Flow Equation Approach to Bosonic Impurity Problems

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Flow Equation Ansatz für bosonische Impurity Probleme

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NOTATION AND SYMBOLS

λ	flow parameter; in the literature sometimes also denoted by B
$\hat{\cdot}$	denotes that $\cdot$ is an operator
1	indicates $1 \in \mathbb{N}$ or the identity operator $\hat{\mathbb{1}} =: \mathbb{1}$
$:\hat{A}:$	normal ordering of operator $\hat{A}$
$\hat{a}_k^\dagger$	k^{th} bosonic creation operator
$\hat{a}_k$	k^{th} bosonic annihilation operator
$[\hat{A}, \hat{B}]$	commutator of operators $\hat{A}, \hat{B}$
$\left\{\hat{A}, \hat{B}\right\}$	anti-commutator of operators $\hat{A}, \hat{B}$
$\hat{A}^\dagger$	adjoint of an operator $\hat{A}$
z^*	complex conjugate of $z \in \mathbb{C}$
$\delta_{\alpha,\beta}$	Kronecker-Delta of α, β
$\delta(x)$	Dirac-Delta of $x \in \mathbb{R}$
∂_x	partial derivative $\frac{\partial}{\partial x}$ w.r.t. x
$\overset{②}{=}$	Equality up to second order, i.e. higher order terms are neglected.
$\hbar = 1$	reduced Planck's constant is set to 1
$+$h.c.	plus the Hermitian conjugate of the previous term
$\sim$	approximately proportional to
$\underline{\underline{E}}_N$	$N \times N$ identity matrix
$\operatorname{sgn}(\cdot)$	signum function
$\mathcal{O}$	Landau Big O
$\gtrsim$	greater than an approximate value
iff	if and only if

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SECTION 1 INTRODUCTION

The flow equation approach was independently discovered by Franz Wegner [1] and by Stanislaw D. Glazek and Kenneth G. Wilson [2] as a new renormalization technique to diagonalize, or at least block-diagonalize, Hamiltonians. It is also known under the names Continuous Unitary Transformation (CUT), Double Bracket Flow, or Isospectral Flow, and has been successfully applied to a variety of physical systems, including the Kondo model, interacting bosons, and electron-phonon interaction [3]. What makes the flow equation approach a particularly powerful and interesting tool for many-body problems is that it can sometimes still be applied in cases where conventional techniques such as perturbation theory fail. It consists of a continuous unitary transformation of the Hamiltonian, guided by a generator that makes the Hamiltonian increasingly diagonal.

This thesis deals with the application of the flow equation method to quadratic bosonic Hamiltonians. Two cases are distinguished: In the first case the Hamiltonian is purely quadratic, in the second case the Hamiltonian still has the same basic structure, but now the matrix elements of the second quantized Hamiltonian depend on the (bosonic) occupation numbers. The latter occurs, for example, in the Bose polaron problem with a movable impurity of finite mass. The dependence on the occupation numbers vanishes in the limit of an infinite impurity mass, that is, when the impurity is fixed.

The structure of this thesis is as follows: First, we will provide a brief introduction to the flow equation approach and elaborate on some of the problems it entails in Section 2. We will also give an overview on the Bose Polaron problem by discussing the Fröhlich Hamiltonian and the Lee-Low-Pines (LLP) transformation. The flow equations for both the purely quadratic case and the case where the coefficients depend on the bosonic occupation numbers will be formulated in Section 3. This section will be supplemented by detailed calculations, which can be found in Appendix A.

In Section 4 the flow equations for the purely quadratic case will be tested on the one dimensional Bose polaron model by comparing its result with the spectrum that can be obtained by an exact diagonalization of the corresponding Hamiltonian with the help of Bogoliubov transformations.

We then close by discussing the advantages and limitations of our method, as well as possible extensions and future applications in Section 5.

SECTION 2 THEORETICAL BACKGROUND

2.1 The Flow Equation Approach

In this section we introduce the mechanism and general idea behind the flow equation approach. Then we will axiomatically define normal ordering for its relevance to our subsequent discussion about truncation schemes.
After that, we will give a brief overview of the Bose polaron problem. The Hamiltonian which will be introduced there can be brought into the purely quadratic form required for our flow equations derived in Section 3 by a Lee-Low-Pines transformation, an introduction to which will be given at the end of this section.

2.1.1 General Mechanism

Since this section is intended to be a concise and rather operational overview on the flow equation approach, we refer to S. Kehrein's in-depth and very pedagogical introduction for further reading [4]. This is also the textbook on which this section is based on, unless indicated otherwise.

Our starting point will be some Hamiltonian $\hat{\mathcal{H}}$ and our goal will be to continuously transform $\hat{\mathcal{H}}$ into an unitarily equivalent diagonal Hamiltonian. This sequence of transformations $\hat{U}$ is ordered by a flow parameter λ with $[\lambda] = \text{Energy}^{-2}$ and will be chosen such that the off-diagonal elements in

$$\hat{\mathcal{H}}(\lambda) = \hat{U}(\lambda)\hat{\mathcal{H}}(\lambda = 0)\hat{U}^{\dagger}(\lambda) \tag{2.1}$$

vanish in the limit $\lambda \to \infty$. $\hat{U}(\lambda)$ is connected to $\hat{\eta}(\lambda)$ by

$$\hat{\eta}(\lambda) := \frac{\mathrm{d}\hat{U}(\lambda)}{\mathrm{d}\lambda}\hat{U}^{\dagger}(\lambda) = -\hat{\eta}^{\dagger}(\lambda) \tag{2.2}$$

where $\hat{\eta}(\lambda)$ is called the antihermitian generator of the unitary transformation $\hat{U}(\lambda)$ or simply the generator of the flow. Applying the Baker-Campbell-Hausdorff formula to equation 2.1, or simply differentiating both sides of equation 2.1 with respect to λ, yields

$$\frac{\mathrm{d}\hat{\mathcal{H}}(\lambda)}{\mathrm{d}\lambda} = \left[\hat{\eta}(\lambda), \hat{\mathcal{H}}(\lambda)\right]. \tag{2.3}$$

This differential equation is what we will refer to as the flow equation for the Hamiltonian $\hat{\mathcal{H}}(\lambda)$. The explicit computation of the unitary transformation from the generator of the transformation is generally complicated and usually not of interest because it is not required for finding the diagonal Hamiltonian. It involves the λ-ordering operator

$$\hat{T}_{\lambda}\left(\hat{\eta}(\lambda_1)\dots\hat{\eta}(\lambda_n)\right) := \hat{\eta}(\max_{i=1,\dots,n}\lambda_i)\dots\hat{\eta}(\min_{i=1,\dots,n}\lambda_i) \tag{2.4}$$

which commutes generators with larger flow parameters further to the left. Then the unitary transformation is given by

$$\hat{U}(\lambda) = \hat{T}_\lambda \exp\left(\int_0^\lambda \mathrm{d}\lambda' \hat{\eta}(\lambda')\right) \tag{2.5}$$

$$= 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \int_0^\lambda \mathrm{d}\lambda_1 \dots \mathrm{d}\lambda_n \hat{T}_\lambda \left(\hat{\eta}(\lambda_1) \dots \hat{\eta}(\lambda_n)\right). \tag{2.6}$$

From now on, the $\lambda-$dependence of $\hat{\eta}, \hat{\mathcal{H}}$ and $\hat{U}$ will usually be notationally dropped.
For every $\hat{U}$ there exists one and only one $\hat{\eta}$ which generates the unitary transformation defined by $\hat{U}$. However, there may be several $\hat{U}$ which let $\hat{\mathcal{H}}(\lambda = 0) =: \hat{\mathcal{H}}^{(0)}$ flow to (the evidently unique) diagonal Hamiltonian $\hat{\mathcal{H}}(\lambda = \infty) =: \hat{\mathcal{H}}^{(\infty)}$ so in general there is more than one good choice for $\hat{\eta}$.
It turns out that in most cases setting

$$\hat{\eta} = \left[\hat{\mathcal{H}}_{\text{diag.}}, \hat{\mathcal{H}}\right], \tag{2.7}$$

where $\hat{\mathcal{H}}_{\text{diag.}}$ is the diagonal part of the Hamiltonian, achieves the desired diagonalization.

We are often in a situation where a given system described by $\hat{\mathcal{H}}_0$ with known eigenenergies and eigenstates is well understood if certain interaction terms $\hat{\mathcal{H}}_{\text{int}}$ are omitted. In this case, we can write $\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{\text{int}}$ and thus

$$\hat{\eta} = \left[\hat{\mathcal{H}}_0, \hat{\mathcal{H}}_{\text{int}}\right]. \tag{2.8}$$

This choice for $\hat{\eta}$ is called the canonical generator and is also the choice for the generator that will be adopted in this thesis..
A good benchmark that indicates how diagonal the interaction Hamiltonian is at a given point in the flow, is to check if the the trace of its square becomes smaller in the flow:

$$\frac{\mathrm{d}}{\mathrm{d}\lambda} \mathrm{Tr}\left(\hat{\mathcal{H}}_{\text{int}}^2\right) \leq 0 \tag{2.9}$$

It can be proved [4, pp. 27-28] that this is always the case iff

$$\mathrm{Tr}\left(\hat{\mathcal{H}}_0 \hat{\mathcal{H}}_{\text{int}}\right) = \mathrm{Tr}\left(\frac{\mathrm{d}\hat{\mathcal{H}}_0}{\mathrm{d}\lambda} \hat{\mathcal{H}}_{\text{int}}\right) = 0 \tag{2.10}$$

Note, however, that a complete diagonalization of the Hamiltonian may not always be worthwhile, since for practically relevant Hamiltonians one almost always has to introduce approximations in order to obtain closed-form flow equations [3]. Thus, in some cases, one might want to perform only weak unitary transformations, making the flow converge only to a block diagonal form [3].
In this thesis we will construct the flow so that it in fact flows to a diagonal Hamiltonian, but it is still good to keep in mind that the flow equation approach can be useful even if it is only used to transform the Hamiltonian into a block diagonal form that may be easier to diagonalize by other methods such as block-wise exact diagonalization.
In the following section, we will introduce normal ordering - an important concept for controlling the error in the aforementioned often-needed approximations.

2.1.2 Normal Ordering

Normal ordering plays an essential role in successfully applying to flow equation approach to realistic Hamiltonians. In our definition of normal ordering, we closely follow [4, pp. 62-63] which in turn is based upon unpublished notes by F. Wegner.
Let $\hat{\alpha}_k \in \{\hat{a}_k, \hat{a}_k^\dagger\}$ and consider some normalized reference state $|\psi_{NO}\rangle$. Moreover, we define the contractions

$$C_{k,l} := \langle\psi_{NO}|\hat{\alpha}_k\hat{\alpha}_l|\psi_{NO}\rangle. \tag{2.11}$$

Then it follows that

$$[\hat{\alpha}_k, \hat{\alpha}_l] = C_{k,l} - C_{l,k} \tag{2.12}$$

which can be proved readily by applying the canonical commutation relations to equation 2.11 and by using the normalization of $|\psi_{NO}\rangle$. The normal ordering of an operator $\hat{O}$ composed of creation and annihilation operators is defined by the following three rules:

1. c-numbers are unaffected by normal ordering:

$$:1:=1 \tag{2.13}$$

2. Linearity:

$$:c\,\hat{O}_1 + \hat{O}_2 := c:\hat{O}_1: + :\hat{O}_2: \;\; \forall c \in \mathbb{C} \tag{2.14}$$

3. Recurrence relation:

$$\hat{\alpha}_k : \hat{O} :=: \hat{\alpha}_k\hat{O} : + \sum_l C_{k,l} : \partial_{\hat{\alpha}_l}\hat{O} : \tag{2.15}$$

   The derivative is performed symbolically w.r.t. $\hat{\alpha}_l$.

An important property of normal ordered operators is that within an normal ordered expression, products of operators can be permuted arbitrarily.
Furthermore, when the normal ordering is performed with respect to the vacuum, normal ordering an operator is equivalent to successively commuting all creation operators to the left and all annihilation operators to the right.

2.1.3 Truncation Schemes

The crux of the flow equation approach lies in the fact that for many Hamiltonians, the flow creates higher and higher interaction terms. To illustrate this, consider a Hamiltonian which can be split into a quadratic $\hat{\mathcal{H}}_0$ and a quartic $\hat{\mathcal{H}}_{\text{int}}$, i.e. they contain terms with two respectively four creation or annihilation operators.
Evaluating the commutator 2.8 yields a generator which is still of the same structure as the original Hamiltonian. However, evaluating equation 2.3 yields fourth order terms from the commutators of quadratic and quartic terms and sixth order terms from the commutators of quartic and quartic terms. This might suggest that the flow Hamiltonian is of order six, but then also the commutators of these sixth order terms with the canonical generator with terms up to quartic order have to be considered, which in turn creates terms of order eight and so forth.

It follows that, for practical purposes, this sequence must be truncated at some point. Normal ordering can be thought of as a procedure to organize the higher order terms generated in the flow, because the normal ordered expression consisting of all quadratic creation or annihilation operator terms contains all the information about the particle energies, and the normal ordered expression consisting of all quartic creation or annihilation operator terms contains all the information about the two-particle interaction and so on [4]. Without normal ordering, for example, fourth-order terms might also contribute to one-particle energies. Thus, a normally ordered expression organizes its terms by the order of their interaction. Since higher order interactions generally contribute less than lower order interactions, this is the correct way to truncate a sequence.

With respect to which state the Hamiltonian should be normal ordered, i.e. with respect to which state the contractions 2.11 should be defined, is subtle. It should be defined with respect to the ground state $|GS\rangle$ of the diagonal Hamiltonian $\hat{\mathcal{H}}^{(\infty)}$, because we want the interaction terms to be ordered by their interaction order in our actual physical system. But there are two problems with this: First, the ground state of the diagonal Hamiltonian is not necessarily known; second, this state changes because the basis changes at each step of the flow, i.e.

$$|GS(\lambda)\rangle = \hat{U}(\lambda)\hat{U}^{\dagger}(\lambda = \infty)|GS\rangle. \tag{2.16}$$

Intuitively, this is clear: We first let the flow run backwards from $\lambda = \infty$ to $\lambda = 0$ and then let $|GS(\lambda = 0)\rangle$ flow until $|GS(\lambda)\rangle$ which is the correct ground state in the basis of a given point λ in the flow.
A possible solution to our two problems is to first start with normal ordering w.r.t. some arbitrary state (e.g. the vacuum) to get a first guess for the ground state of the diagonal Hamiltonian and to iteratively improve that guess by repeatedly traversing the flow.

Although this method has not found widespread adoption when using the flow equation approach because the error induced by a “naïve“ normal ordering prescription is usually not large [4], and it may sometimes be easier just to consider more terms in the flow instead of working with the correct normal ordering prescription, it is important not to forget that not all normal ordered expansions and truncation schemes are equally well-behaved and can introduce differently sized errors.

2.2 The Bose Polaron Problem

2.2.1 (Beyond) The Fröhlich Hamiltonian

The Fröhlich Hamiltonian is a model Hamiltonian that describes the interaction between a single quantum particle and a phonon reservoir, such as a crystal lattice.It was introduced by Herbert Fröhlich in 1954 to study the effect of electron-phonon coupling on the electrical conductivity of polar crystals [5] but can also be used to describe the interaction of an impurity with the Bogoliubov phonons of an BEC [6].This interaction leads to the formation of a quasiparticle called the Bose polaron because the impurity atom becomes “dressed“ in a cloud of phonons, which changes important properties of the impurity, such as its effective mass and mobility [7]. We follow Grusdt *et al.* [7] and write the Fröhlich Hamiltonian in one dimension in the following form:

$$\hat{\mathcal{H}}_F = g_{IB}n_0 + \frac{\hat{p}^2}{2M} + \int \mathrm{d}k\omega_k\hat{a}_k^{\dagger}\hat{a}_k + \sqrt{\frac{n_0}{2\pi}}g_{IB}\int \mathrm{d}kW_k e^{ik\hat{x}}\left(\hat{a}_k + \hat{a}_{-k}^{\dagger}\right) \tag{2.17}$$

Here g_{IB} is the boson-impurity coupling constant which characterizes the strength of their interaction and n_0 is the density of the Bose gas. The second term describes the kinetic energy of the impurity of mass M in first quantized form. The third term accounts for the energy of the Bogoliubov phonons with the Bogoliubov dispersion given by

$$w_k = ck\sqrt{1 + \frac{1}{2}\xi^2k^2} \tag{2.18}$$

where we introduced ξ as the healing length and c as the speed of sound. The last term describes interactions between the impurity and the phonons. It can be thought of modeling a process where a phonon in mode k is first absorbed and then reemitted as a phonon in mode $-k$ with an appropriate change in both amplitude and phase. For this process, the scattering amplitude is

$$W_k = \left(\frac{(\xi k)^2}{2 + (\xi k)^2} \right)^{1/4} \tag{2.19}$$

and the change in phase depends on the position operator of the impurity (again in first quantization).

It has been shown that in order to accurately describe the effective mass of Bose polarons, the Fröhlich Hamiltonian alone does not suffice and two-phonon scattering terms have to be included in the Hamiltonian [7]. Then the full Hamiltonian reads

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_F + \hat{\mathcal{H}}_{\text{2ph}}. \tag{2.20}$$

It should be noted at this point that a 1D model is not only interesting from a theoretical perspective, since experimental setups in one dimension are possible and have successfully been realized [8]. The inclusion of two-phonon scattering terms leads to very good agreement of experiment and theory when the coupling between the impurity and the phonons is not too strong [7].
The aforementioned two-phonon scattering terms are quadratic and are again proportional to the boson-impurity coupling constant [7, 9]:

$$\hat{\mathcal{H}}_{\text{2ph}} = \frac{g_{IB}}{2\pi} \int \mathrm{d}k \mathrm{d}k' \left(c_k \hat{a}_k^\dagger - s_k \hat{a}_{-k} \right) \left(c_{k'} \hat{a}_{k'} - s_{k'} \hat{a}_{-k'}^\dagger \right) e^{i(k-k')x} \tag{2.21}$$

The coefficients c_k and s_k can be obtained from

$$W_k = c_k - s_k \tag{2.22a}$$
$$W_k^{-1} = c_k + s_k \tag{2.22b}$$

In principle, additional interactions between the Bogoliubov phonons have to be accounted for. However, those only become relevant when the boson-boson interaction constant g_{BB} becomes large, the density n_0 becomes small or, equivalently, the coupling strength

$$\gamma := \frac{m_B g_{BB}}{n_0} \tag{2.23}$$

is large. Because this regime will not be considered in this thesis, $\hat{\mathcal{H}}_F$ and $\hat{\mathcal{H}}_{\text{2ph}}$ model the polaron problem well for our purposes.
For future reference, we will now also introduce the 1D boson–boson s-wave scattering length

$$a_{BB} = -\frac{2}{m_B g_{BB}} \tag{2.24}$$

where

$$m_B = \frac{1}{\sqrt{2c\xi}} \tag{2.25}$$

is the mass of the bosons and the dimensionless parameter

$$\eta := \frac{g_{IB}}{g_{BB}} \tag{2.26}$$

to quantify how the interaction strength between impurity and boson compares to the strength of the boson-boson interactions.

