb{Z} \cap [0, N-1]$ and $\widetilde{\beta} = \beta/N$.

9.2: Yoshida's sixth-order symplectic integrator

To test the scaling of β for performing the canonical transformation, we first do numerical simulations for the β-FPUT model using the sixth order symplectic integrator method [73] based on the canonical equations of motion (9.4) and (9.5). We set $m = 1, \kappa = 1$ for all simulations to be performed. The Hamiltonian is:

$$H(q,p) = T(p) + V(q), \tag{9.6}$$

$$T(p) = \sum_{j=0}^{N-1} \frac{p_j^2}{2m}, \tag{9.7}$$

$$V(q) = \sum_{j=0}^{N-1} \Big[\frac{\kappa}{2} \big(q_{j+1} - q_j\big)^2 + \frac{\widetilde{\beta}}{4} \big(q_{j+1} - q_j\big)^4 \Big], \tag{9.8}$$

Let $z = (q,p) = (q_0, \ldots, q_{N-1}, p_0, \ldots, p_{N-1})$ denote the $2N$-dimensional phase-space vector and let $f(z)$ be any smooth observable. The Poisson bracket of f with the Hamiltonian H is defined as

$$\{f, H\} = \sum_{j=0}^{N-1} \Big(\frac{\partial f}{\partial q_j} \frac{\partial H}{\partial p_j} - \frac{\partial f}{\partial p_j} \frac{\partial H}{\partial q_j} \Big).$$

Let A and B be Poisson brackets $A = \{\cdot, T\},\ B = \{\cdot, V\}$ so that we can write the Hamilton equations (9.4) and (9.5) into:

$$\dot{z} = (A + B)z.$$

We get the approximated solution $z(h) = \exp\big(h(A+B)\big)z(0)$. Since A and B do not commute, we cannot evaluate $\exp\big(h(A+B)\big)$ in closed form and instead investigate $\exp(hA)$ and $\exp(hB)$. The mapping $\exp(hA)$ and $\exp(hB)$ with time step h are defined by:

$$\begin{aligned} \exp(hA) \ &: \ (q,p) \mapsto \big(q + h\nabla_p T(p),\, p\big), \\ \exp(hB) \ &: \ (q,p) \mapsto (q,\, p - h\nabla_q V(q)) \end{aligned}$$

A symplectic integrator of sixth order is obtained by composing these flows with coefficients $\{c_i, d_i\}_{i=1}^{8}$:

$$\exp\big(h(A+B)\big) = \prod_{i=1}^{8} \exp(c_i hA) \exp(d_i hB) + O(h^6) \tag{9.9}$$

where Yoshida's sixth-order coefficients [73] are listed below:

$$
\begin{aligned}
c_1 &= 0.392256805238780, & d_1 &= 0.784513610477560,\\
c_2 &= 0.510043411918458, & d_2 &= 0.235573213359357,\\
c_3 &= -0.471053385409757, & d_3 &= -1.177679984178870,\\
c_4 &= 0.068753168252518, & d_4 &= 1.315186320683906,\\
c_5 &= 0.068753168252518, & d_5 &= -1.177679984178870,\\
c_6 &= -0.471053385409757, & d_6 &= 0.235573213359357,\\
c_7 &= 0.510043411918458, & d_7 &= 0.784513610477560,\\
c_8 &= 0.392256805238780, & d_8 &= 0.
\end{aligned}
$$

Compared with the classical fourth-order Runge–Kutta scheme, the Yoshida integrator retains the symplectic structure exactly and exhibits energy conservation, which is essential when we analyze the FPUT system at long time scales.