2.2.2 The Lee-Low-Pines (LLP) Transformation

The Lee-Low-Pines (LLP) transformation [10] dramatically simplifies solving the full Hamiltonian 2.20. By making use of the fact that the total system momentum is conserved (which follows from the translational invariance of $\hat{\mathcal{H}}$) it allows us to transform to a reference frame co-moving to the impurity with the impurity in its center.
Let $\hat{p}$ be the momentum operator of the impurity and

$$\hat{p}_b = \int \mathrm{d}k k \hat{a}_k^\dagger \hat{a}_k \tag{2.27}$$

be the momentum operator of the bosons. We take advantage of the fact that the total system momentum operator is

$$\hat{P}_{\text{tot}} = \hat{p}_b + \hat{p}. \tag{2.28}$$

and then define

$$\hat{U}_{\text{LLP}} := \exp\left(i\hat{x} \cdot \hat{p}_b\right) \tag{2.29}$$

Intuitively, it is clear why this performs the desired transformation: $\hat{p}_b$ is the generator of translations for the bosons and therefore $\hat{U}_{\text{LLP}}$ translates all bosons by the (correct) amount $\hat{x}$, which is the position operator of the impurity. On the other hand, $\hat{x}$ generates translations in momentum space for the impurity and therefore $\hat{U}_{\text{LLP}}$ shifts the impurity momentum by the boson momentum.
Hence, upon applying the transformation, we have indeed transformed into a frame co-moving with the impurity where the impurity is in the center.
Lee, Low and Pines [10, eq. (8)] then went on to show that

$$\hat{U}_{\text{LLP}}^\dagger \hat{p} \hat{U}_{\text{LLP}} = \hat{p} - \hat{p}_b \tag{2.30a}$$
$$\hat{U}_{\text{LLP}}^\dagger \hat{a}_k \hat{U}_{\text{LLP}} = \hat{a} e^{ik\hat{x}}. \tag{2.30b}$$

Therefore the Hamiltonian under the LLP transformation reads:

$$\begin{aligned} \hat{U}_{\text{LLP}}^\dagger \hat{\mathcal{H}} \hat{U}_{\text{LLP}} := \hat{\mathcal{H}}_{\text{LLP}}(p) = g_{IB} n_0 + \frac{1}{2M}\left(p - \int \mathrm{d}k k \hat{a}_k^\dagger \hat{a}_k\right)^2 + \int \mathrm{d}k \omega_k \hat{a}_k^\dagger \hat{a}_k \\ + \sqrt{\frac{n_0}{2\pi}} g_{IB} \int \mathrm{d}k W_k \left(\hat{a}_k + \hat{a}_{-k}^\dagger\right) + \frac{g_{IB}}{2\pi} \int \mathrm{d}k \mathrm{d}k' \left(c_k \hat{a}_k^\dagger - s_k \hat{a}_{-k}\right)\left(c_{k'} \hat{a}_{k'} - s_{k'} \hat{a}_{-k'}^\dagger\right) \end{aligned} \tag{2.31}$$

In the new frame the impurity momentum is a constant of motion because in the original frame the total momentum was a constant of motion. This allows us to replace the impurity momentum with the c-number p in the Hamiltonian 2.31 which will be referred to as LLP-Hamiltonian.

SECTION 3 DERIVING THE FLOW EQUATIONS

This section explains how the flow equations can be derived. For detailed calculations, please refer to the Appendix A.
First, we will consider the purely quadratic case without $\hat{n}$-dependencies and discuss how the flow equations can be applied to the Bose polaron problem in the heavy impurity limit. Then a possible exact diagonalization procedure will be explained, as it will serve as our benchmark for the flow equations in Section 4.
Second, we will consider the case with $\hat{n}$-dependence, such as the LLP-Hamiltonian with finite impurity mass. Again, we will only sketch the steps necessary to arrive at the flow equations while the full calculations can be found in the Appendix A.2. These equations will not be put to the test in the scope of this thesis, but we will try to assess the prospects of successfully applying them to the LLP-Hamiltonian at the end of this section.

3.1 Purely Quadratic Case

3.1.1 Applying the Formalism

In the purely quadratic case where the coefficients do not depend on the occupation numbers and where a static impurity is considered, exact flow equations A.14a-A.14e can be derived. In particular, the flow Hamiltonian $\hat{\mathcal{H}}(\lambda)$ is of the same quadratic form as the original Hamiltonian

$$\hat{\mathcal{H}} := \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{\text{int}} := \sum_k \omega_k \hat{a}_k^\dagger \hat{a}_k + \sum_{q\neq q'} V_{q,q'} \hat{a}_q^\dagger \hat{a}_{q'} + \sum_{p,p'} \left(W_{p,p'} \hat{a}_p^\dagger \hat{a}_{p'}^\dagger + \text{h.c.} \right) \tag{3.1}$$

and no truncation scheme as discussed in Section 2.1.3 has to be employed. For details on the calculations, see Section A.1.

We followed precisely the recipe introduced in Section 2.1.1: First the canonical generator 2.7 is evaluated (see equation A.2). Then the derivative of the flow Hamiltonian is determined by the commutator of the generator and the Hamiltonian in equation 2.3. The relevant terms A.5-A.8 are evaluated separately by only making use of the bosonic commutation relations. The flow equations then follow by a simple comparison of coefficients from the quadratic (plus a constant energy ϵ) ansatz for the flow Hamiltonian.

Note that the resulting flow equations A.14a-A.14e suggest that they are exact in the sense that if the flow is completely traversed, the flow Hamiltonian will be exactly diagonal because in first order

$$V_{q,q'} \sim \exp\left(-(\omega_q - \omega_{q'})^2\right) \xrightarrow{\lambda\to\infty} 0 \tag{3.2a}$$

$$W_{p,p'} \sim \exp\left(-(\omega_p + \omega_{p'})^2\right) \xrightarrow{\lambda\to\infty} 0, \tag{3.2b}$$

assuming that there are no degeneracies. If there were, it would mean that $(\omega_q - \omega_{q'})^2 = 0$ for some pair q, q' and that the corresponding matrix element $V_{q,q'}$ is not exponentially suppressed in first order of the flow equations. Alternatively, near-degeneracies may render the convergence

so slow that the corresponding matrix elements decay so slowly that the flow would have to be traversed an unreasonable or impractical distance to achieve sufficient suppression. Fortunately, the flow equations *can* still be successful in some cases [11] because the second order terms (terms that come from the commutator of $\hat{\eta}$ and $\hat{\mathcal{H}}_{\text{int}}$) coupling the ODEs for the different matrix elements are non-trivial and might, depending on the initial condition, even sufficiently suppress degenerate matrix elements. It follows that applying the equations to a concrete problem provides the best test of their performance and convergence properties.
Also, checking the condition 2.9 is indeed a strong indicator for good convergence properties but does not necessarily imply that all elements in $\hat{\mathcal{H}}_{\text{int}}$ converge to 0 when degeneracies are present, which is why we do not explicitly evaluate of the conditions 2.10 that in turn imply 2.9.

3.1.2 Application to the 1D Bose Polaron Model

In the heavy impurity limit $M \to \infty$, the dependence of the occupation numbers in the LLP-Hamiltonian 2.31 vanishes and we get an Hamiltonian which differs from the purely quadratic form we discussed in the last section only by linear terms. Before we discuss the significance of these linear term we will address the fact that the integrals in there have to discretized for numerical treatment.
To this end, we will restrict ourselves to a discrete number of modes k where $0 < \Lambda_{IR} \leq |k| \leq \Lambda_{UV} < \infty$. Λ_{IR} denotes the infrared and Λ_{UV} denotes the ultraviolet cut-off. We will work with values $\Lambda_{IR}\xi = 10^{-1}$ and $\Lambda_{UV}\xi = 10^{1}$ because this range includes phonons with momenta $k \sim 1/\xi$ which are critical for defining essential properties of the Bose polaron [7].
Of course, considering a larger number of k values is generally better, but involves significant computational cost. That is why the spacing $\Delta k = \frac{2\pi}{L}$ (where L is a constant which describes the size of the system) between two adjacent k values will be not be chosen too small. Reasonable values are of order $\Delta k \sim 10^{-1}\xi$.
These values are small enough that we are allowed to approximate integrals by sums

$$\int \mathrm{d}k \to \Delta k \sum_k \tag{3.3}$$

ranging over a discrete and finite grid of size $N \in \mathbb{N}$. The commutation relations of the creation and annihilation operators in $\hat{\mathcal{H}}_{\text{LLP}}$ are $\left[\hat{a}_k, \hat{a}^\dagger_{k'}\right] = \delta(k-k')$. Our new discrete operators will obey the same commutation relation with a Kronecker-delta instead of the Dirac-delta. The transition from the continuous to the discrete case is done by coarsening the annihilation and creation operators

$$\hat{a}_k^{(\dagger)} \to \frac{1}{\sqrt{\Delta k}} \hat{a}_k^{(\dagger)} \tag{3.4}$$

(see [9, eq. (7)]) and the LLP-Hamiltonian becomes:

$$\begin{aligned} \hat{\mathcal{H}}_{\text{LLP}}^{\text{discr.}} &= g_{IB} n_0 + \sum_k \omega_k \hat{a}_k^\dagger \hat{a}_k + \sqrt{\frac{n_0 \Delta k}{2\pi}} g_{IB} \sum_k W_k \left(\hat{a}_k + \hat{a}^\dagger_{-k}\right) \\ &+ \frac{g_{IB}\Delta k}{2\pi} \sum_{k,k'} \left(c_k \hat{a}^\dagger_k - s_k \hat{a}_{-k}\right)\left(c_{k'}\hat{a}_{k'} - s_{k'}\hat{a}^\dagger_{-k'}\right) \end{aligned} \tag{3.5}$$

It would be conceivable to extend our flow equations to allow for linear terms in our Hamiltonian. In this case, it would again be possible to obtain a closed set of flow equations.

However, this can be avoided because the linear terms $W_k \left(\hat{a}_k + \hat{a}^\dagger_{-k}\right)$ can be eliminated by applying the displacement operator

$$\hat{D}(\underline{\alpha}) := \exp\left(\sum_k \alpha_k \hat{a}^\dagger_k - \text{h.c.}\right) = \exp\left(-\underline{\alpha}^\dagger \underline{\underline{\Omega}}\ \underline{\hat{a}}\right) \tag{3.6}$$

to the discrete LLP-Hamiltonian [9]. Here we introduced the symplectic $2N \times 2N$ matrix

$$\underline{\underline{\Omega}} = \begin{pmatrix} \underline{\underline{E}}_N & 0 \\ 0 & -\underline{\underline{E}}_N \end{pmatrix} \tag{3.7}$$

and the notation

$$\underline{\hat{a}} = \left(\hat{a}_{k_1}, ..., \hat{a}_{k_N}, \hat{a}^\dagger_{k_1}, ..., \hat{a}^\dagger_{k_N}\right)^T \tag{3.8}$$

for vectors of creation and annihilation operators as well as

$$\underline{\alpha} = \left(\alpha_{k_1}, ..., \alpha_{k_N}, \alpha^*_{k_1}, ..., \alpha^*_{k_N}\right)^T \in \mathbb{C}^{2N} \tag{3.9}$$

for vectors of c-numbers.

The displacement operator shifts creation and annihilation operators by a given c-number:

$$\hat{D}^\dagger(\underline{\alpha})\hat{a}_{k_i}\hat{D}(\underline{\alpha}) = \hat{a}_{k_i} + \alpha_{k_i} \tag{3.10a}$$
$$\hat{D}^\dagger(\underline{\alpha})\hat{a}^\dagger_{k_i}\hat{D}(\underline{\alpha}) = \hat{a}^\dagger_{k_i} + \alpha^*_{k_i} \tag{3.10b}$$

This can be proved readily with the help of the Baker-Campbell-Hausdorff formula. Simliarly, one can convince oneself that

$$\hat{D}(\underline{\alpha})\hat{a}_{k_i}\hat{D}^\dagger(\underline{\alpha}) = \hat{a}_{k_i} - \alpha_{k_i} \tag{3.11a}$$
$$\hat{D}(\underline{\alpha})\hat{a}^\dagger_{k_i}\hat{D}^\dagger(\underline{\alpha}) = \hat{a}^\dagger_{k_i} - \alpha^*_{k_i}. \tag{3.11b}$$

From this it follows immediately that the displacement operator is unitary, and therefore applying it to the discrete LLP-Hamiltonian does not change its spectrum. We obtain:

$$\begin{aligned}\hat{D}^\dagger(\underline{\alpha})\hat{\mathcal{H}}^{\text{discr.}}_{\text{LLP}}\hat{D}(\underline{\alpha}) = g_{IB}n_0 &+ \sum_k \omega_k(\hat{a}^\dagger_k + \alpha^*_k)(\hat{a}_k + \alpha_k) \\ &+ \sqrt{\frac{n_0\Delta k}{2\pi}}g_{IB}\sum_k W_k\left(\hat{a}_k + \hat{a}^\dagger_{-k} + \alpha_k + \alpha^*_{-k}\right) \\ &+ \frac{g_{IB}\Delta k}{2\pi}\sum_{k,k'}\left(c_k(\hat{a}^\dagger_k + \alpha^*_k) - s_k(\hat{a}_{-k} + \alpha_{-k})\right)\left(c_{k'}(\hat{a}_{k'} + \alpha_{k'}) - s_{k'}(\hat{a}^\dagger_{-k'} + \alpha^*_{-k'})\right)\end{aligned} \tag{3.12}$$

After using of the symmetry $W_k = W_{-k}$ and the associated symmetries for c_k and s_k and reordering the terms, the condition that the displacement transformation turns our discrete LLP-Hamiltonian into a purely quadratic Hamiltonian reads:

$$\forall k:\ 0 \stackrel{!}{=} \omega_k\alpha^*_k + \tilde{W}^{(0)}_k + \sum_{k'} V^{(0)}_{k',k}\alpha^*_{k'} + \sum_{k'}\alpha_{k'}\left(W^{(0)}_{k,k'} + W^{(0)}_{k',k}\right) \tag{3.13}$$

Here we defined

$$\tilde{W}^{(0)}_k := \frac{g_{IB}}{2\pi}\sqrt{n_0\Delta k}W_k \tag{3.14a}$$

$$V^{(0)}_{k,k'} := \frac{g_{IB}}{2\pi}\Delta k(c_k c_{k'} + s_k s_{k'}) \tag{3.14b}$$
$$W^{(0)}_{k,k'} := -\frac{g_{IB}}{2\pi}\Delta k s_k c_{k'}, \tag{3.14c}$$

adopting the notation in the generic quadratic Hamiltonian 3.1.
The condition 3.13 can be solved very efficiently and inexpensively using existing solvers for linear systems of equations, which is why the approach involving the displacement operator is generally favored to solving a larger set of ODEs to also suppress the linear parts in the flow. The solution $\underline{\alpha}$ obtained this way can be substituted into the Hamiltonian which is then of purely quadratic form: [(1)]

$$\hat{\mathcal{H}}^{\text{quadr.}}_{\text{LLP}} = \sum_k (\omega_k + V^{(0)}_{k,k})\hat{a}^\dagger_k \hat{a}_k + \sum_{q\neq q'} V^{(0)}_{q,q'}\hat{a}^\dagger_q \hat{a}_{q'} + \sum_{p,p'}\left(W^{(0)}_{p,p'}\hat{a}^\dagger_p \hat{a}^\dagger_{p'} + \text{h.c.}\right) + g_{IB}n_0 + \frac{g_{IB}}{2\pi}\Delta k \sum_k s_k^2 \tag{3.15}$$

The flow equations A.14a-A.14e for $\hat{\mathcal{H}}^{\text{quadr.}}_{\text{LLP}}$ define a system of $(2N^2+N+1) \in \mathcal{O}(N^2)$ ODEs and can be solved numerically using preexisting ODE solvers. We will use the `ODEProblem` class from julia's `DifferentialEquations.jl` library in combination with the `Tsit5` integrator, a Runge-Kutta integrator of order 5(4) [12], for its general robustness and versatility[(2)].

Finally, concrete parameters for $c, \xi, \eta, \gamma, n_0$ have to be chosen. We refer to Catani's experimental results and set $\gamma = 0.438$, $n_0\xi = 1.05$ and choose our units s.t. $c = \xi = 1$ [7, 8]. Then the other constants introduced before can be calculated using the expressions introduced in Section 2.2.1.

3.1.3 Benchmark: Exact Diagonalization via Bogoliubov Transformation

The purely quadratic Hamiltonian 3.15 can be exactly diagonalized by Bogoliubov Transformations [9, 13, 14]. Using the short hand notations 3.8 and 3.9 as well as 3.7, our quadratic Hamiltonian can be written in the form:

$$\hat{\mathcal{H}} = E_0 + \sum_{k,k'}\hat{a}^\dagger_k A_{k,k'}\hat{a}_{k'} + \frac{1}{2}\sum_{k,k'}\left(\hat{a}^\dagger_k B_{k,k'}\hat{a}^\dagger_{k'} + \text{h.c.}\right) \tag{3.16}$$
$$= E_0 - \frac{1}{2}\sum_k A_{k,k} + \frac{1}{2}\underline{\hat{a}^\dagger}\begin{pmatrix} A & B \\ B^* & A^*\end{pmatrix}\underline{\hat{a}} \tag{3.17}$$
$$= E_0 - \frac{1}{2}\sum_k A_{k,k} + \frac{1}{2}\underline{\hat{a}^\dagger}\;\underline{\underline{\Omega}}\;\underline{\underline{\mathscr{H}}}\;\underline{\hat{a}} \tag{3.18}$$

where we introduced

$$\underline{\underline{\mathscr{H}}} := \begin{pmatrix} A & B \\ -B^* & -A^*\end{pmatrix} \in \mathbb{C}^{2N\times 2N} \tag{3.19}$$

and

$$A = \left(A_{k,k'}\right)_{k,k'=1,\dots,N}\,,\; B = \left(B_{k,k'}\right)_{k,k'=1,\dots,N}\,. \tag{3.20}$$

Hermiticity of the Hamiltonian requires $A^\dagger = A$ and B can and must always be chosen s.t. $B^T = B$. This is because $[\hat{a}^\dagger_k, \hat{a}^\dagger_{k'}] = [\hat{a}_k, \hat{a}_{k'}] = 0$, so if we start with a non-symmetric B we can

(1) The relevant source code "displacement_transformation.jl" for performing the displacement transformation and initializing the parameters can be found in the GitHub Repository `https://github.com/SufficientlySmooth/Bachelor-Thesis-Numerics`.

(2) For the numerics we again refer to the source code "Solve_Flow_Equations.jl" in `https://github.com/SufficientlySmooth/Bachelor-Thesis-Numerics`

always symmetrize $B \to \frac{1}{2}\left(B + B^T\right)$.
As shown in [9, 13], the Bogoliubov Transformation

$$\underline{\hat{a}} \mapsto \underline{\underline{U_B}}\,\underline{\hat{a}} \tag{3.21}$$

defined by the matrix

$$\underline{\underline{U_B}} := \begin{pmatrix} U^* & -V^* \\ -V & U \end{pmatrix} \tag{3.22}$$

conserves the bosonic commutation relations iff $\underline{\underline{U_B}}$ is a symplectic matrix:

$$\underline{\underline{U_B}}\,\underline{\underline{\Omega}}\,\underline{\underline{U_B}}^\dagger = \underline{\underline{\Omega}}. \tag{3.23}$$

There exists an $\underline{\underline{U_B}}$ s.t.

$$\underline{\underline{U_B}}^\dagger \underline{\underline{\Omega}}\,\underline{\underline{\mathscr{H}}}\,\underline{\underline{U_B}} = \mathrm{diag}\left(\lambda_1, ..., \lambda_N, \lambda_1^*, ..., \lambda_N^*\right) \tag{3.24}$$

The values $\{\lambda_j^{(*)}\}_{j=1,...,N}$ can be obtained by solving the eigenvalue problem of $\underline{\underline{\mathscr{H}}}$. The eigenvectors then constitute the columns $\underline{\underline{U_B}}$. If all eigenvalues are real, the ground state energy reads:

$$E_{GS} = E_0 - \frac{1}{2}\sum_k A_{k,k} + \sum_k \lambda_k \tag{3.25}$$

Furthermore, we can make use of the fact that the real eigenvalues always occur in pairs $(\lambda_j, -\lambda_j^*)$. To see this, we introduce the operator

$$\underline{\underline{\vartheta}} : \mathbb{C}^{2N} \to \mathbb{C}^{2N}, \begin{pmatrix} \underline{u} \\ \underline{v} \end{pmatrix} \mapsto \begin{pmatrix} \underline{v}^* \\ \underline{u}^* \end{pmatrix} \text{ where } \underline{u}, \underline{v} \in \mathbb{C}^N. \tag{3.26}$$

The relations

$$\left\{\underline{\underline{\vartheta}}, \underline{\underline{\Omega}}\right\} = 0 \tag{3.27}$$

and

$$\left[\underline{\underline{\Omega}}\,\underline{\underline{\mathscr{H}}}, \underline{\underline{\vartheta}}\right] = 0 \tag{3.28}$$

imply that if $\underline{x}$ is an eigenvector of $\underline{\underline{\Omega}}\,\underline{\underline{\mathscr{H}}}$ corresponding to the eigenvalue λ, then $\underline{\underline{\vartheta}}\,\underline{x}$ is an eigenvector corresponding to the eigenvalue $-\lambda^*$. The λ_j in equation 3.24 are characterized by the fact that their associated eigenvectors $\underline{w}_j$ have positive matrix elements:

$$\underline{w}_j^\dagger \underline{\underline{\Omega}}\,\underline{w}_j > 0 \tag{3.29}$$

The corresponding eigenvector to $-\lambda_j^*$ always has a negative matrix element. This follows immediately from the relation 3.27 and the fact that obviously $\underline{\underline{\vartheta}}^2 = \underline{\underline{E}}_{2N}$.
It is necessary to classify the eigenvalues in this way, because only then the symplectic condition 3.22 holds.

This condition cannot be satisfied if not all eigenvalues are real. For example, if one eigenvalue is in $i\mathbb{R}$, the corresponding state is clearly not describable by ladder operators, i.e. the spectrum is no longer discretized, and is (dynamically) unstable. Then any small perturbation might irreversibly change the systems state from equilibrium [14]. If at least one real eigenvalue is strictly negative, this indicates "a state [which] cannot be created adiabatically by gradually reducing the entropy associated with the thermal energy" [14]. This is called a thermodynamic instability. In our case this means the existence of a bound state whose binding energy is given by the (single) negative eigenvalue.
Both types of instabilities are observed when the results of a Bogoliubov transformation are compared with the flow equations in Section 4.

3.2 With Dependence on the Occupation Numbers

3.2.1 Useful Preliminaries

Consider some operator $\hat{f}$ which depends on a single number operator $\hat{n} = \hat{a}^\dagger \hat{a}$. The following relations will be used when deriving the flow equations:

$$\left[\hat{a}^\dagger, \hat{f}(\hat{n})\right] = \hat{a}^\dagger \left(\hat{f}(\hat{n}) - \hat{f}(\hat{n}+1)\right) \tag{3.30a}$$

$$\left[\hat{a}, \hat{f}(\hat{n})\right] = \hat{a} \left(\hat{f}(\hat{n}) - \hat{f}(\hat{n}-1)\right) \tag{3.30b}$$

$$\left[\hat{f}(\hat{n}), \hat{a}^\dagger\right] = \left(\hat{f}(\hat{n}) - \hat{f}(\hat{n}-1)\right) \hat{a}^\dagger \tag{3.30c}$$

$$\left[\hat{f}(\hat{n}), \hat{a}\right] = \left(\hat{f}(\hat{n}) - \hat{f}(\hat{n}+1)\right) \hat{a} \tag{3.30d}$$

These can be proved by induction for $\hat{f}(\hat{n}) = \hat{n}^k, k \in \mathbb{N}$ and from there simply extended to well-behaved $\hat{f}$ via power series. Equations 3.30 are still valid for functions depending on $\{\hat{n}_k\}_k$, because all $\hat{n}_k$ pairwise commute.
We will write $\hat{f}\left(\hat{n}_1, \hat{n}_2, \ldots\right) =: \hat{f}$ and $\hat{f}\left(\hat{n}_1, \hat{n}_2, \ldots, \hat{n}_k \pm 1, \hat{n}_{k+1}, \ldots\right) =: \hat{f}(\hat{n}_k \pm 1)$. Moreover, we define $\hat{f}(\hat{n}_k \pm 1, \hat{n}_k \pm 1) := \hat{f}(\hat{n}_k \pm 2)$ in this notation.
A simple induction for $n_1, n_2 \in \mathbb{N}_0$ yields the following useful relation:

$$\begin{aligned}&\left[\hat{f}(\hat{n}), \hat{a}^\dagger_{k_1}\hat{a}^\dagger_{k_2}\cdots\hat{a}^\dagger_{k_{n_1}}\hat{a}_{k_1}\hat{a}_{k_2}\cdots\hat{a}_{k_{n_2}}\right]\\ &= \left(\hat{f} - \hat{f}\left(\hat{n}_{k_1}-1, \hat{n}_{k_2}-1, \ldots, \hat{n}_{k_{n_1}}, \hat{n}_{k_1}+1, \hat{n}_{k_2}+1 \ldots \hat{n}_{k_{n_2}}+1\right)\right) \hat{a}^\dagger_{k_1}\hat{a}^\dagger_{k_2}\cdots\hat{a}^\dagger_{k_{n_1}}\hat{a}_{k_1}\hat{a}_{k_2}\cdots\hat{a}_{k_{n_2}}\end{aligned} \tag{3.31}$$

Furthermore, applying the recurrence relation 2.15 can be used to successively normal order operators. Let $\hat{O} := \hat{a}^\dagger_{k_1}\hat{a}^\dagger_{k_2}\cdots\hat{a}^\dagger_{k_{n_1}}\hat{a}_{k_1}\hat{a}_{k_2}\cdots\hat{a}_{k_{n_2}}$. Then normal ordering w.r.t. the vacuum yields:

$$\begin{aligned}\hat{a}_q : \hat{O} : &=: \hat{O}\hat{a}_q : + \sum_k : \frac{\partial \hat{O}}{\partial \hat{a}^\dagger_k} :\\ &=: \hat{O}\hat{a}_q : + \sum_{i=1}^{n_1} \delta_{k_i,q} : \hat{a}^\dagger_{k_1}\hat{a}^\dagger_{k_2}\cdots\hat{a}^\dagger_{k_{i-1}}\hat{a}^\dagger_{k_{i+1}}\cdots\hat{a}^\dagger_{k_{n_1}}\hat{a}_{k_1}\hat{a}_{k_2}\cdots\hat{a}_{k_{n_2}} :\end{aligned} \tag{3.32a}$$

$$\hat{a}^\dagger_q : \hat{O} : =: \hat{a}^\dagger_q \hat{O} : \tag{3.32b}$$

3.2.2 Applying the Formalism

Following the same same procedure as in the heavy impurity limit, we first start by evaluating the canonical generator. It turns out that $\hat{\eta}$ conserves the structure of the original Hamiltonian (cf. eq. A.22) while the flow Hamiltonian does not (cf. eq. A.25a ff.). Therefore, the sequence of higher and higher order terms has to be truncated at some point as discussed in Section 2.1.3. Three simplifications will be made in order to obtain closed expressions for the flow equations:

- We will use a naïve and only partial normal ordering prescription where the contractions are defined with respect to the vacuum state and not the ground state of the diagonal Hamiltonian.
- The expressions we consider will not be fully normal ordered because the coefficients $\hat{\omega}_k$, $\hat{W}_{p,p'}$, and $\hat{V}_{q,q'}$ are not normal ordered. This saves the rather tedious process of normal

ordering arbitrary functions of number operators, which involves expanding the operator into a Newton series [15], but may render the sequence less well-behaved when truncated to an order as low as two.

- We will neglect all terms of order four or higher, i.e. terms which contain products of four creation/ annihilation operators or more.

After evaluating the commutator of $\hat{\eta}$ and the full Hamiltonian where we made frequent use of the equations in 3.30, we arrive at the flow equations A.59a-A.59d. In first order, we can expect the off-diagonal elements to vanish if $\hat{H} \neq \hat{H}(\hat{n}_q - 1, \hat{n}_{q'} + 1)\ \forall q, q', q \neq q'$ and $\hat{H} \neq \hat{H}(\hat{n}_p \pm 1, \hat{n}_{p'} \pm 1)\ \forall p, p'$ with

$$\hat{H} := \sum_k \hat{\omega}_k : \hat{a}_k^\dagger \hat{a}_k : + \hat{\epsilon}. \tag{3.33}$$

The next section will address whether we can expect this to hold true.

3.2.3 Discussion of the Applicability of the Flow Equations

Discretizing $\hat{\mathcal{H}}_{\mathrm{LLP}}(p)$ can be done analogously to how it was done in the heavy impurity limit. We obtain:

$$\begin{aligned}\hat{\mathcal{H}}_{\mathrm{LLP}}^{\mathrm{discr.}}(P) &= g_{IB} n_0 + \frac{1}{2M}\left(p - \sum_k k \hat{a}_k^\dagger \hat{a}_k\right)^2 + \sum_k \omega_k \hat{a}_k^\dagger \hat{a}_k \\ &+ \sqrt{\frac{n_0 \Delta k}{2\pi}} g_{IB} \sum_k W_k \left(\hat{a}_k + \hat{a}_{-k}^\dagger\right) + \frac{g_{IB}\Delta k}{2\pi} \sum_{k,k'} \left(c_k \hat{a}_k^\dagger - s_k \hat{a}_{-k}\right)\left(c_{k'} \hat{a}_{k'} - s_{k'} \hat{a}_{-k'}^\dagger\right)\end{aligned} \tag{3.34}$$

Because $\hat{n}_k = \hat{a}_k^\dagger \hat{a}_k$ this can be written in the following way:

$$\begin{aligned}\hat{\mathcal{H}}_{\mathrm{LLP}}^{\mathrm{discr.}}(p) &= \hat{H}(p) + \frac{g_{IB}\Delta k}{2\pi} \sum_{k \neq k'} (c_k c_{k'} + s_k s_{k'}) \hat{a}_k^\dagger \hat{a}_{k'} \\ &+ \sqrt{\frac{n_0 \Delta k}{2\pi}} g_{IB} \sum_k W_k \left(\hat{a}_k + \hat{a}_{-k}^\dagger\right) - \frac{g_{IB}\Delta k}{2\pi} \sum_{k,k'} \left(c_k s_{k'} \hat{a}_k^\dagger \hat{a}_{k'}^\dagger + s_k c_{k'} \hat{a}_k \hat{a}_{k'}\right)\end{aligned} \tag{3.35}$$

$\hat{H}$ contains the parts of the Hamiltonian which can be written in terms of number operators:

$$\hat{H}(p) := g_{IB} n_0 + \frac{g_{IB}}{2\pi}\Delta k \sum_k s_k^2 + \frac{1}{2M}\left(p - \sum_k k \hat{n}_k\right)^2 + \sum_k \omega_k \hat{n}_k + \frac{g_{IB}\Delta k}{2\pi} \sum_k (c_k^2 + s_k^2)\hat{n}_k \tag{3.36}$$

Then for $q, q', q \neq q'$ we get:

$$\begin{aligned}\hat{H}(p, \hat{n}_q - 1, \hat{n}_{q'} + 1) - \hat{H}(p) &= \frac{1}{2M}\left(p + q - q' - \sum_k k \hat{n}_k\right)^2 - \frac{1}{2M}\left(p - \sum_k k \hat{n}_k\right)^2 \\ &+ \omega_{q'} - \omega_q + \frac{g_{IB}\Delta k}{2\pi}(c_{q'}^2 + s_{q'}^2 - c_q^2 - s_q^2) \end{aligned} \tag{3.37}$$

$$= \frac{q - q'}{2M}\left(2p - 2\sum_k k \hat{n}_k + q - q'\right) + \omega_{q'} - \omega_q + \frac{g_{IB}\Delta k}{2\pi}(c_{q'}^2 + s_{q'}^2 - c_q^2 - s_q^2) \tag{3.38}$$

So in first order we can expect:

$$\hat{V}_{q,q'} \sim \exp\left(-\left(\frac{q-q'}{2M}\left(2p - 2\sum_k k\hat{n}_k + q - q'\right) + \omega_{q'} - \omega_q + \frac{g_{IB}\Delta k}{2\pi}(c_{q'}^2 + s_{q'}^2 - c_q^2 - s_q^2)\right)^2\right) \tag{3.39}$$

Not worrying too much about the mathematical details like the fact that 3.38 defines an unbounded operator because the number operators are unbounded, we can, loosely using the spectral mapping theorem [16] and the spectral radius formula, conclude that $\hat{V}_{q,q'}$ should vanish if the spectrum of the argument of the exponential is a subset of $\mathbb{R}_{<0}$. Due to the square in the exponent the inclusion in $\mathbb{R}_{\leq 0}$ is clear.
Considering the vacuum, 0 is in the spectrum of 3.38 iff

$$\frac{q-q'}{2M}\left(2p + q - q'\right) + \omega_{q'} - \omega_q + \frac{g_{IB}\Delta k}{2\pi}(c_{q'}^2 + s_{q'}^2 - c_q^2 - s_q^2) = 0. \tag{3.40}$$

For fixed q, q' this condition can hold for at most one p. For most other values of p, 3.39 should be relatively well-behaved. The same reasoning applies to $\hat{H}(p, \hat{n}_p \pm 1, \hat{n}_{p'} \pm 1) - \hat{H}(p)$ and $\hat{W}_{p,p'}$ to reach a similar conclusion. Of course, for the countable number of original eigenstates different from the vacuum analogous conditions to equation 3.40 can be derived.
This gives hope that flow equations A.59a-A.59d converge to a diagonal Hamiltonian as desired for all but a countable number of values of p. Even if not, the second order terms of the flow equations may be enough to suppress the off-diagonal elements. So again, the convergence is best tested by numerically solving the flow equations, which will not be done in this thesis.

This involves the following steps:

1. First, the displacement operator has to be applied to the full Hamiltonian. The condition that we want all linear terms to vanish will give a set of N non-linear equations which are again to be solved for $\underline{\alpha}$.

2. Then each coefficient appearing in the full Hamiltonian must be expanded in powers of $\hat{n}_k$. The resulting power series should not be truncated at less than quadratic order, otherwise nonlinearities will not be captured and the problem can be reduced to the case where none of the coefficients depend on the occupation numbers.
Even the coefficients which do not depend on the occupation numbers (such as ω_k, c_k, s_k) must be expanded in terms of $\hat{n}_k$ because they can (and generally will) pick up non-trivial $\hat{n}$-dependencies during the flow.

3. The flow equations A.59a-A.59d (which define the flow for *operators*) must be reduced to flow equations for the *expansion coefficients* (see Appendix A.2.4). A unpleasant but crucial point is that when the operators are expanded to order n, the number of evolution coefficients is $\mathcal{O}(N^n)$. But the number of operators is already $\mathcal{O}(N^2)$, so solving the resulting $\mathcal{O}(N^{2n})$ ODEs will be computationally intensive.

4. The resulting system of coupled ODEs can then be solved as in the heavy impurity limit.

Instead of steps 2 and 3, an alternative and promising simplification of the flow equations might be to expand them in order $1/M$: The flow equations with $\hat{n}$-dependence contain the case without $\hat{n}$-dependence as a special case, and we know that these flow equations are exact for $1/M = 0$. Dropping all terms of $\mathcal{O}(1/M^2)$ or higher may lead to flow equations that do not require strict assumptions about or simplifications of the exact $\hat{n}$-dependence of the matrix elements to solve, as had to be made in step 2 above.

SECTION 4
APPLYING THE FLOW EQUATIONS: 1D BOSE POLARON IN THE HEAVY IMPURITY LIMIT

In this section we will present the results of applying the flow equations the LLP-Hamiltonian in the heavy impurity limit. We will see that under certain conditions excellent agreement of the ground state energy and the full spectrum as determined by the flow equations can be obtained when compared with the result of exact diagonalization using a Bogoliubov transformation. The quality of the agreement depends strongly on how long the flow is traversed, which is why we will close by qualitatively analyzing the convergence properties of the flow equations.

4.1 In Combination with a Bogoliubov Transformation

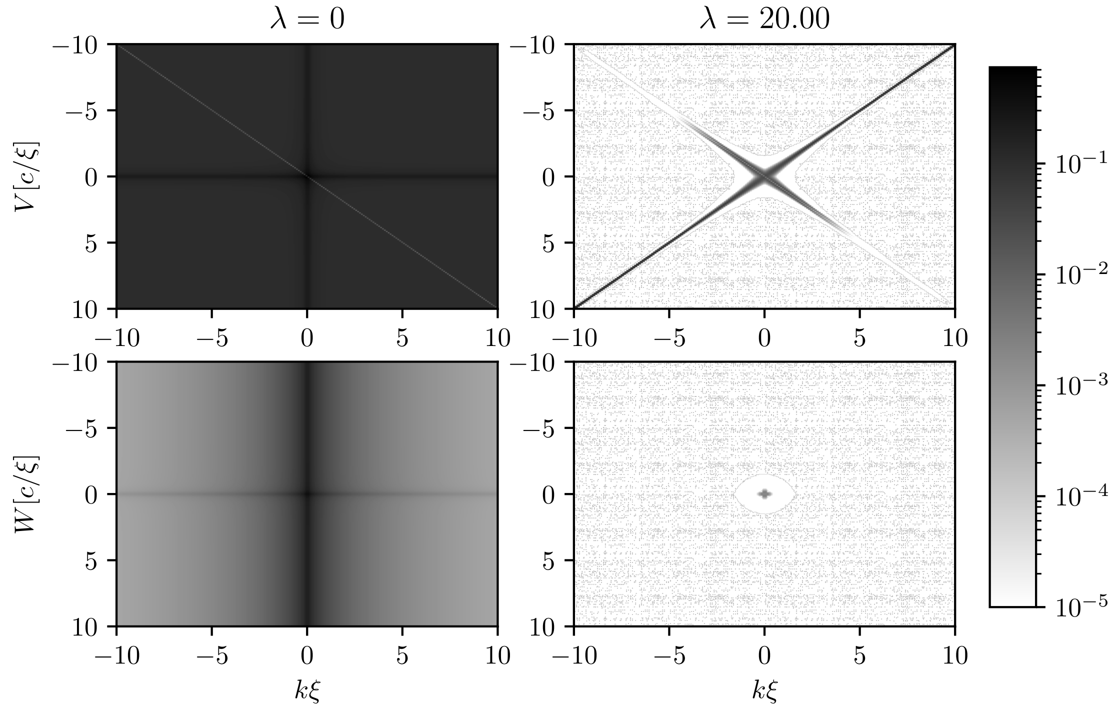

Figure 4.1: Visualization of how the flow progresses for $\eta = 10$, by shading larger absolute values for $V_{k,k'}, W_{k,k'}$ darker. It is of note that on the ordinate and abscissa $0 \hat{=} \pm \lambda_{IR}\xi = \pm 0.1$. We see that good suppression occurs for all $W_{k,k'}$, with slower convergence for smaller $|k|, |k'|$. Meanwhile, the matrix elements near the diagonal $V_{k,k}$ decay significantly slower than most off-diagonal elements. Also, matrix elements $V_{k,-k}$ converge, but to a value different from zero. Note that the values of V near the main diagonal would become even smaller if the flow were to progress further. This can be checked numerically by checking if $\text{sgn}\,(V_{k,k'}) = -\text{sgn}\,(\partial_\lambda V_{k,k'})$.

As seen in Figure 4.1, the flow equations achieve the desired diagonalization except for terms $V_{k,-k}$. This is because $\omega_k = \omega_{-k} \forall k$ implies that the first order contribution in $\partial_\lambda V_{k,-k} = ...$ vanishes. This is not a problem for the main diagonal terms $V_{k,k}$ because those have been "manually" set to zero by moving them in the diagonal part $\hat{\mathcal{H}}_0$ of the Hamiltonian.
We can conclude that if we were not to stop the flow at a finite λ, our Hamiltonian would be approximately of the form

$$\hat{\mathcal{H}}' := \sum_k \left(\tilde{\omega}_k \hat{a}_k^\dagger \hat{a}_k + \tilde{V}_{k,-k} \hat{a}_k^\dagger \hat{a}_{-k} \right) \tag{4.1}$$

for some $\tilde{\omega}_k, \tilde{V}_{k,-k}$.
In principle, this could be brought into diagonal form by performing a Bogoliubov transformation for each summand by hand. But we will use the more general Bogoliubov transformation 3.21[(1)] instead because, as can be seen in the Figure 4.2, there are interaction strengths where not all $W_{k,k'}$ vanish.