9.3: Setup for the initial data

We set the discrete Fourier Transform $Q_k(0)$ and $P_k(0)$'s at the initial state in the following steps. First we set $Q_k^{(0)}$ and $P_k^{(0)}$ as:

$$
Q_k^{(0)}, P_k^{(0)} = \begin{cases} 0 & \text{if } k = 0, \\ 1 & \text{otherwise,} \end{cases}
$$

We would like to choose $Q_k(0)$ and $P_k(0)$ so that they share the same spectral profile as $Q_k^{(0)}$ and $P_k^{(0)}$, while still physically admissible and consistent with the real-space variables. Next we calculate the spectrum $E_k^{(0)}$:

$$
E_k^{(0)} = \frac{1}{2}\left(\left| P_k^{(0)}(t) \right|^2 + \left| \omega_k Q_k^{(0)}(t) \right|^2 \right),
$$

Next we set the action variable $b_k(0)$:

$$
b_k(0) = \begin{cases} 0 & \text{if } k = 0, \\ \sqrt{E_k^{(0)}/\omega_k} \cdot \exp(i\varphi_k) & \text{otherwise,} \end{cases}
$$

with phases $\varphi_k \sim \text{Unif}[0, 2\pi)$ for all $k \in \mathbb{Z} \cap (0, N)$. Note that here we have $\|b_k\|_{\ell^2} \sim O(\log N)$ and we just consider it to be $O(1)$ for $N \leq 1000$. Next we calculate $Q_k(0), P_k(0)$:

$$Q_k(0) = (2\omega_k)^{-\frac{1}{2}}[b_k(0) + b^*_{N-k}(0))] \tag{9.10}$$

$$P_k(0) = -i(2\omega_k)^{-\frac{1}{2}}[b_k(0) - b^*_{N-k}(0)]. \tag{9.11}$$

Then we can use the inverse Fourier Transform to get the initial conditions:

$$q_j(0) = \sum_{k=0}^{N-1} Q_k(0) e^{i2\pi jk/N}, \; p_j(0) = \sum_{k=0}^{N-1} P_k(0) e^{i2\pi jk/N}. \tag{9.12}$$

9.4: Simulation

Starting from $(q^{(0)}, p^{(0)}) = (q(t), p(t))$, the discrete updating algorithm of Yoshida's sixth order symplectic integrator method is shown as follows for $i = 1, \ldots, 8$:

$$q^{(i)} \leftarrow q^{(i-1)} + c_i h p^{(i-1)}, \tag{9.13}$$

$$p^{(i)} \leftarrow p^{(i-1)} - d_i h \nabla_q V(q^{(i)}), \tag{9.14}$$

After the loop, we get the updated data $q(t + h) := q^{(8)}$, $p(t + h) := p^{(8)}$. The fundamental period can be found as: $T_f = \frac{2\pi}{\omega_1} \approx N$. We simulate the model for a time $t_{\max} = 10N \approx 10T_f$. We set the time step $h = 0.01$ and simulate the β-FPUT system for $1000N \times h$ time steps from $t = 0$ to $t = t_{\max}$ so that the relative errors of Hamiltonian can be limited by 10^{-8}.

9.5: Ratio of non-resonant to resonant sums

We want to study whether equation (R-FPUT) correctly represents the β-FPUT model after removing the non-resonant sums in (9.1). In order to verify the feasibility of canonical transformation, we calculate the weight of non-resonant sums in nonlinear sums of the Hamiltonian. Plugging in the Fourier transforms Q_k and P_k for (9.2), we get:

$$H = \frac{P_0^2}{2m} + \frac{1}{2m} \sum_{k=1}^{N-1} \left(|P_k|^2 + m^2 \omega_k^2 |Q_k|^2 \right) + \frac{\widetilde{\beta}}{4} \sum_{k_1,k_2,k_3,k_4=1}^{N-1} \tilde{T}_{1,2,3,4} Q_1 Q_2 Q_3 Q_4 \delta_{1+2+3+4}.$$

We further substitute the normal modes b_k and omit the P_0 term:

$$H = \sum_{k=1}^{N-1} \omega_k |b_k|^2 + \widetilde{\beta} \sum_{k_1,k_2,k_3,k_4} \Big[\tilde{T}_{-1,2,3,4}(b_1^* b_2 b_3 b_4 + c.c.)\delta_{1-2-3-4} + \frac{3}{2}\tilde{T}_{-1,2,-3,4} b_1^* b_2 b_3^* b_4 \delta_{1-2+3-4} + \frac{1}{4}\tilde{T}_{1,2,3,4}(b_1^* b_2^* b_3^* b_4^* + c.c.)\delta_{1+2+3+4} \Big], \tag{9.15}$$