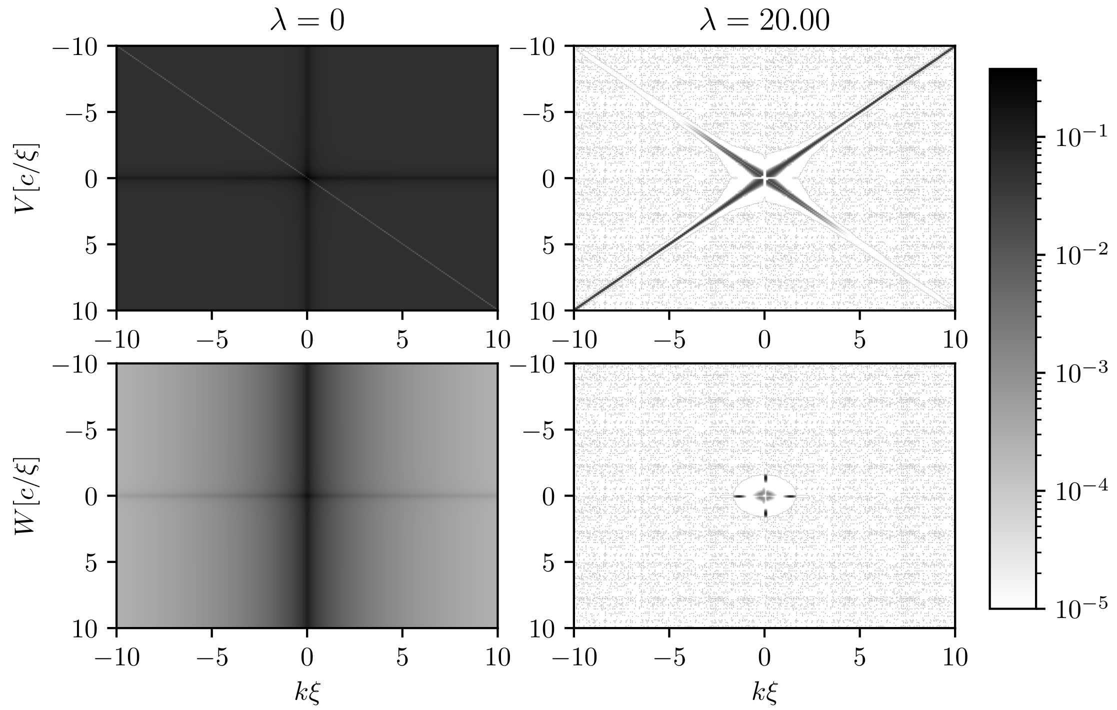

Figure 4.2: Visualization of the flow progression for $\eta = -5.1$ analogous to Figure 4.1. We can see that for this η not all of the $W_{k,k'}$ vanish, which may be related to the fact that we are now observing a system with a thermodynamic instability, as will become clear later on. The entailing negative eigenenergies can lead to unexpected behavior of the second order terms in the flow equations.

4.1.1 Ground State Energy for Different Interaction Strengths

One might think that we are therefore at an inherently poor starting point for making predictions about interesting system properties such as the ground state energy. However, it turns out that the many matrix elements that are actually suppressed sufficiently quickly dominate

(1) For the numerics we refer to the source code "Bogoliubov_Transformation.py" in `https://github.com/SufficientlySmooth/Bachelor-Thesis-Numerics`

the behavior for the ground state energy to such an extent that if one discards all off-diagonal elements (regardless of their magnitude) after a certain point in the flow, very good agreement with the ground state energy predicted by a Bogoliubov transformation can be reached.

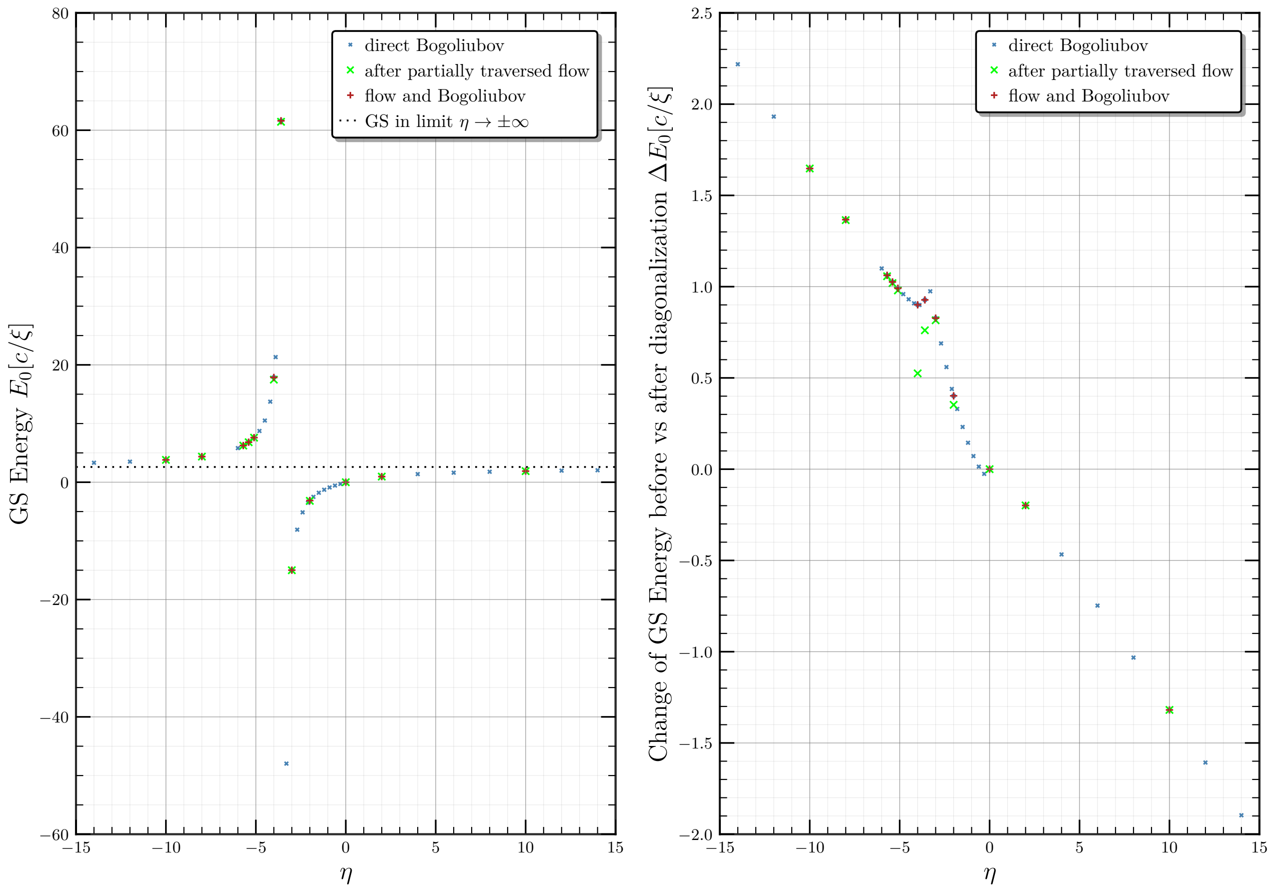

Figure 4.3: The left subplot shows the ground state energy for different η. The results are obtained via three different approaches: First a Bogoliubov transformation is applied directly to the Hamiltonian 3.15. Second, the ground state energy is given by the constant ϵ in the flow Hamiltonian A.13 if all off-diagonal elements are neglected after a sufficiently long traversal of the flow. Third, the off-diagonal elements are not neglected but instead set to zero by a Bogoliubov Transformation of the flow Hamiltonian after traversing the flow for as long as in the second case. The right subplot shows the difference between the ground state energy and the constant terms in the Hamiltonian 3.15 to better highlight the (slight) differences between the three approaches.

The agreement of the first and third approach in Figure 4.3 is not surprising, since the flow equation approach transforms the Hamiltonian in infinitesimal *unitary* steps. The good behavior of the second method (stand-alone flow equations) seems plausible once we consider that $\mathcal{O}(N^2)$ matrix elements flow towards the diagonal, where of course the unitarity of the transformation conserves the trace of Hamiltonian (i.e. the sum of its eigenenergies). The number of $V_{k,k'}$ that do not converge to 0 is only $\mathcal{O}(N)$, and the number of $W_{k,k'}$ that do not converge to 0 is $\mathcal{O}(1)$. Therefore, assuming that these terms converge to values that are too large and do not diverge, we expect negligible contributions of these terms to the sum of the eigenenergies if a unitary transformation were performed that would actually make these

terms vanish. Now, because the ground state energy depends on the sum of the eigenvalues (see eq. 3.25), the prediction for the ground state energy for our system is very accurate. It is noteworthy that the ground state energy in the limit $\eta \to \pm\infty$ is the same. This is because the two branches are adiabatically connected [7, 14]. This can, for example, be shown by noticing that the ground state energy is a smooth function of $1/\eta$ at $1/\eta = 0$ [14, Fig. 1].
An accurate prediction of the ground state energy does not necessarily imply that all eigenenergies are predicted accurately too.

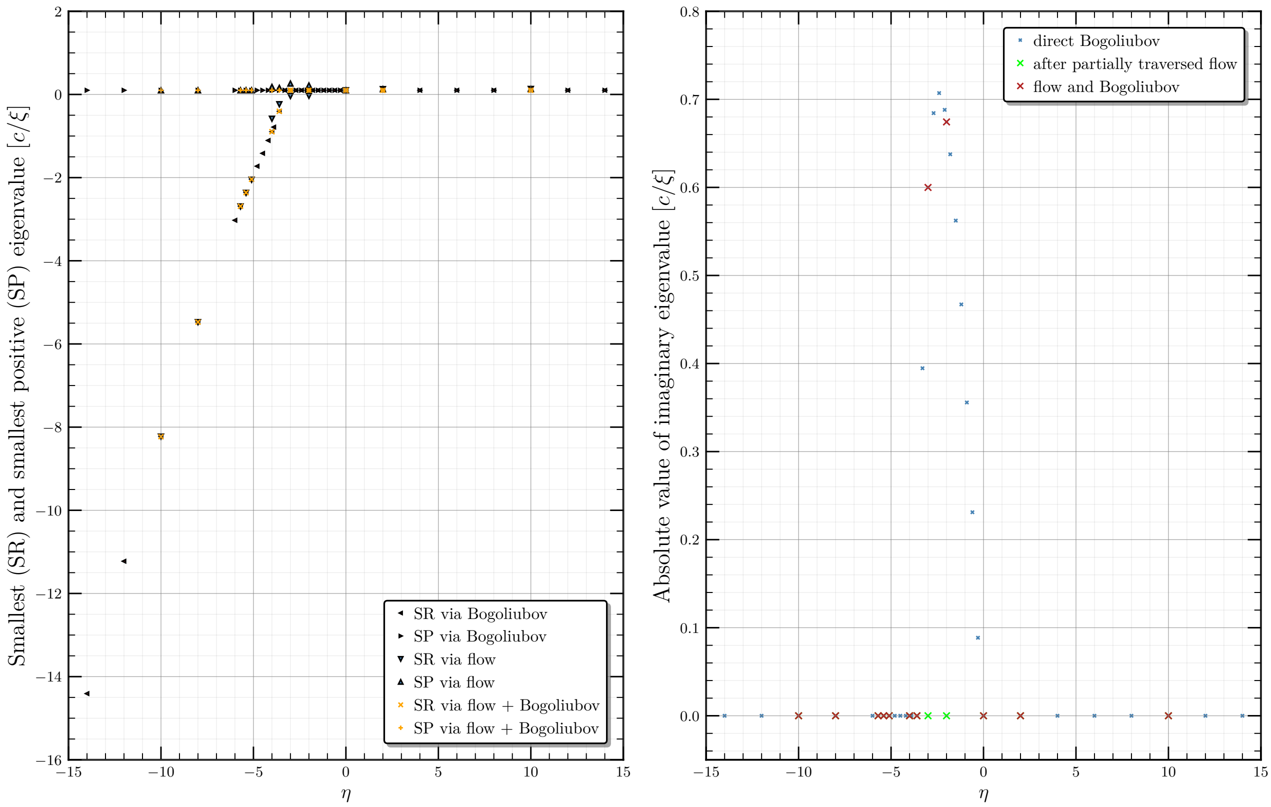

Figure 4.4: The left subplot shows the smallest real (SR) and smallest real positive (SP) eigenvalues of the Hamiltonian for different η. If an negative eigenvalue occurs, this indicates the existence of a bound state whose binding energy is then given by the (single) negative eigenvalue.
The right subplot illustrates in which regime dynamical instabilities (i.e. imaginary eigenvalues) occur.

For example, the difference in the ground state energy in Figure 4.3 for $\eta \approx -3.5$, which becomes especially clear when looking at the right subplot, can be explained by the fact that in this regime imaginary eigenvalues are to be expected (see Figure 4.4). The flow equations cannot "see" these eigenvalues because the original Hamiltonian is real and the flow equations are algebraically closed in the sense that the flow cannot generate terms from $\mathbb{C} \setminus \mathbb{R}$ if it starts with purely real terms. If the flow equation approach is when complex eigenvalues occur, those will be encoded in behaviour as seen in Figure 4.2 where not all off-diagonal terms vanish.
An important side note: The fact that imaginary eigenvalues occur principally means that formula 3.25 does not hold. However, Kain and Ling [14] argued that it is still applicable if the imaginary parts are relatively small. Looking at the maximal eigenvalues $\sim 70c/\xi$ and the imaginary parts $\sim 1c/\xi$ in Figure 4.4 justifies our use of formula 3.25 when calculating the

ground state energy for Figure 4.3.
The thermodynamic instability region for $-3.5 \gtrsim \eta$, on the other hand, is correctly predicted in accordance with the results obtained by a Bogoliubov transformation, since negative eigenvalues are generally unproblematic for the flow equations, even though a more complicated convergence behavior may result from these negative eigenvalues, as we observed in Figure 4.2.

4.1.2 Analysis of the Spectrum

We have seen that the flow equation approach allows for accurate predictions of the ground state energy. The fact that the flow equations simply gloss over the imaginary eigenvalues that can be seen by a Bogoliubov Transformation leads to less good predictions in a small regime around the η where the ground state energy diverges. Yet the relative error of these predictions is still small because the absolute error of ΔE_0 in Figure 4.3 is bounded whereas the ground energy is not.

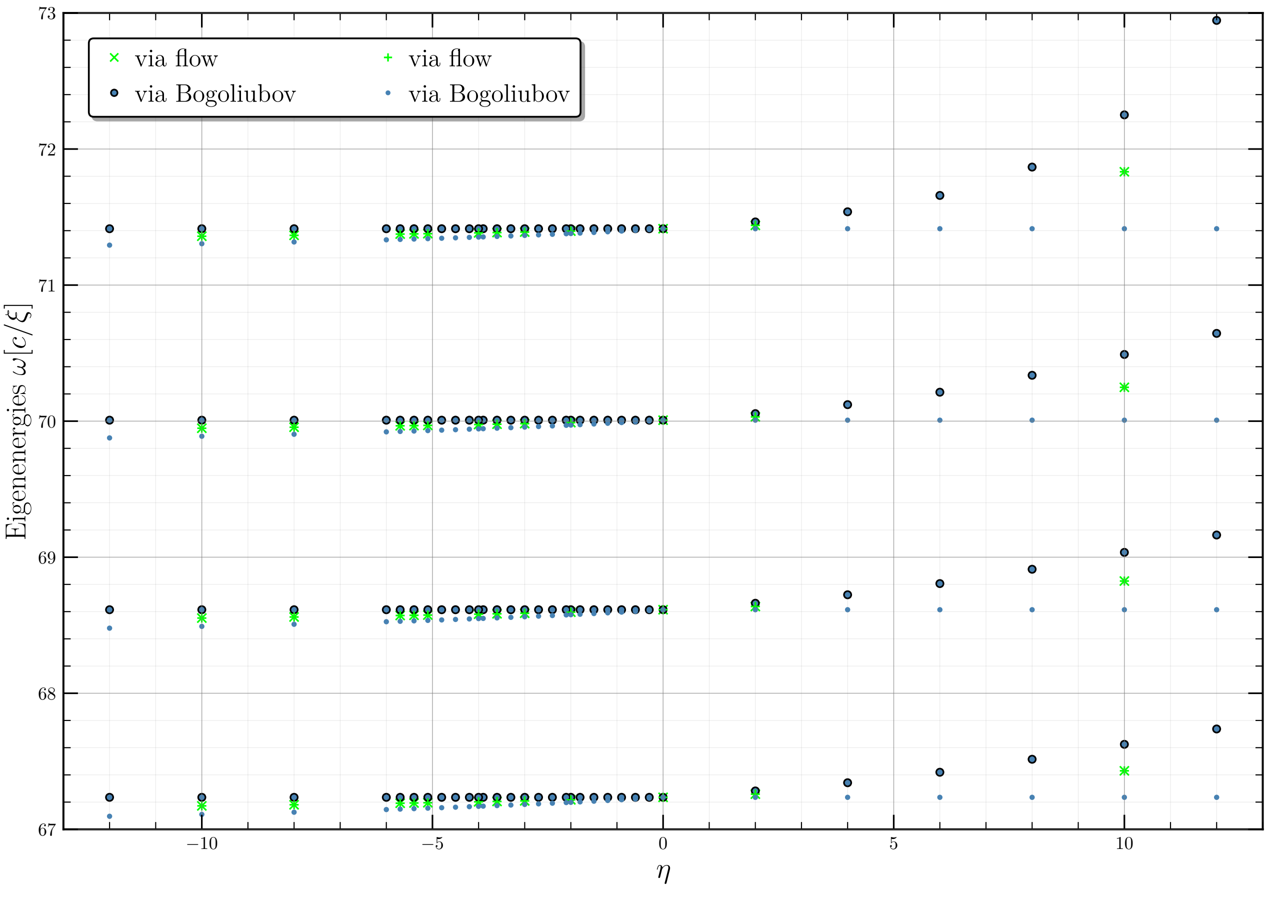

Figure 4.5: This plot shows how the largest eigenvalues change in η. It has been refrained from performing a Bogoliubov transformation after the flow, since this would only reproduce the values of a direct Bogoliubov transformation anyway due to the unitarity of the flow transformation.

In the previous section we have also seen that the flow equations predict the negative eigenvalues correctly. Moreover, Figure 4.4 showed that the smallest positive real eigenvalue is (almost) constant across the range of η we investigated. This is also true for most of the other positive eigenvalues, and only the end of the spectrum shows interesting behavior, so we will take a closer look at that. Figure 4.5 reveals the following features of the spectrum:

- The smaller the eigenvalue, the less it changes for different values of η. This is consistent with the fact, as noted above, that the smallest positive real eigenvalue remains virtually unchanged for different values interaction strengths.

- In the spectrum we get from the flow equations, each eigenvalue appears exactly twice, i.e. each eigenvalue is twofold degenerate. Therefore the flow does not lift the original degeneracy $\omega_k = \omega_{-k}$.

- In the spectrum we get from the Bogoliubov transformation, the eigenvalues come in pairs too where one eigenvalue remains exactly constant across different interaction strengths. The other increases strictly monotonically with η.

- The eigenvalues from the flow spectrum are almost exactly the mean value between the two different values corresponding to a pair in the Bogoliubov spectrum.

If this pattern can be continued, it seems plausible, even without knowing details about the flow equations, that no imaginary eigenvalues can be observed with them: Since the original Hamiltonian is purely real, its characteristic polynomial is also purely real, and its zeros must occur in pairs λ, λ^*. But since $\lambda + \lambda^* \in \mathbb{R}$, the flow equations do not see complex eigenvalues. In the next section, we will try to remove the degeneracy in the flow equations, in the hope that better agreement with the spectrum obtained via the Bogoliubov transformation can be achieved.

4.2 Introducing Twisted Boundary Conditions

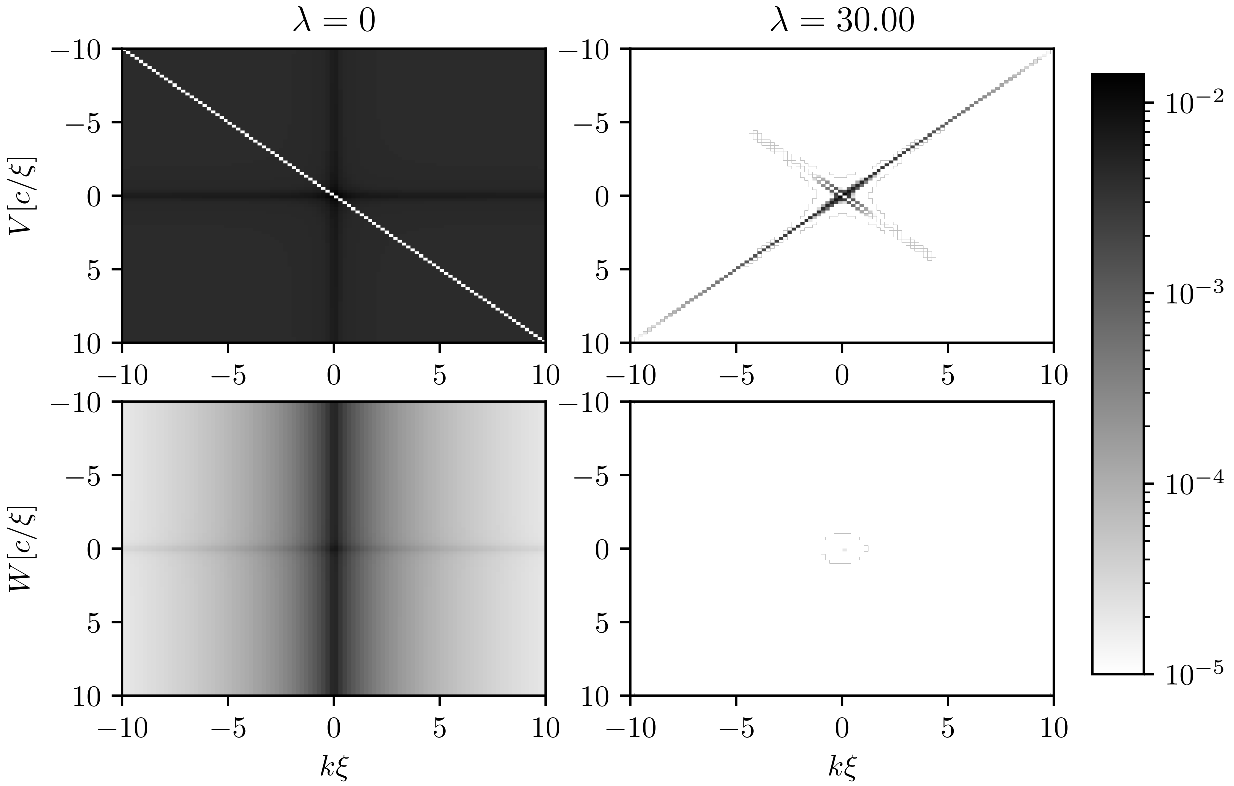

Figure 4.6: Visualization of the flow progression for $\eta = 0.2$ and $\varphi = 1$ analogous to Figure 4.1. We can see that by introducing the symmetry breaking parameter φ, all $V_{k,k'}$ decay from the outside, albeit slowly. Yet, considering the shading scale is logarithmic, many $V_{k,k'}$ can be well suppressed even if the flow is stopped at $\lambda = 30$.

We will now try to improve the convergence properties of the off-diagonal matrix elements using the transformation

$$\{\Delta k_n\}_{n\in\mathbb{Z}} \to \left\{\Delta k_n + \frac{\varphi}{L}\right\}_{n\in\mathbb{Z}} \tag{4.2}$$

which (slightly) shifts the grid of k-values and thereby breaks the symmetry $k \leftrightarrow -k$ by introducing a phase parameter $\varphi \in \mathbb{R}$. Obviously, the original, symmetrical grid is recovered in the limit $\varphi \to 0$. This transformation is not merely a mathematically convenient trick but is also physically meaningful. If we consider our bosonic bath in which the impurity is immersed arranged in circular form, we expect periodic boundary conditions

$$\psi(x) = \psi(x + L) \tag{4.3}$$

on a wave function ψ describing some part of the system. However, introducing a magnetic flux θ in the ring imposes *twisted* periodic boundary conditions:

$$\psi(x) = e^{i\varphi}\psi(x + L) \tag{4.4}$$

It can then be shown [17] that these twisted boundary conditions are equivalent to the shift

$$-i\partial_x \to -i\partial x + \frac{\varphi}{L} \tag{4.5}$$

or, after recognizing the momentum operator in position representation,

$$k \to k + \frac{\varphi}{L}. \tag{4.6}$$

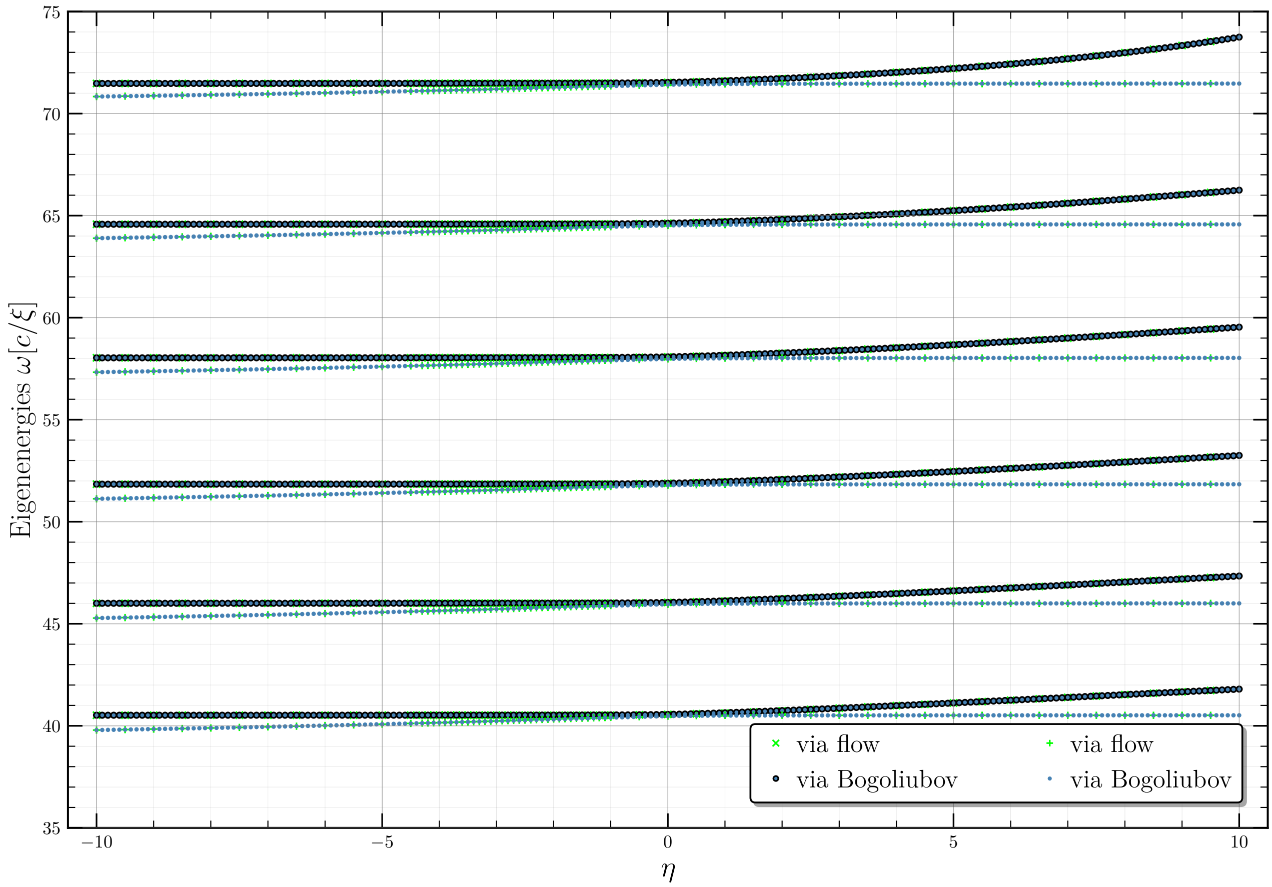

Figure 4.7: This plot shows how the largest eigenvalues change in η analogously to Figure 4.5 when twisted boundary conditions are in place. We can see that the symmetry breaking helps the convergence of the flow equations to the diagonal Hamiltonian.

Indeed, shifting the $k-$grid improves the convergence properties of the $V_{k,k'}$, as seen in Figure 4.6. There the calculations were still based on a $N = 200$ grid of k-values, just like in the previous section.
In the following, we will significantly coarsen the grid to $N = 40$ for computational reasons. This is acceptable to get a general idea of the convergence behavior and how the spectrum looks qualitatively, but probably does not allow for quantitatively exact conclusions. For Figure 4.9 we chose $\varphi := 0.1$. This is a reasonable value because it is large enough to break the symmetry sufficiently much while introducing only a very moderate error of $\sim 1.6\%$ for the smallest $|k|$-value. Hence, the ω_k, $V_{k,k'}$ and $W_{k,k'}$ in the original Hamiltonian have an error of the same order.
Since the symmetry of the diagonal part of the original Hamiltonian is now broken, the eigenvalues of the flow Hamiltonian are also no longer degenerate. We obtain a quantitatively very good agreement between the eigenvalues resulting from a Bogoliubov transformation and the predictions of the flow equations for large eigenvalues. Unfortunately, this does not hold for small eigenvalues.

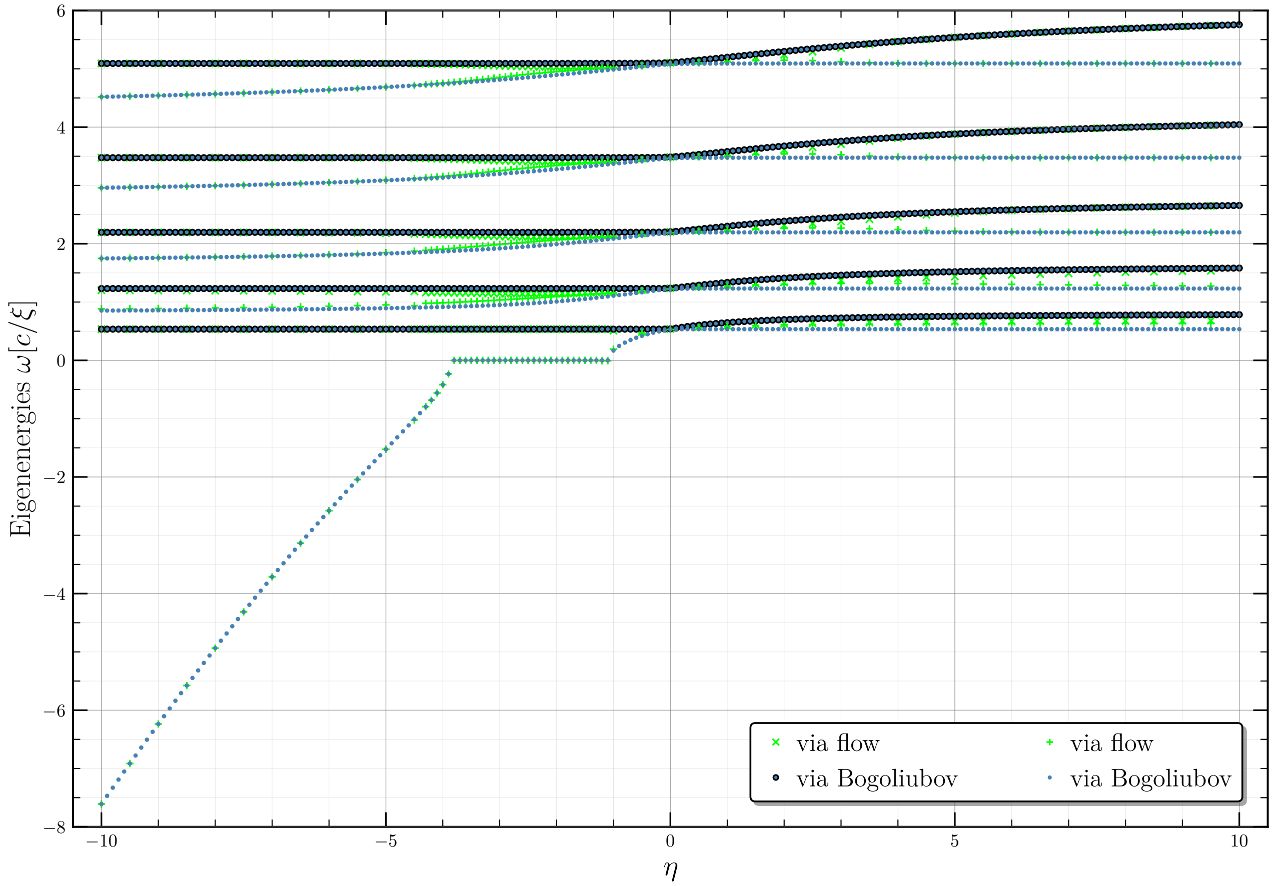

Figure 4.8: This plot shows how the smallest eigenvalues change in η analogously to Figure 4.5 when twisted boundary conditions are in place. We notice a slight discrepancy between the results obtained via Bogoliubov Transformation and via the Flow Equations.

However, it is assumed that these discrepancies in Figure 4.8 can be largely resolved by refining the k-grid, since we have very good agreement between the two methods for the top and bottom eigenvalues. Smaller distances between neighboring k-values mean, of course, smaller distances between the eigenvalues of the Hamiltonian and thus smaller distances between the eigenvalues we obtain via the flow equations and the Bogoliubov transformation, respectively. The right convergence to the spectrum of the Hamiltonian thanks to the twisted boundary conditions also resolves the discrepancies we observed in Figure 4.3, and almost perfect agreement of the ground state energies via Bogoliubov transformation and the flow equations can be obtained, as seen in Figure 4.9.

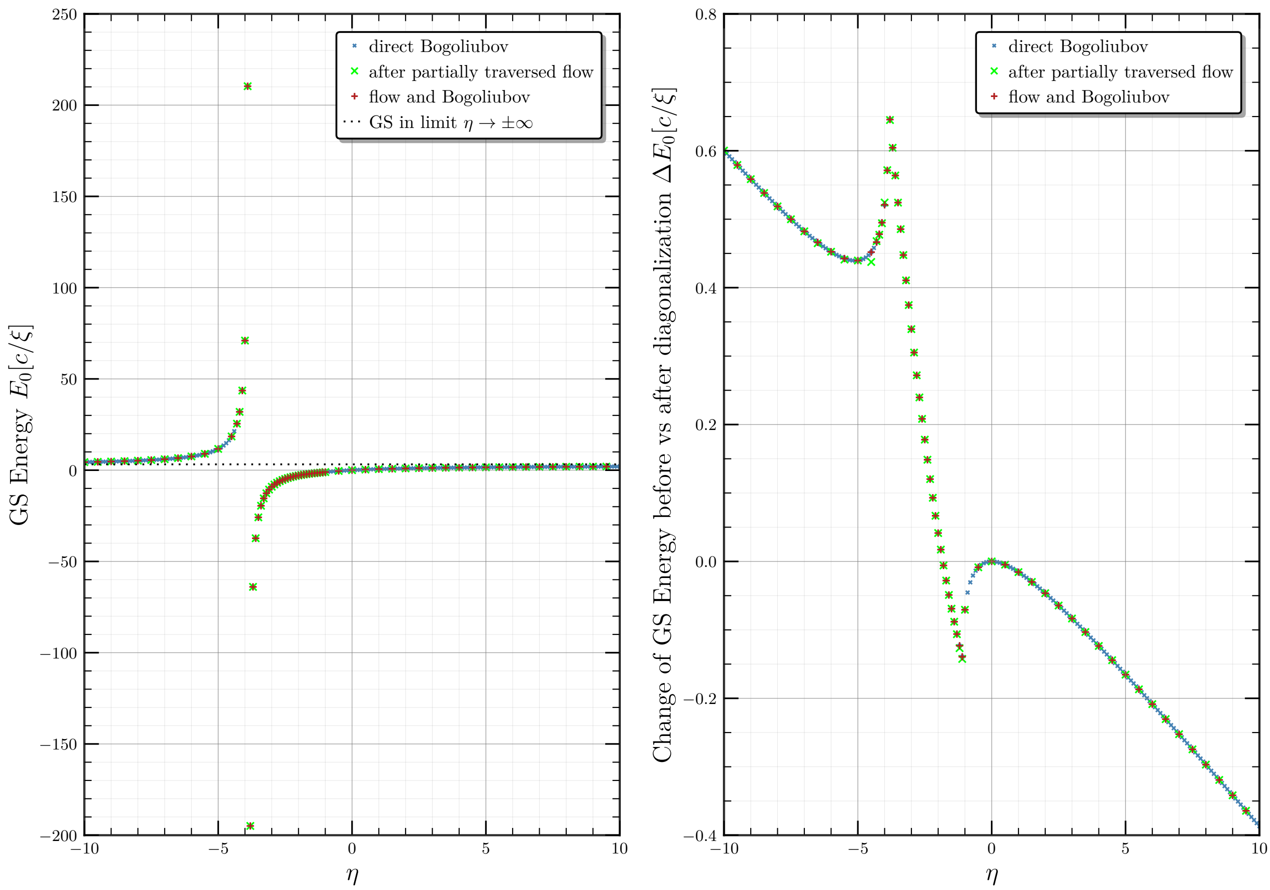

Figure 4.9: This plot shows how the ground state energy changes in η analogously to Figure 4.3 when twisted boundary conditions are in place. We can see that the symmetry breaking helps in reaching agreement between the Bogoliubov transformation and the flow equations. The quantitative disagreement to Figure 4.3 is grounded in the significantly coarser grid for this plot here and, to a lesser extend, the error introduced by the twisted boundary conditions.

4.3 Qualitative Convergence Analysis

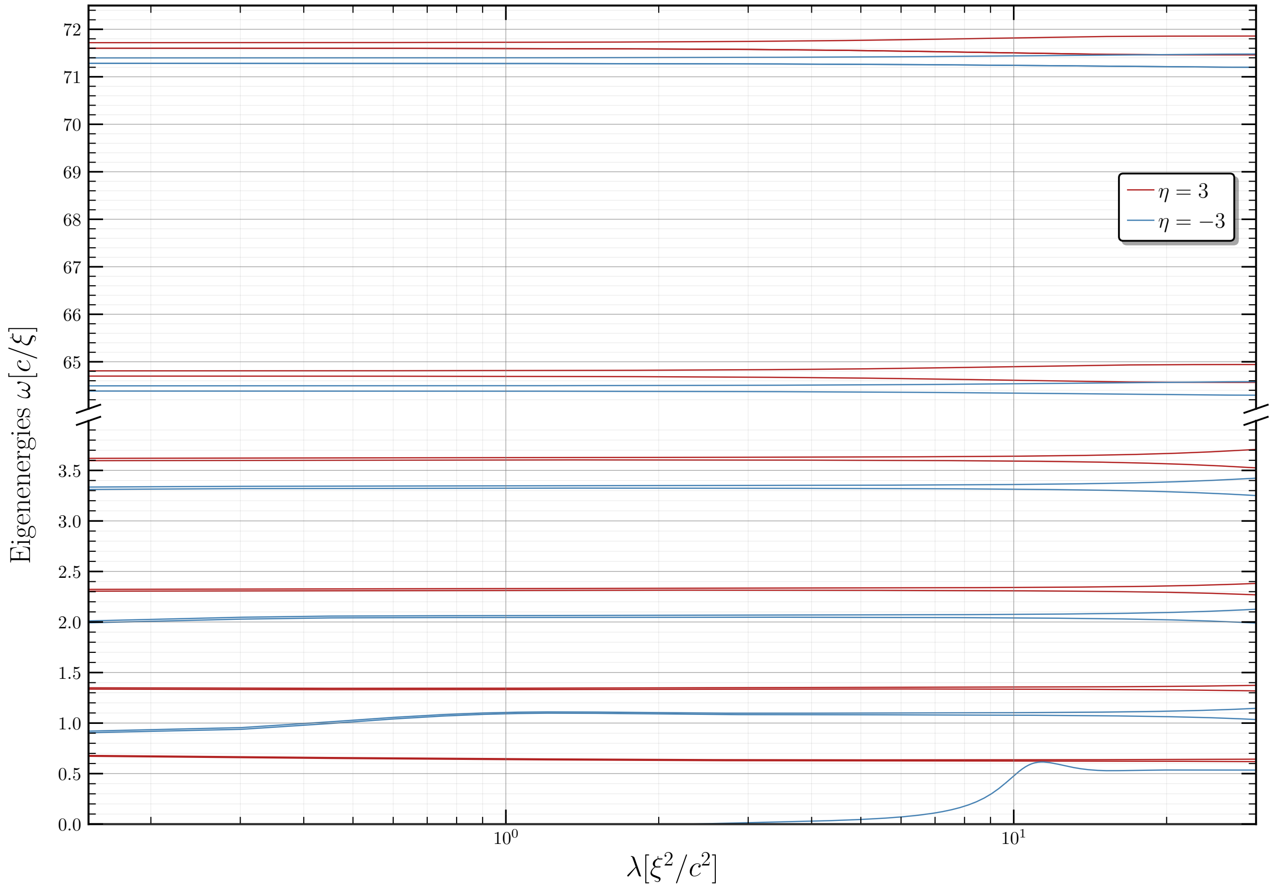

Figure 4.10: This plot illustrates that the rate of convergence is not uniform across the spectrum by plotting how the largest and smallest positive eigenvalues for two selected η evolve in the flow. It becomes evident that larger eigenvalues converge considerably faster than smaller eigenvalues.