where *c.c.* denotes the complex conjugate of the previous term. We choose to calculate and record the following sums in each k_1 when $t = 0 \pmod{10}$ or every 1000 time steps for enough data points:

$$S_{k_1}^{(1)} = 2\mathrm{Re} \sum_{k_2,k_3,k_4} \tilde{T}_{-1,2,3,4} b_1^* b_2 b_3 b_4 \delta(k_1 - k_2 - k_3 - k_4), \tag{9.16}$$

$$S_{k_1}^{(2)} = 2\mathrm{Re} \sum_{k_2,k_3,k_4} \tilde{T}_{-1,2,-3,4} 3 b_1^* b_2 b_3^* b_4 \delta(k_1 - k_2 + k_3 - k_4), \tag{9.17}$$

$$S_{k_1}^{(3)} = 2\mathrm{Re} \sum_{k_2,k_3,k_4} \tilde{T}_{1,2,3,-4} 3 b_1^* b_2^* b_3^* b_4 \delta(k_1 + k_2 + k_3 - k_4), \tag{9.18}$$

$$S_{k_1}^{(4)} = 2\mathrm{Re} \sum_{k_2,k_3,k_4} \tilde{T}_{1,2,3,4} b_1^* b_2^* b_3^* b_4^* \delta(k_1 + k_2 + k_3 + k_4). \tag{9.19}$$

so that with index relabeling and permutation, we can recover:

$$H = \sum_{k=1}^{N-1} \omega_k |b_k|^2 + \frac{\widetilde{\beta}}{4} \sum_{k=1}^{N-1} \sum_{m=1}^{4} S_k^{(m)}. \tag{9.20}$$

To reduce the number of iterations when summing over (k_2, k_3, k_4), we first find all of the quartets (k_2, k_3, k_4) that satisfy $\delta(k_1 - k_2 - k_3 - k_4)$, $\delta(k_1 - k_2 + k_3 - k_4)$, $\delta(k_1 + k_2 + k_3 - k_4)$, and $\delta(k_1 + k_2 + k_3 + k_4)$ respectively. Next, we calculate all the sums (9.16-9.19) at the time points $t_n = 10n$, we then get the sums at a total number of N time points: $10 = t_1 < ..... < t_N = t_{\max}$. We take averages of the sums over the time points in the second half of the time interval and the ensemble average over 5 random phases $j = 1, 2, 3, 4, 5$ for the initial condition to get:

$$AS_k^{(m)} = \frac{2}{5N} \sum_{j=1}^{5} \sum_{i=\frac{N}{2}+1}^{N} S_{k,j}^{(m)}(t_i), \tag{9.21}$$

for $m = 1, 2, 3, 4$. We then can get the ratio of the averaged non-resonant sums to averaged resonant sums for mode k:

$$r_k = \left| \frac{AS_k^{(1)} + AS_k^{(3)} + AS_k^{(4)}}{AS_k^{(2)}} \right|. \tag{9.22}$$