Looking qualitatively at the convergence behavior of the eigenvalues whose flow evolution is shown in Figure 4.10, it seems likely that the discrepancies between the flow equation approach and the exact solution for small eigenvalues are largely due to the fact that the lower end of the spectrum converges much slower than the upper part of the spectrum. This is to be expected since $\partial_\lambda \omega_k$ in the flow equation A.14a is smaller for smaller $|\omega_k|$. Furthermore, when using the canonical generator, the flow equation approach always works by first decoupling matrix elements that couple modes with large energy differences. This means that $V_{k,k'}, W_{k,k'}$ generally converge faster if $\omega_k, \omega_{k'}$ are larger and that the flow equations work their way through Hilbert space starting by transforming states whose energies are high. Thus, the flow transforms the states associated with lower energies later, and the corresponding eigenvalues also settle to a constant value later in the flow.

SECTION 5
CONCLUSION AND OUTLOOK

The overarching goal of this project was to test whether the flow equation approach can be successfully applied to quadratic bosonic Hamiltonians. We can confirm this for the purely quadratic case where none of the coefficients of the second quantized Hamiltonian depend on the occupation numbers, since we were able to reproduce the spectrum as is obtained by exact diagonalization for the 1D Bose Polaron Problem in the heavy impurity limit. We showed that convergence to the spectrum can only be achieved by introducing twisted boundary conditions which (ever so slightly) break the symmetry of the Bogoliubov dispersion. This should not be considered a particularly large limitation of the method, since an arbitrarily small perturbation is sufficient to break the symmetry. We also want to point out that the fact that we have only considered the one-dimensional Bose polaron is not a major limitation of the method either, since increasing it would only increase the number of k-modes and thus the number of ODEs to be solved. In fact, in two or three dimensions we might see an even faster convergence to the spectrum, because the number of off-diagonal matrix elements that do not vanish would be even smaller compared to those that do.

A far more significant drawback of flow equations is that solving them has turned out to be computationally expensive. $\mathcal{O}(N^2)$ coupled ODEs have to be solved which is far more intricate than solving the eigenvalue problem for a matrix of size $2N$ when performing a Bogoliubov transformation. It is therefore explicitly not to be recommended to use the flow equations to diagonalize a purely quadratic bosonic Hamiltonian. At the same time, however, it should be noted that the eigenvalue problems to be solved for the Bogoliubov transform have been numerically optimized for decades, while the code written for this thesis is not necessarily particularly efficient or well optimized. The biggest attempt to improve performance made here was done by switching the programming language from Python to Julia.

Due to the computational complexity of the flow equation approach, it is not reasonable to apply it to a significantly finer grid, or to a grid with increased UV cutoff or decreased IR cutoff while maintaining the same spacing Δk. A grid with adaptive spacing might be a good way to overcome this issue. By introducing logarithmic spacing between the $k-$values it would be possible to cover a large part of momentum space with reasonable computational effort. The changes that would need to be made to the existing code to implement such a grid and solving the flow equations on that grid would be minimal.

Another good approach to improve the performance of the flow equations would be to adaptively stop the flow when convergence is reached by implementing an appropriate termination condition for the numerical integrator, i.e. to check if the change of a matrix element during the last integration steps has fallen below a certain threshold. It is even conceivable to use different termination points for matrix elements. As discussed in the last section, this would mean that high energy parts of the Hilbert space would be terminated first, because they settle relatively quickly to a constant value for the matrix elements and the spectrum. Of course, care must be taken that the overhead for the integrator to check for a termination condition is not greater than the computational savings from reducing the effective number of ODEs. If implemented well, this promises to reduce the computational complexity of solving the flow equations very substantially. However, this would require equally substantial changes to the code developed for this project.

To summarize, we are particularly pleased that in this thesis a very good agreement between the ground state energy via exact diagonalization and the flow equations was found. This gives hope that even after introducing some approximations the flow equations are still close to the exact solution for other more complex problems.

So the prospect of applying the flow equation approach to other problems where coefficients of the second quantized Hamiltonian depend on the occupation numbers is promising. In this case, exact diagonalization is no longer possible, whereas the generic flow equations derived in this thesis are still applicable. Whether they exhibit the desired convergence behavior must be tested for each specific application and may involve intricacies such as the necessity to introduce twisted boundary conditions. Those possible future applications may include the Bose polaron problem at finite impurity mass in one or higher dimensions or the description of magnons in antiferromagnets [18].

APPENDIX A

DETAILED CALCULATIONS

A.1 Deriving the Flow Equations Without n-Dependence

First the canonical generator $\hat{\eta}$ has to be evaluated:

$$\hat{\eta} := \hat{\eta}(\lambda) := \left[\hat{\mathcal{H}}_0, \hat{\mathcal{H}}_{\text{int}}\right] = \left[\sum_k \omega_k \hat{a}_k^\dagger \hat{a}_k, \sum_{q\neq q'} V_{q,q'} \hat{a}_q^\dagger \hat{a}_{q'} + \sum_{p,p'} \left(W_{p,p'} \hat{a}_p^\dagger \hat{a}_{p'}^\dagger + W_{p,p'}^* \hat{a}_p \hat{a}_{p'}\right)\right] \tag{A.1}$$

$$= \sum_k \sum_{q,q'} \omega_k V_{q,q'} \left[\hat{a}_k^\dagger \hat{a}_k, \hat{a}_q^\dagger \hat{a}_{q'}\right] + \sum_k \sum_{p,p'} \left(\omega_k W_{p,p'} \left[\hat{a}_k^\dagger \hat{a}_k, \hat{a}_p^\dagger \hat{a}_{p'}^\dagger\right] + \omega_k W_{p,p'}^* \left[\hat{a}_k^\dagger \hat{a}_k, \hat{a}_p \hat{a}_{p'}\right]\right)$$

$$= \sum_k \sum_{q,q'} \omega_k V_{q,q'} \left(\hat{a}_k^\dagger \hat{a}_{q'} \delta_{k,q} - \hat{a}_q^\dagger \hat{a}_k \delta_{k,q'}\right)$$

$$+ \sum_k \sum_{p,p'} \left(\omega_k W_{p,p'} \left(\hat{a}_k^\dagger \hat{a}_p^\dagger \delta_{k,p'} + \hat{a}_k^\dagger \hat{a}_{p'}^\dagger \delta_{k,p}\right) - \omega_k W_{p,p'}^* \left(\hat{a}_p \hat{a}_k \delta_{k,p'} + \hat{a}_{p'} \hat{a}_k \delta_{k,p}\right)\right)$$

$$= \sum_{q\neq q'} V_{q,q'} (\omega_q - \omega_{q'}) \hat{a}_q^\dagger \hat{a}_{q'} + \sum_{p,p'} \left(W_{p,p'} (\omega_p + \omega_{p'}) \hat{a}_p^\dagger \hat{a}_{p'}^\dagger - W_{p,p'}^* (\omega_p + \omega_{p'}) \hat{a}_p \hat{a}_{p'}\right) \tag{A.2}$$

Since $\hat{\eta}$ has the same form as $\hat{\mathcal{H}}_{\text{int}}$, $\left[\hat{\eta}, \hat{\mathcal{H}}_0\right]$ follows by inspection of A.2:

$$\left[\hat{\eta}, \hat{\mathcal{H}}_0\right] = -\sum_{q\neq q'} V_{q,q'} (\omega_q - \omega_{q'})^2 \hat{a}_q^\dagger \hat{a}_{q'}$$
$$-\sum_{p,p'} \left(W_{p,p'} (\omega_p + \omega_{p'})^2 \hat{a}_p^\dagger \hat{a}_{p'}^\dagger + W_{p,p'}^* (\omega_p + \omega_{p'})^2 \hat{a}_p \hat{a}_{p'}\right) \tag{A.3}$$

The commutator of the generator and $\hat{\mathcal{H}}_{\text{int}}$ needs more work:

$$\left[\hat{\eta}, \hat{\mathcal{H}}_{\text{int}}\right] = \Bigg[\sum_{q\neq q'} V_{q,q'} (\omega_q - \omega_{q'}) \hat{a}_q^\dagger \hat{a}_{q'} + \sum_{p,p'} \Big(W_{p,p'} (\omega_p + \omega_{p'}) \hat{a}_p^\dagger \hat{a}_{p'}^\dagger \tag{A.4}$$

$$- W_{p,p'}^* (\omega_p + \omega_{p'}) \hat{a}_p \hat{a}_{p'}\Big), \sum_{\tilde{q}\neq\tilde{q}'} V_{\tilde{q},\tilde{q}'} \hat{a}_{\tilde{q}}^\dagger \hat{a}_{\tilde{q}'} + \sum_{\tilde{p},\tilde{p}'} \left(W_{\tilde{p},\tilde{p}'} \hat{a}_{\tilde{p}}^\dagger \hat{a}_{\tilde{p}'}^\dagger + W_{\tilde{p},\tilde{p}'}^* \hat{a}_{\tilde{p}} \hat{a}_{\tilde{p}'}\right)\Bigg]$$

$$= \left[\sum_{q\neq q'} V_{q,q'} (\omega_q - \omega_{q'}) \hat{a}_q^\dagger \hat{a}_{q'}, \sum_{\tilde{q}\neq\tilde{q}'} V_{\tilde{q},\tilde{q}'} \hat{a}_{\tilde{q}}^\dagger \hat{a}_{\tilde{q}'}\right] \tag{A.5}$$

$$+ \left[\sum_{q\neq q'} V_{q,q'} (\omega_q - \omega_{q'}) \hat{a}_q^\dagger \hat{a}_{q'}, \sum_{\tilde{p},\tilde{p}'} \left(W_{\tilde{p},\tilde{p}'} \hat{a}_{\tilde{p}}^\dagger \hat{a}_{\tilde{p}'}^\dagger + W_{\tilde{p},\tilde{p}'}^* \hat{a}_{\tilde{p}} \hat{a}_{\tilde{p}'}\right)\right] \tag{A.6}$$

$$+ \left[\sum_{p,p'} \left(W_{p,p'} (\omega_p + \omega_{p'}) \hat{a}_p^\dagger \hat{a}_{p'}^\dagger - W_{p,p'}^* (\omega_p + \omega_{p'}) \hat{a}_p \hat{a}_{p'}\right), \sum_{\tilde{q}\neq\tilde{q}'} V_{\tilde{q},\tilde{q}'} \hat{a}_{\tilde{q}}^\dagger \hat{a}_{\tilde{q}'}\right] \tag{A.7}$$

$$+ \left[\sum_{p,p'} \left(W_{p,p'} (\omega_p + \omega_{p'}) \hat{a}_p^\dagger \hat{a}_{p'}^\dagger - W_{p,p'}^* (\omega_p + \omega_{p'}) \hat{a}_p \hat{a}_{p'}\right), \sum_{\tilde{p},\tilde{p}'} \left(W_{\tilde{p},\tilde{p}'} \hat{a}_{\tilde{p}}^\dagger \hat{a}_{\tilde{p}'}^\dagger + W_{\tilde{p},\tilde{p}'}^* \hat{a}_{\tilde{p}} \hat{a}_{\tilde{p}'}\right)\right] \tag{A.8}$$

In the following, A.5-A.8 will be evaluated separately. There will occur sums with $V_{q,q'}$ where $q = q'$. In this case, we define $V_{k,k} := 0\ \forall k$. This saves the rather tedious declaration of the constraints of several sum indices.

A.5:

$$
\begin{aligned}
&\left[\sum_{q\neq q'} V_{q,q'}(\omega_q - \omega_{q'})\hat{a}_q^\dagger \hat{a}_{q'}, \sum_{\tilde{q}\neq\tilde{q}'} V_{\tilde{q},\tilde{q}'}\hat{a}_{\tilde{q}}^\dagger \hat{a}_{\tilde{q}'}\right] \\
&= \sum_{q\neq q'}\sum_{\tilde{q}\neq\tilde{q}'} V_{\tilde{q},\tilde{q}'}V_{q,q'}(\omega_q - \omega_{q'})\left[\hat{a}_q^\dagger \hat{a}_{q'}, \hat{a}_{\tilde{q}}^\dagger \hat{a}_{\tilde{q}'}\right] \\
&= \sum_{q\neq q'}\sum_{\tilde{q}\neq\tilde{q}'} V_{\tilde{q},\tilde{q}'}V_{q,q'}(\omega_q - \omega_{q'})\left(\hat{a}_q^\dagger \hat{a}_{\tilde{q}'}\delta_{q',\tilde{q}} - \hat{a}_{\tilde{q}}^\dagger \hat{a}_{q'}\delta_{q,\tilde{q}'}\right) \\
&= \sum_{q\neq q'}\sum_{\tilde{q}'} V_{q',\tilde{q}'}V_{q,q'}(\omega_q - \omega_{q'})\hat{a}_q^\dagger \hat{a}_{\tilde{q}'} - \sum_{q\neq q'}\sum_{\tilde{q}} V_{\tilde{q},q}V_{q,q'}(\omega_q - \omega_{q'})\hat{a}_{\tilde{q}}^\dagger \hat{a}_{q'} \\
&= \sum_{q,q'}\sum_{\tilde{q}'} V_{q',\tilde{q}'}V_{q,q'}(\omega_q - \omega_{q'})\hat{a}_q^\dagger \hat{a}_{\tilde{q}'} - \sum_{q,q'}\sum_{\tilde{q}} V_{\tilde{q},q}V_{q,q'}(\omega_q - \omega_{q'})\hat{a}_{\tilde{q}}^\dagger \hat{a}_{q'} \\
&= \sum_{q,q'}\sum_{\tilde{q}} V_{\tilde{q},q'}V_{q,\tilde{q}}(\omega_q - \omega_{\tilde{q}})\hat{a}_q^\dagger \hat{a}_{q'} - \sum_{q,q'}\sum_{\tilde{q}} V_{q,\tilde{q}}V_{\tilde{q},q'}(\omega_{\tilde{q}} - \omega_{q'})\hat{a}_q^\dagger \hat{a}_{q'} \\
&= \sum_{q\neq q'}\sum_{\tilde{q}} V_{\tilde{q},q'}V_{q,\tilde{q}}(\omega_q - \omega_{\tilde{q}})\hat{a}_q^\dagger \hat{a}_{q'} - \sum_{q\neq q'}\sum_{\tilde{q}} V_{q,\tilde{q}}V_{\tilde{q},q'}(\omega_{\tilde{q}} - \omega_{q'})\hat{a}_q^\dagger \hat{a}_{q'} \\
&+ \sum_{k}\sum_{\tilde{q}} V_{\tilde{q},k}V_{k,\tilde{q}}(\omega_k - \omega_{\tilde{q}})\hat{a}_k^\dagger \hat{a}_k - \sum_{k}\sum_{\tilde{q}} V_{k,\tilde{q}}V_{\tilde{q},k}(\omega_{\tilde{q}} - \omega_k)\hat{a}_k^\dagger \hat{a}_k \\
&= \sum_{q\neq q'}\sum_{\tilde{q}} V_{\tilde{q},q'}V_{q,\tilde{q}}(\omega_q - \omega_{\tilde{q}})\hat{a}_q^\dagger \hat{a}_{q'} - \sum_{q\neq q'}\sum_{\tilde{q}} V_{q,\tilde{q}}V_{\tilde{q},q'}(\omega_{\tilde{q}} - \omega_{q'})\hat{a}_q^\dagger \hat{a}_{q'} \\
&+ \sum_{k}\sum_{\tilde{q}} 2V_{\tilde{q},k}V_{k,\tilde{q}}(\omega_k - \omega_{\tilde{q}})\hat{a}_k^\dagger \hat{a}_k
\end{aligned}
\tag{A.9}
$$

A.6:

$$
\begin{aligned}
&\left[\sum_{q\neq q'} V_{q,q'}(\omega_q - \omega_{q'})\hat{a}_q^\dagger \hat{a}_{q'}, \sum_{\tilde{p},\tilde{p}'}\left(W_{\tilde{p},\tilde{p}'}\hat{a}_{\tilde{p}}^\dagger \hat{a}_{\tilde{p}'}^\dagger + W_{\tilde{p},\tilde{p}'}^*\hat{a}_{\tilde{p}}\hat{a}_{\tilde{p}'}\right)\right] \\
&= \sum_{q\neq q'}\sum_{\tilde{p},\tilde{p}'} V_{q,q'}(\omega_q - \omega_{q'})\left(W_{\tilde{p},\tilde{p}'}\left[\hat{a}_q^\dagger \hat{a}_{q'}, \hat{a}_{\tilde{p}}^\dagger \hat{a}_{\tilde{p}'}^\dagger\right] + W_{\tilde{p},\tilde{p}'}^*\left[\hat{a}_q^\dagger \hat{a}_{q'}, \hat{a}_{\tilde{p}}\hat{a}_{\tilde{p}'}\right]\right) \\
&= \sum_{q,q'}\sum_{\tilde{p},\tilde{p}'} V_{q,q'}(\omega_q - \omega_{q'})\left(W_{\tilde{p},\tilde{p}'}\left(\hat{a}_q^\dagger \hat{a}_{\tilde{p}}^\dagger\delta_{q',\tilde{p}'} + \hat{a}_q^\dagger \hat{a}_{\tilde{p}'}^\dagger\delta_{q',\tilde{p}}\right) - W_{\tilde{p},\tilde{p}'}^*\hat{a}_{\tilde{p}}\left(\hat{a}_{\tilde{p}'}\hat{a}_{q'}\delta_{q,\tilde{p}} + \hat{a}_{\tilde{p}}\hat{a}_{q'}\delta_{\tilde{p}',q}\right)\right) \\
&= \sum_{p,p'}\sum_{q} V_{q,p'}(\omega_q - \omega_{p'})W_{p,p'}\hat{a}_q^\dagger \hat{a}_p^\dagger + \sum_{p,p'}\sum_{q} V_{q,p}(\omega_q - \omega_p)W_{p,p'}\hat{a}_q^\dagger \hat{a}_{p'}^\dagger \\
&- \sum_{p,p'}\sum_{q'} V_{p,q'}(\omega_p - \omega_{q'})W_{p,p'}^*\hat{a}_{p'}\hat{a}_{q'} - \sum_{p,p'}\sum_{q'} V_{p',q'}(\omega_{p'} - \omega_{q'})W_{p,p'}^*\hat{a}_p\hat{a}_{q'} \\
&= \sum_{p,p'}\sum_{q} V_{p',q}(\omega_{p'} - \omega_q)W_{p,q}\hat{a}_p^\dagger \hat{a}_{p'}^\dagger + \sum_{p,p'}\sum_{q} V_{p,q}(\omega_p - \omega_q)W_{q,p'}\hat{a}_p^\dagger \hat{a}_{p'}^\dagger \\
&- \sum_{p,p'}\sum_{q} V_{q,p}(\omega_q - \omega_p)W_{q,p'}^*\hat{a}_p\hat{a}_{p'} - \sum_{p,p'}\sum_{q} V_{q,p'}(\omega_q - \omega_{p'})W_{p,q}^*\hat{a}_p\hat{a}_{p'} \\
&= \sum_{p,p'}\sum_{q} V_{p',q}(\omega_{p'} - \omega_q)W_{p,q}\hat{a}_p^\dagger \hat{a}_{p'}^\dagger + \sum_{p,p'}\sum_{q} V_{p,q}(\omega_p - \omega_q)W_{q,p'}\hat{a}_p^\dagger \hat{a}_{p'}^\dagger \\
&- \sum_{p,p'}\sum_{q} V_{q,p}(\omega_q - \omega_p)W_{q,p'}^*\hat{a}_p\hat{a}_{p'} - \sum_{p,p'}\sum_{q} V_{q,p'}(\omega_q - \omega_{p'})W_{p,q}^*\hat{a}_p\hat{a}_{p'} \\
&= \sum_{p,p'}\sum_{q} V_{p,q}(\omega_p - \omega_q)(W_{q,p'} + W_{p',q})\hat{a}_p^\dagger \hat{a}_{p'}^\dagger
\end{aligned}
$$

$$+\sum_{p,p'}\sum_{q} V_{q,p}(\omega_p-\omega_q)(W^*_{q,p'}+W^*_{p',q})\hat{a}_p\hat{a}_{p'} \tag{A.10}$$

A.7:

$$\begin{aligned}
&\left[\sum_{p,p'}\left(W_{p,p'}(\omega_p+\omega_{p'})\hat{a}^\dagger_p\hat{a}^\dagger_{p'}-W^*_{p,p'}(\omega_p+\omega_{p'})\hat{a}_p\hat{a}_{p'}\right),\sum_{\tilde{q}\neq\tilde{q}'}V_{\tilde{q},\tilde{q}'}\hat{a}^\dagger_{\tilde{q}}\hat{a}_{\tilde{q}'}\right]\\
&=\sum_{p,p'}\sum_{\tilde{q}\neq\tilde{q}'}V_{\tilde{q},\tilde{q}'}(\omega_p+\omega_{p'})\left(W_{p,p'}\left[\hat{a}^\dagger_p\hat{a}^\dagger_{p'},\hat{a}^\dagger_{\tilde{q}}\hat{a}_{\tilde{q}'}\right]-W^*_{p,p'}\left[\hat{a}_p\hat{a}_{p'},\hat{a}^\dagger_{\tilde{q}}\hat{a}_{\tilde{q}'}\right]\right)\\
&=-\sum_{p,p'}\sum_{q\neq q'}V_{q,q'}(\omega_p+\omega_{p'})W_{p,p'}\left(\hat{a}^\dagger_q\hat{a}^\dagger_p\delta_{q',p'}+\hat{a}^\dagger_q\hat{a}^\dagger_{p'}\delta_{q',p}\right)\\
&-\sum_{p,p'}\sum_{q\neq q'}V_{q,q'}(\omega_p+\omega_{p'})W^*_{p,p'}\left(\hat{a}_p\hat{a}_{q'}\delta_{q,p'}+\hat{a}_{p'}\hat{a}_{q'}\delta_{q,p}\right)\\
&=-\sum_{p,p'}\sum_{q}V_{q,p'}(\omega_p+\omega_{p'})W_{p,p'}\hat{a}^\dagger_q\hat{a}^\dagger_p-\sum_{p,p'}\sum_{q}V_{q,p}(\omega_p+\omega_{p'})W_{p,p'}\hat{a}^\dagger_q\hat{a}^\dagger_{p'}\\
&-\sum_{p,p'}\sum_{q'}V_{p',q'}(\omega_p+\omega_{p'})W^*_{p,p'}\hat{a}_p\hat{a}_{q'}-\sum_{p,p'}\sum_{q'}V_{p,q'}(\omega_p+\omega_{p'})W^*_{p,p'}\hat{a}_{p'}\hat{a}_{q'}\\
&=-\sum_{p,p'}\sum_{q}V_{p',q}(\omega_p+\omega_q)W_{p,q}\hat{a}^\dagger_p\hat{a}^\dagger_{p'}-\sum_{p,p'}\sum_{q}V_{p,q}(\omega_q+\omega_{p'})W_{q,p'}\hat{a}^\dagger_p\hat{a}^\dagger_{p'}\\
&-\sum_{p,p'}\sum_{q'}V_{q',p'}(\omega_p+\omega_{q'})W^*_{p,q'}\hat{a}_p\hat{a}_{p'}-\sum_{p,p'}\sum_{q'}V_{q',p}(\omega_{q'}+\omega_{p'})W^*_{q',p'}\hat{a}_p\hat{a}_{p'}\\
&=-\sum_{p,p'}\sum_{q}V_{p,q}(\omega_q+\omega_{p'})(W_{p',q}+W_{q,p'})\hat{a}^\dagger_p\hat{a}^\dagger_{p'}\\
&-\sum_{p,p'}\sum_{q}V_{q,p}(\omega_q+\omega_{p'})(W^*_{p',q}+W^*_{q,p'})\hat{a}_p\hat{a}_{p'}
\end{aligned} \tag{A.11}$$

A.8:

$$\begin{aligned}
&\left[\sum_{p,p'}\left(W_{p,p'}(\omega_p+\omega_{p'})\hat{a}^\dagger_p\hat{a}^\dagger_{p'}-W^*_{p,p'}(\omega_p+\omega_{p'})\hat{a}_p\hat{a}_{p'}\right),\sum_{\tilde{p},\tilde{p}'}\left(W_{\tilde{p},\tilde{p}'}\hat{a}^\dagger_{\tilde{p}}\hat{a}^\dagger_{\tilde{p}'}+W^*_{\tilde{p},\tilde{p}'}\hat{a}_{\tilde{p}}\hat{a}_{\tilde{p}'}\right)\right]\\
&=\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}W_{p,p'}(\omega_p+\omega_{p'})W^*_{\tilde{p},\tilde{p}'}\left[\hat{a}^\dagger_p\hat{a}^\dagger_{p'},\hat{a}_{\tilde{p}}\hat{a}_{\tilde{p}'}\right]-\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}W^*_{p,p'}W_{\tilde{p},\tilde{p}'}(\omega_p+\omega_{p'})\left[\hat{a}_p\hat{a}_{p'},\hat{a}^\dagger_{\tilde{p}}\hat{a}^\dagger_{\tilde{p}'}\right]\\
&=-\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}W_{p,p'}(\omega_p+\omega_{p'}+\omega_{\tilde{p}}+\omega_{\tilde{p}'})W^*_{\tilde{p},\tilde{p}'}\left[\hat{a}_{\tilde{p}}\hat{a}_{\tilde{p}'},\hat{a}^\dagger_p\hat{a}^\dagger_{p'}\right]\\
&=-\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}W_{p,p'}(\omega_p+\omega_{p'}+\omega_{\tilde{p}}+\omega_{\tilde{p}'})W^*_{\tilde{p},\tilde{p}'}\hat{a}_{\tilde{p}}\hat{a}^\dagger_p\delta_{\tilde{p}',p'}\\
&-\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}W_{p,p'}(\omega_p+\omega_{p'}+\omega_{\tilde{p}}+\omega_{\tilde{p}'})W^*_{\tilde{p},\tilde{p}'}\hat{a}_{\tilde{p}}\hat{a}^\dagger_{p'}\delta_{\tilde{p}',p}\\
&-\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}W_{p,p'}(\omega_p+\omega_{p'}+\omega_{\tilde{p}}+\omega_{\tilde{p}'})W^*_{\tilde{p},\tilde{p}'}\hat{a}^\dagger_p\hat{a}_{\tilde{p}'}\delta_{\tilde{p},p'}\\
&-\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}W_{p,p'}(\omega_p+\omega_{p'}+\omega_{\tilde{p}}+\omega_{\tilde{p}'})W^*_{\tilde{p},\tilde{p}'}\hat{a}^\dagger_{p'}\hat{a}_{\tilde{p}'}\delta_{\tilde{p},p}\\
&=-\sum_{p,p'}\sum_{\tilde{p}}W_{p,p'}(\omega_p+2\omega_{p'}+\omega_{\tilde{p}})W^*_{\tilde{p},p'}\hat{a}_{\tilde{p}}\hat{a}^\dagger_p-\sum_{p,p'}\sum_{\tilde{p}}W_{p,p'}(2\omega_p+\omega_{p'}+\omega_{\tilde{p}})W^*_{\tilde{p},p}\hat{a}_{\tilde{p}}\hat{a}^\dagger_{p'}\\
&-\sum_{p,p'}\sum_{\tilde{p}'}W_{p,p'}(\omega_p+2\omega_{p'}+\omega_{\tilde{p}'})W^*_{p',\tilde{p}'}\hat{a}^\dagger_p\hat{a}_{\tilde{p}'}-\sum_{p,p'}\sum_{\tilde{p}'}W_{p,p'}(2\omega_p+\omega_{p'}+\omega_{\tilde{p}'})W^*_{p,\tilde{p}'}\hat{a}^\dagger_{p'}\hat{a}_{\tilde{p}'}\\
&=-\sum_{p,p'}\sum_{\tilde{p}}W_{p,\tilde{p}}(\omega_p+2\omega_{\tilde{p}}+\omega_{p'})W^*_{p',\tilde{p}}\hat{a}_{p'}\hat{a}^\dagger_p-\sum_{p,p'}\sum_{\tilde{p}}W_{\tilde{p},p}(2\omega_{\tilde{p}}+\omega_p+\omega_{p'})W^*_{p',\tilde{p}}\hat{a}_{p'}\hat{a}^\dagger_p
\end{aligned}$$

$$
\begin{aligned}
&-\sum_{p,p'}\sum_{\tilde{p}'} W_{p,\tilde{p}'}(\omega_p + 2\omega_{\tilde{p}'} + \omega_{p'})W^*_{\tilde{p}',p'}\hat{a}^\dagger_p\hat{a}_{p'} - \sum_{p,p'}\sum_{\tilde{p}'} W_{\tilde{p}',p}(2\omega_{\tilde{p}'} + \omega_p + \omega_{p'})W^*_{\tilde{p}',p'}\hat{a}^\dagger_p\hat{a}_{p'} \\
&= -\sum_{p,p'}\sum_{\tilde{p}}(W_{p,\tilde{p}} + W_{\tilde{p},p})(\omega_p + 2\omega_{\tilde{p}} + \omega_{p'})W^*_{p',\tilde{p}}\hat{a}_{p'}\hat{a}^\dagger_p \\
&-\sum_{p,p'}\sum_{\tilde{p}'}(W_{p,\tilde{p}'} + W_{\tilde{p}',p})(\omega_p + 2\omega_{\tilde{p}'} + \omega_{p'})W^*_{\tilde{p}',p'}\hat{a}^\dagger_p\hat{a}_{p'} \\
&= -\sum_{p,p'}\sum_{\tilde{p}}(W_{p,\tilde{p}} + W_{\tilde{p},p})(\omega_p + 2\omega_{\tilde{p}} + \omega_{p'})W^*_{p',\tilde{p}}(\delta_{p,p'} + \hat{a}^\dagger_p\hat{a}_{p'}) \\
&-\sum_{p,p'}\sum_{\tilde{p}}(W_{p,\tilde{p}} + W_{\tilde{p},p})(\omega_p + 2\omega_{\tilde{p}} + \omega_{p'})W^*_{\tilde{p},p'}\hat{a}^\dagger_p\hat{a}_{p'} \\
&= -\sum_{p,p'}\sum_{\tilde{p}}(W_{p,\tilde{p}} + W_{\tilde{p},p})(\omega_p + 2\omega_{\tilde{p}} + \omega_{p'})(W^*_{\tilde{p},p'} + W^*_{p',\tilde{p}})\hat{a}^\dagger_p\hat{a}_{p'} \\
&-2\sum_{k}\sum_{\tilde{p}}(W_{k,\tilde{p}} + W_{\tilde{p},k})(\omega_k + \omega_{\tilde{p}})W^*_{k,\tilde{p}} \\
&= -\sum_{q\neq q'}\sum_{\tilde{p}}(W_{q,\tilde{p}} + W_{\tilde{p},q})(\omega_q + 2\omega_{\tilde{p}} + \omega_{q'})(W^*_{\tilde{p},q'} + W^*_{q',\tilde{p}})\hat{a}^\dagger_q\hat{a}_{q'} \\
&-2\sum_{k}\sum_{\tilde{p}}(W_{k,\tilde{p}} + W_{\tilde{p},k})(\omega_k + \omega_{\tilde{p}})(W^*_{\tilde{p},k} + W^*_{k,\tilde{p}})\hat{a}^\dagger_k\hat{a}_k \\
&-2\sum_{k}\sum_{\tilde{p}}(W_{k,\tilde{p}} + W_{\tilde{p},k})(\omega_k + \omega_{\tilde{p}})W^*_{k,\tilde{p}} \qquad \text{(A.12)}
\end{aligned}
$$

We conclude that $\hat{\mathcal{H}}(\lambda)$ is of the form

$$
\hat{\mathcal{H}}(\lambda) = \sum_k \omega_k(\lambda)\hat{a}^\dagger_k\hat{a}_k + \sum_{q\neq q'} V_{q,q'}(\lambda)\hat{a}^\dagger_q\hat{a}_{q'} + \sum_{p,p'}\Big(W_{p,p'}(\lambda)\hat{a}^\dagger_p\hat{a}^\dagger_{p'} + W^*_{p,p'}(\lambda)\hat{a}_p\hat{a}_{p'}\Big) + \epsilon(\lambda) \qquad \text{(A.13)}
$$

where $\epsilon(\lambda)$ is a constant shift in the energy scale.
Using the expressions for the commutators of the generator and $\hat{\mathcal{H}}_0$ respectively $\hat{\mathcal{H}}_{\text{int}}$ derived above, the flow $\partial_\lambda\hat{\mathcal{H}}(\lambda) = [\hat{\eta}(\lambda), \hat{\mathcal{H}}(\lambda)]$ yields the following flow equations $\forall k, p, p', q, q'$ where $q \neq q'$:

$$
\partial_\lambda\omega_k = \sum_{\tilde{q}} 2V_{\tilde{q},k}V_{k,\tilde{q}}(\omega_k - \omega_{\tilde{q}}) - 2\sum_{\tilde{p}}(W_{k,\tilde{p}} + W_{\tilde{p},k})(\omega_k + \omega_{\tilde{p}})(W^*_{\tilde{p},k} + W^*_{k,\tilde{p}}) \qquad \text{(A.14a)}
$$

$$
\begin{aligned}
\partial_\lambda V_{q,q'} &= -V_{q,q'}(\omega_q - \omega_{q'})^2 - \sum_{\tilde{p}}(W_{q,\tilde{p}} + W_{\tilde{p},q})(\omega_q + \omega_{q'} + 2\omega_{\tilde{p}})(W^*_{\tilde{p},q'} + W^*_{q',\tilde{p}}) \\
&\quad + \sum_{\tilde{q}} V_{\tilde{q},q'}V_{q,\tilde{q}}(\omega_q + \omega_{q'} - 2\omega_{\tilde{q}}) \qquad \text{(A.14b)}
\end{aligned}
$$

$$
\begin{aligned}
\partial_\lambda W_{p,p'} &= -W_{p,p'}(\omega_p + \omega_{p'})^2 - \sum_q V_{p,q}(\omega_q + \omega_{p'})(W_{p',q} + W_{q,p'}) \\
&\quad + \sum_q V_{p,q}(\omega_p - \omega_q)(W_{q,p'} + W_{p',q}) \qquad \text{(A.14c)}
\end{aligned}
$$

$$
\begin{aligned}
\partial_\lambda W^*_{p,p'} &= -W^*_{p,p'}(\omega_p + \omega_{p'})^2 - \sum_q V_{q,p}(\omega_q + \omega_{p'})(W^*_{p',q} + W^*_{q,p'}) \\
&\quad + \sum_q V_{q,p}(\omega_p - \omega_q)(W^*_{q,p'} + W^*_{p',q}) \qquad \text{(A.14d)}
\end{aligned}
$$

$$
\partial_\lambda\varepsilon = -2\sum_{p,p'}(W_{p,p'} + W_{p',p})(\omega_p + \omega_{p'})W^*_{p,p'} \qquad \text{(A.14e)}
$$

Obviously, equations A.14c and A.14d are not independent from each other, since they are related by complex conjugation. Seeing this is a good consistency check because complex conjugation was not explicitly used in the derivation of the these two equations.

A.2 Deriving the Flow Equations with n-Dependence

A.2.1 The Canonical Generator

Our Hamiltonian $\hat{\mathcal{H}}$ is of the form:

$$\hat{\mathcal{H}} = \sum_k \hat{\omega}_k : \hat{a}_k^\dagger \hat{a}_k : + \sum_{p,p'} \left(\hat{W}_{p,p'} : \hat{a}_p^\dagger \hat{a}_{p'}^\dagger : + \sum_{q \neq q'} \hat{V}_{q,q'} : \hat{a}_q^\dagger \hat{a}_{q'} : + \hat{W}'_{p,p'} : \hat{a}_p \hat{a}_{p'} : \right) + \hat{\epsilon} \tag{A.15}$$

Upon realizing that $\sum_k \hat{\omega}_k : \hat{a}_k^\dagger \hat{a}_k :$ is also just a function of the number operators, we can consider $\hat{\mathcal{H}}_0 := \hat{H} := \sum_k \hat{\omega}_k : \hat{a}_k^\dagger \hat{a}_k : + \hat{\epsilon}$ as the diagonal part of $\hat{\mathcal{H}}$.
The first step in the calculating the flow equations is again to calculate the canonical commutator $\hat{\eta} := \left[\hat{\mathcal{H}}_0, \hat{\mathcal{H}}_{\text{int}}\right]$:

$$\begin{aligned}
\hat{\eta} &= \left[\hat{H}, \sum_{q \neq q'} \hat{V}_{q,q'} : \hat{a}_q^\dagger \hat{a}_{q'} : + \sum_{p,p'} \left(\hat{W}_{p,p'} : \hat{a}_p^\dagger \hat{a}_{p'}^\dagger : + \hat{W}'_{p,p'} : \hat{a}_p \hat{a}_{p'} : \right) \right] \\
&= \sum_{q \neq q'} \left[\hat{H}, \hat{V}_{q,q'} : \hat{a}_q^\dagger \hat{a}_{q'} :\right] && \text{(A.16a)} \\
&+ \sum_{p,p'} \left[\hat{H}, \hat{W}_{p,p'} : \hat{a}_p^\dagger \hat{a}_{p'}^\dagger :\right] && \text{(A.16b)} \\
&+ \sum_{p,p'} \left[\hat{H}, \hat{W}'_{p,p'} : \hat{a}_p \hat{a}_{p'} :\right] && \text{(A.16c)}
\end{aligned}$$

In the following, the terms A.16a-A.16c will be evaluated separately:

A.16a

$$\begin{aligned}
&\sum_{q \neq q'} \left[\hat{H}, \hat{V}_{q,q'} : \hat{a}_q^\dagger \hat{a}_{q'} :\right] \\
&= \sum_{q \neq q'} V_{q,q'} \left[\hat{H}, : \hat{a}_q^\dagger \hat{a}_{q'} :\right] \\
&= \sum_{q \neq q'} \hat{V}_{q,q'} \left(\hat{H} - \hat{H}(\hat{n}_q - 1, \hat{n}_{q'} + 1)\right) : \hat{a}_q^\dagger \hat{a}_{q'} : && \text{(A.17)} \\
& && \text{(A.18)}
\end{aligned}$$

A.16b

$$\begin{aligned}
&\sum_{p,p'} \left[\hat{H}, \hat{W}_{p,p'} : \hat{a}_p^\dagger \hat{a}_{p'}^\dagger :\right] \\
&= \sum_{p,p'} \hat{W}_{p,p'} \left[\hat{H}, : \hat{a}_p^\dagger \hat{a}_{p'}^\dagger :\right] \\
&= \sum_{p,p'} \hat{W}_{p,p'} \left(\hat{H} - \hat{H}(\hat{n}_{p'} - 1, \hat{n}_p - 1)\right) : \hat{a}_p^\dagger \hat{a}_{p'}^\dagger : && \text{(A.19)}
\end{aligned}$$

A.16c

$$\sum_{p,p'} \left[\hat{H}, \hat{W}'_{p,p'} :\hat{a}_p \hat{a}_{p'}:\right] = \sum_{p,p'} \hat{W}'_{p,p'} \left(\hat{H} - \hat{H}(\hat{n}_{p'}+1, \hat{n}_p+1)\right) :\hat{a}_p \hat{a}_{p'}: \tag{A.20}$$

This gives the canonical generator as:

$$\hat{\eta} = \sum_{q\neq q'} \hat{V}_{q,q'} \left(\hat{H} - \hat{H}(\hat{n}_q - 1, \hat{n}_{q'}+1)\right) :\hat{a}_q^\dagger \hat{a}_{q'}: \tag{A.21}$$
$$+ \sum_{p,p'} \hat{W}_{p,p'} \left(\hat{H} - \hat{H}(\hat{n}_{p'} - 1, \hat{n}_p - 1)\right) :\hat{a}_p^\dagger \hat{a}_{p'}^\dagger:$$
$$+ \sum_{p,p'} \hat{W}'_{p,p'} \left(\hat{H} - \hat{H}(\hat{n}_{p'} + 1, \hat{n}_p + 1)\right) :\hat{a}_p \hat{a}_{p'}:$$
$$=: \sum_{q\neq q'} \hat{\theta}_{q,q'} :\hat{a}_q^\dagger \hat{a}_{q'}: + \sum_{p,p'} \left(\hat{\phi}_{p,p'} :\hat{a}_p^\dagger \hat{a}_{p'}^\dagger: + \hat{\psi}_{p,p'} :\hat{a}_p \hat{a}_{p'}:\right) \tag{A.22}$$