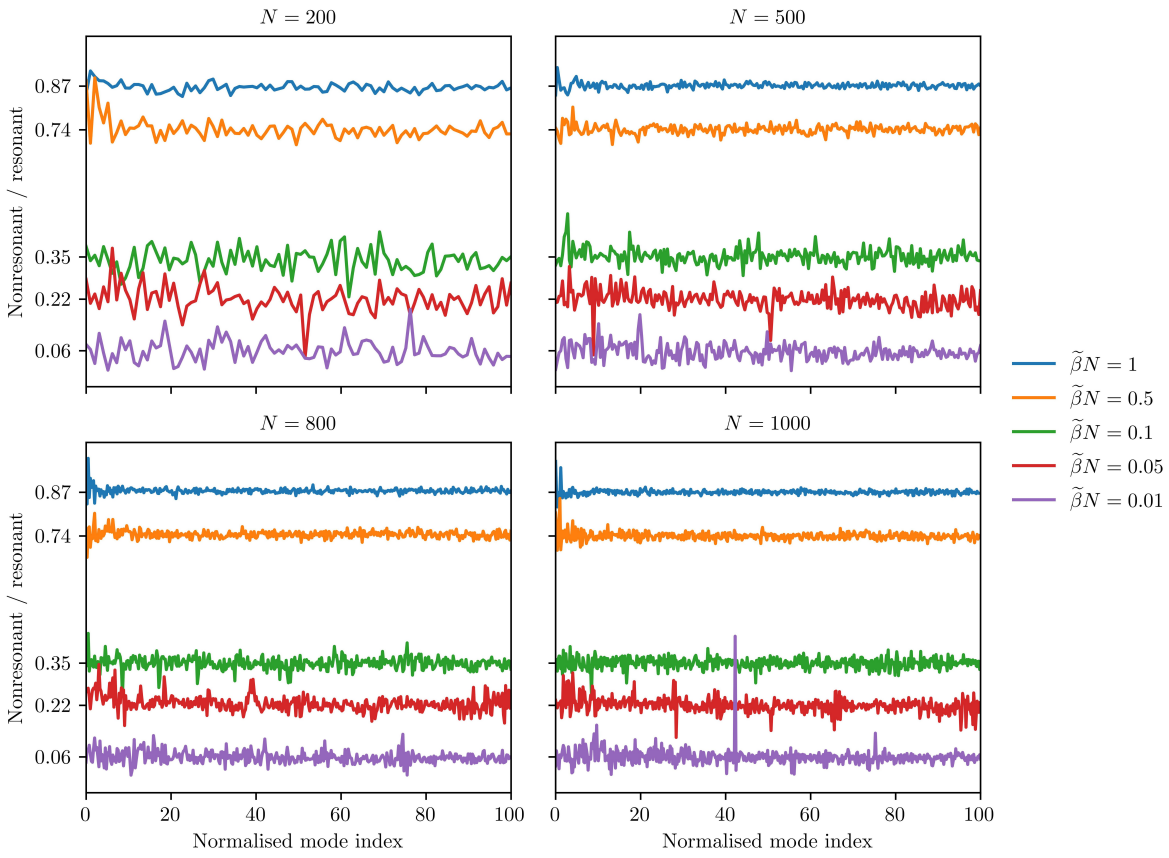


Figure 9.1: Ratio r_k of averaged non-resonant to resonant sums in Hamiltonian versus the normalised mode index $\frac{2k}{N} \times 100\%$ up to $k = \frac{N}{2}$ for $N = 200$, 500, 800, and 1000. In every subplot the product of nonlinearity and number of particles is scaled as $\widetilde{\beta}N = 1$, 0.5, 0.1, 0.05, and 0.01. The ratio on average decreases from 87% to 6% as $\widetilde{\beta}N$ decreases from 1 to 0.01 for each tested particle number N.

We perform the above steps for $N = 200$, 500, 800, and 1000 and nonlinearity $\widetilde{\beta} = \frac{\beta}{N}$, where $\widetilde{\beta}N = 1$, 0.5, 0.1, 0.05, and 0.01. We observe from plots in Figure 9.1:

- Sharing the same $\beta_0 = \widetilde{\beta}N$, the absolute ratios of non-resonant sums to the resonant sums against the percentage of mode number for different N are approximately the same in the same time period. The ratio also retains a consistent shape or pattern

across different particle numbers when the nonlinearity $\widetilde{\beta}$ is proportional to $\frac{1}{N}$.

- As $\widetilde{\beta}N$ decreases from 1 to 0.01, the ratio of averaged non-resonant sums to resonant sums in the Hamiltonian also decreases from 87% to 6%, consistently across various particle numbers N.
- The threshold of nonlinearity $\widetilde{\beta}$ for performing the canonical transformation without removing relatively large non-resonant sums: $\widetilde{\beta} < \frac{0.01}{N}$ as the ratio of non-resonant sums to resonant sums decreasing below 10%.

Note that these findings are consistent with the theoretical bound $\beta = \widetilde{\beta}N \ll N^{-\epsilon}$ after the change of variables we did in Sections 1.4.4 and 8.1: $b_k := \sqrt{N}a_k$.

On the other hand, in our numerical simulations, the action variables are updated every 10 time steps and the initial data are endowed with independent random phases, the hypercontractivity estimates that underlie the theory remain valid for the simulated trajectories as well.

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