A.2.2 Evaluating the Commutator of the Generator with the Hamiltonian

If one notices that η is structurally identical to $\hat{\mathcal{H}}_{\mathrm{int}}$, the commutator of $\hat{\mathcal{H}}_0$ and η can be written down immediately:

$$\left[\eta^{(2)}, \hat{\mathcal{H}}_0\right] = - \sum_{q\neq q'} \hat{\theta}_{q,q'} \left(\hat{H} - \hat{H}(\hat{n}_q - 1, \hat{n}_{q'}+1)\right) :\hat{a}_q^\dagger \hat{a}_{q'}: \tag{A.23}$$
$$- \sum_{p,p'} \hat{\phi}_{p,p'} \left(\hat{H} - \hat{H}(\hat{n}_{p'} - 1, \hat{n}_p - 1)\right) :\hat{a}_p^\dagger \hat{a}_{p'}^\dagger:$$
$$- \sum_{p,p'} \hat{\psi}_{p,p'} \left(\hat{H} - \hat{H}(\hat{n}_{p'} + 1, \hat{n}_p + 1)\right) :\hat{a}_p \hat{a}_{p'}:$$
$$= - \sum_{q\neq q'} \hat{V}_{q,q'} \left(\hat{H} - \hat{H}(\hat{n}_q - 1, \hat{n}_{q'}+1)\right)^2 :\hat{a}_q^\dagger \hat{a}_{q'}: \tag{A.24}$$
$$- \sum_{p,p'} \hat{W}_{p,p'} \left(\hat{H} - \hat{H}(\hat{n}_{p'} - 1, \hat{n}_p - 1)\right)^2 :\hat{a}_p^\dagger \hat{a}_{p'}^\dagger:$$
$$- \sum_{p,p'} \hat{W}'_{p,p'} \left(\hat{H} - \hat{H}(\hat{n}_{p'} + 1, \hat{n}_p + 1)\right)^2 :\hat{a}_p \hat{a}_{p'}:$$

The commutator of $\hat{\mathcal{H}}_{\mathrm{int}}$ and η requires significantly more work:

$$\left[\eta^{(2)}, \hat{\mathcal{H}}_{\mathrm{int}}\right] = \sum_{q\neq q'} \sum_{\tilde{q}\neq\tilde{q}'} \left[\hat{\theta}_{\tilde{q},\tilde{q}'} :\hat{a}_{\tilde{q}}^\dagger \hat{a}_{\tilde{q}'}:, \hat{V}_{q,q'} :\hat{a}_q^\dagger \hat{a}_{q'}:\right] \tag{A.25a}$$
$$+ \sum_{p,p'} \sum_{\tilde{q}\neq\tilde{q}'} \left[\hat{\theta}_{\tilde{q},\tilde{q}'} :\hat{a}_{\tilde{q}}^\dagger \hat{a}_{\tilde{q}'}:, \hat{W}_{p,p'} :\hat{a}_p^\dagger \hat{a}_{p'}^\dagger:\right] \tag{A.25b}$$
$$+ \sum_{p,p'} \sum_{\tilde{q}\neq\tilde{q}'} \left[\hat{\theta}_{\tilde{q},\tilde{q}'} :\hat{a}_{\tilde{q}}^\dagger \hat{a}_{\tilde{q}'}:, \hat{W}'_{p,p'} :\hat{a}_p \hat{a}_{p'}:\right] \tag{A.25c}$$
$$+ \sum_{q\neq q'} \sum_{\tilde{p},\tilde{p}'} \left[\hat{\phi}_{\tilde{p},\tilde{p}'} :\hat{a}_{\tilde{p}}^\dagger \hat{a}_{\tilde{p}'}^\dagger:, \hat{V}_{q,q'} :\hat{a}_q^\dagger \hat{a}_{q'}:\right] \tag{A.25d}$$
$$+ \sum_{p,p'} \sum_{\tilde{p},\tilde{p}'} \left[\hat{\phi}_{\tilde{p},\tilde{p}'} :\hat{a}_{\tilde{p}}^\dagger \hat{a}_{\tilde{p}'}^\dagger:, \hat{W}_{p,p'} :\hat{a}_p^\dagger \hat{a}_{p'}^\dagger:\right] \tag{A.25e}$$

$$+\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\left[\hat{\phi}_{\tilde{p},\tilde{p}'}:\hat{a}^\dagger_{\tilde{p}}\hat{a}^\dagger_{\tilde{p}'}:,\hat{W}'_{p,p'}:\hat{a}_p\hat{a}_{p'}:\right] \tag{A.25f}$$

$$+\sum_{q\neq q'}\sum_{\tilde{p},\tilde{p}'}\left[\hat{\psi}_{\tilde{p},\tilde{p}'}:\hat{a}_{\tilde{p}}\hat{a}_{\tilde{p}'}:,\hat{V}_{q,q'}:\hat{a}^\dagger_q\hat{a}_{q'}:\right] \tag{A.25g}$$

$$+\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\left[\hat{\psi}_{\tilde{p},\tilde{p}'}:\hat{a}_{\tilde{p}}\hat{a}_{\tilde{p}'}:,\hat{W}_{p,p'}:\hat{a}^\dagger_p\hat{a}^\dagger_{p'}:\right] \tag{A.25h}$$

$$+\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\left[\hat{\psi}_{\tilde{p},\tilde{p}'}:\hat{a}_{\tilde{p}}\hat{a}_{\tilde{p}'}:,\hat{W}'_{p,p'}:\hat{a}_p\hat{a}_{p'}:\right] \tag{A.25i}$$

For the sake of clarity, the terms A.25a-A.25i will again be evaluated one by one.

A.25a:

$$\begin{aligned}
&\sum_{q\neq q'}\sum_{\tilde{q}\neq\tilde{q}'}\left[\hat{\theta}_{\tilde{q},\tilde{q}'}:\hat{a}^\dagger_{\tilde{q}}\hat{a}_{\tilde{q}'}:,\hat{V}_{q,q'}:\hat{a}^\dagger_q\hat{a}_{q'}:\right]\\
&=\sum_{q\neq q'}\sum_{\tilde{q}\neq\tilde{q}'}\hat{\theta}_{\tilde{q},\tilde{q}'}\hat{V}_{q,q'}\left[:\hat{a}^\dagger_{\tilde{q}}\hat{a}_{\tilde{q}'}:,:\hat{a}^\dagger_q\hat{a}_{q'}:\right]\\
&+\sum_{q\neq q'}\sum_{\tilde{q}\neq\tilde{q}'}\hat{V}_{q,q'}\left[\hat{\theta}_{\tilde{q},\tilde{q}'},:\hat{a}^\dagger_q\hat{a}_{q'}:\right]:\hat{a}^\dagger_{\tilde{q}}\hat{a}_{\tilde{q}'}:\\
&+\sum_{q\neq q'}\sum_{\tilde{q}\neq\tilde{q}'}\hat{\theta}_{\tilde{q},\tilde{q}'}\left[:\hat{a}^\dagger_{\tilde{q}}\hat{a}_{\tilde{q}'}:,\hat{V}_{q,q'}\right]:\hat{a}^\dagger_q\hat{a}_{q'}:\\
&=\sum_{q\neq q'}\sum_{\tilde{q}\neq\tilde{q}'}\hat{\theta}_{\tilde{q},\tilde{q}'}\hat{V}_{q,q'}\left(\delta_{\tilde{q}',q}:\hat{a}^\dagger_{\tilde{q}}\hat{a}_q:-\delta_{\tilde{q},q'}:\hat{a}^\dagger_q\hat{a}_{\tilde{q}'}:\right) &\text{(A.26)}\\
&+\sum_{q\neq q'}\sum_{\tilde{q}\neq\tilde{q}'}\hat{V}_{q,q'}\left(\hat{\theta}_{\tilde{q},\tilde{q}'}-\hat{\theta}_{\tilde{q},\tilde{q}'}(\hat{n}_{q'}+1,\hat{n}_q-1)\right)\underbrace{:\hat{a}^\dagger_q\hat{a}_{q'}::\hat{a}^\dagger_{\tilde{q}}\hat{a}_{\tilde{q}'}:}_{\overset{2}{=}\delta_{q',\tilde{q}}:\hat{a}^\dagger_q\hat{a}_{\tilde{q}'}:}\\
&-\sum_{q\neq q'}\sum_{\tilde{q}\neq\tilde{q}'}\hat{\theta}_{q,q'}\left[\hat{V}_{\tilde{q},\tilde{q}'},:\hat{a}^\dagger_q\hat{a}_{q'}:\right]:\hat{a}^\dagger_{\tilde{q}}\hat{a}_{\tilde{q}'}:\\
&\overset{2}{=}\sum_{q\neq q'}\sum_{\tilde{q}}\left(\hat{\theta}_{\tilde{q},q}\hat{V}_{q,q'}:\hat{a}^\dagger_{\tilde{q}}\hat{a}_q:-\hat{\theta}_{q',\tilde{q}}\hat{V}_{q,q'}:\hat{a}^\dagger_q\hat{a}_{\tilde{q}}:\right)\\
&+\sum_{q\neq q'}\sum_{\tilde{q}}\hat{V}_{q,q'}\left(\hat{\theta}_{q',\tilde{q}}-\hat{\theta}_{q',\tilde{q}}(\hat{n}_{q'}+1,\hat{n}_q-1)\right):\hat{a}^\dagger_q\hat{a}_{\tilde{q}}:\\
&-\sum_{q\neq q'}\sum_{\tilde{q}\neq\tilde{q}'}\hat{\theta}_{q,q'}\left[\hat{V}_{\tilde{q},\tilde{q}'},:\hat{a}^\dagger_q\hat{a}_{q'}:\right]:\hat{a}^\dagger_{\tilde{q}}\hat{a}_{\tilde{q}'}:\\
&=\sum_{q,q'}\sum_{\tilde{q}}\left(\hat{\theta}_{q,q'}\hat{V}_{q',\tilde{q}}:\hat{a}^\dagger_q\hat{a}_{q'}:-\hat{\theta}_{\tilde{q},q'}\hat{V}_{q,\tilde{q}}:\hat{a}^\dagger_q\hat{a}_{q'}:\right) &\text{(A.27)}\\
&\underbrace{-\sum_{k}\sum_{\tilde{q}}\left(\hat{\theta}_{\tilde{q},k}\hat{V}_{k,k}:\hat{a}^\dagger_{\tilde{q}}\hat{a}_k:-\hat{\theta}_{k,\tilde{q}}\hat{V}_{k,k}:\hat{a}^\dagger_k\hat{a}_{\tilde{q}}:\right)}_{=0}\\
&+\sum_{q,q'}\sum_{\tilde{q}}\hat{V}_{q,\tilde{q}}\left(\hat{\theta}_{\tilde{q},q'}-\hat{\theta}_{\tilde{q},q'}(\hat{n}_{\tilde{q}}+1,\hat{n}_q-1)\right):\hat{a}^\dagger_q\hat{a}_{q'}:\\
&\underbrace{-\sum_{k}\sum_{\tilde{q}}\hat{V}_{k,k}\left(\hat{\theta}_{k,\tilde{q}}-\hat{\theta}_{k,\tilde{q}}(\hat{n}_k+1,\hat{n}_k-1)\right):\hat{a}^\dagger_k\hat{a}_{\tilde{q}}:}_{=0}\\
&-\sum_{q\neq q'}\sum_{\tilde{q}\neq\tilde{q}'}\hat{\theta}_{q,q'}\left[\hat{V}_{\tilde{q},\tilde{q}'},:\hat{a}^\dagger_q\hat{a}_{q'}:\right]:\hat{a}^\dagger_{\tilde{q}}\hat{a}_{\tilde{q}'}:\\
&=\sum_{q\neq q'}\sum_{\tilde{q}}\left(\hat{\theta}_{q,q'}\hat{V}_{q',\tilde{q}}:\hat{a}^\dagger_q\hat{a}_{q'}:-\hat{\theta}_{\tilde{q},q'}\hat{V}_{q,\tilde{q}}:\hat{a}^\dagger_q\hat{a}_{q'}:\right) &\text{(A.28)}
\end{aligned}$$

$$
\begin{aligned}
&+\sum_{k}\sum_{\tilde q}\left(\hat\theta_{k,k}\hat V_{k,\tilde q} :\hat a_k^\dagger \hat a_k: -\hat\theta_{\tilde q,k}\hat V_{k,\tilde q} :\hat a_k^\dagger \hat a_k:\right)\\
&+\sum_{q\neq q'}\sum_{\tilde q}\hat V_{q,\tilde q}\left(\hat\theta_{\tilde q,q'}-\hat\theta_{\tilde q,q'}(\hat n_{\tilde q}+1,\hat n_q-1)\right) :\hat a_q^\dagger \hat a_{q'}:\\
&+\sum_{k}\sum_{\tilde q}\hat V_{k,\tilde q}\left(\hat\theta_{\tilde q,k}-\hat\theta_{\tilde q,k}(\hat n_{\tilde q}+1,\hat n_k-1)\right) :\hat a_k^\dagger \hat a_k:\\
&-\sum_{q\neq q'}\sum_{\tilde q\neq\tilde q'}\hat\theta_{q,q'}\left[\hat V_{\tilde q,\tilde q'}, :\hat a_q^\dagger \hat a_{q'}:\right] :\hat a_{\tilde q}^\dagger \hat a_{\tilde q'}:\\
&=\sum_{q\neq q'}\sum_{\tilde q}\left(\hat\theta_{q,q'}\hat V_{q',\tilde q}-\hat\theta_{\tilde q,q'}\hat V_{q,\tilde q}\right) :\hat a_q^\dagger \hat a_{q'}: \qquad \text{(A.29)}\\
&+\sum_{k}\sum_{\tilde q}\left(\hat\theta_{k,k}\hat V_{k,\tilde q}-\hat\theta_{\tilde q,k}\hat V_{k,\tilde q}\right) :\hat a_k^\dagger \hat a_k:\\
&+\sum_{q\neq q'}\sum_{\tilde q}\hat V_{q,\tilde q}\left(\hat\theta_{\tilde q,q'}-\hat\theta_{\tilde q,q'}(\hat n_{\tilde q}+1,\hat n_q-1)\right) :\hat a_q^\dagger \hat a_{q'}:\\
&+\sum_{k}\sum_{\tilde q}\hat V_{k,\tilde q}\left(\hat\theta_{\tilde q,k}-\hat\theta_{\tilde q,k}(\hat n_{\tilde q}+1,\hat n_k-1)\right) :\hat a_k^\dagger \hat a_k:\\
&-\sum_{q\neq q'}\sum_{\tilde q}\hat\theta_{q,\tilde q}\left(\hat V_{\tilde q,q'}-\hat V_{\tilde q,q'}(\hat n_{\tilde q}+1,\hat n_q-1)\right) :\hat a_q^\dagger \hat a_{q'}:\\
&-\sum_{k}\sum_{\tilde q}\hat\theta_{k,\tilde q}\left(\hat V_{\tilde q,k}-\hat V_{\tilde q,k}(\hat n_{\tilde q}+1,\hat n_k-1)\right) :\hat a_k^\dagger \hat a_k:
\end{aligned}
$$

Here we introduced the symbol $\overset{②}{=}$ which is used for equalities which are exact up to second order.

A.25b:

$$
\begin{aligned}
&\sum_{p,p'}\sum_{\tilde q\neq\tilde q'}\left[\hat\theta_{\tilde q,\tilde q'} :\hat a_{\tilde q}^\dagger \hat a_{\tilde q'}:, \hat W_{p,p'} :\hat a_p^\dagger \hat a_{p'}^\dagger:\right]\\
&=\sum_{p,p'}\sum_{\tilde q\neq\tilde q'}\hat\theta_{\tilde q,\tilde q'}\hat W_{p,p'}\left[:\hat a_{\tilde q}^\dagger \hat a_{\tilde q'}:, :\hat a_p^\dagger \hat a_{p'}^\dagger:\right] \qquad \text{(A.30a)}\\
&+\sum_{p,p'}\sum_{\tilde q\neq\tilde q'}\hat\theta_{\tilde q,\tilde q'}\left[:\hat a_{\tilde q}^\dagger \hat a_{\tilde q'}:, \hat W_{p,p'}\right] :\hat a_p^\dagger \hat a_{p'}^\dagger: \qquad \text{(A.30b)}\\
&+\sum_{p,p'}\sum_{\tilde q\neq\tilde q'}\hat W_{p,p'}\left[\hat\theta_{\tilde q,\tilde q'}, :\hat a_p^\dagger \hat a_{p'}^\dagger:\right] :\hat a_{\tilde q}^\dagger \hat a_{\tilde q'}: \qquad \text{(A.30c)}
\end{aligned}
$$

We start by evaluating A.30a:

$$
\begin{aligned}
&\sum_{p,p'}\sum_{\tilde q\neq\tilde q'}\hat\theta_{\tilde q,\tilde q'}\hat W_{p,p'}\left[:\hat a_{\tilde q}^\dagger \hat a_{\tilde q'}:, :\hat a_p^\dagger \hat a_{p'}^\dagger:\right]\\
&=\sum_{p,p'}\sum_{q\neq q'}\hat\theta_{q,q'}\hat W_{p,p'}\left(\delta_{q',p'} :\hat a_q^\dagger \hat a_p^\dagger: +\delta_{q',p} :\hat a_q^\dagger \hat a_{p'}^\dagger:\right)\\
&=\sum_{p,p'}\sum_{q}\hat\theta_{q,p'}\hat W_{p,p'} :\hat a_q^\dagger \hat a_p^\dagger: +\sum_{p,p'}\sum_{q}\hat\theta_{q,p}\hat W_{p,p'} :\hat a_q^\dagger \hat a_{p'}^\dagger:\\
&=\sum_{p,p'}\sum_{q}\left(\hat\theta_{p',q}\hat W_{p,q}+\hat\theta_{p,q}\hat W_{q,p'}\right) :\hat a_p^\dagger \hat a_{p'}^\dagger: \qquad \text{(A.31)}
\end{aligned}
$$

Next is A.30b:

$$
\sum_{p,p'}\sum_{q\neq q'}\hat\theta_{q,q'}\left[:\hat a_q^\dagger \hat a_{q'}:, \hat W_{p,p'}\right] :\hat a_p^\dagger \hat a_{p'}^\dagger:
$$

$$
\begin{aligned}
&= \sum_{p,p'} \sum_{q\neq q'} \hat{\theta}_{q,q'} \left(\hat{W}_{p,p'}(\hat{n}_{q'}+1, \hat{n}_q - 1) - \hat{W}_{p,p'} \right) \quad \underbrace{: \hat{a}^\dagger_q \hat{a}_{q'} :: \hat{a}^\dagger_p \hat{a}^\dagger_{p'} :}_{\overset{②}{=} \delta_{q',p} : \hat{a}^\dagger_{p'} \hat{a}^\dagger_q : + \delta_{q',p'} : \hat{a}^\dagger_p \hat{a}^\dagger_q :} \\
&\overset{②}{=} \sum_{p,p'} \sum_{q} \hat{\theta}_{q,p} \left(\hat{W}_{p,p'}(\hat{n}_p+1, \hat{n}_q - 1) - \hat{W}_{p,p'} \right) : \hat{a}^\dagger_{p'} \hat{a}^\dagger_q : \\
&+ \sum_{p,p'} \sum_{q} \hat{\theta}_{q,p'} \left(\hat{W}_{p,p'}(\hat{n}_{p'}+1, \hat{n}_q - 1) - \hat{W}_{p,p'} \right) : \hat{a}^\dagger_p \hat{a}^\dagger_q : \\
&= \sum_{p,p'} \sum_{q} \hat{\theta}_{p,q} \left(\hat{W}_{q,p'}(\hat{n}_q+1, \hat{n}_p - 1) - \hat{W}_{q,p'} \right) : \hat{a}^\dagger_p \hat{a}^\dagger_{p'} : \\
&+ \sum_{p,p'} \sum_{q} \hat{\theta}_{p',q} \left(\hat{W}_{p,q}(\hat{n}_q+1, \hat{n}_{p'} - 1) - \hat{W}_{p,q} \right) : \hat{a}^\dagger_p \hat{a}^\dagger_{p'} :
\end{aligned} \tag{A.32}
$$

A.30c gives no quadratic contribution:

$$
\begin{aligned}
&\sum_{p,p'} \sum_{\tilde{q}\neq\tilde{q}'} \hat{W}_{p,p'} \left[\hat{\theta}_{\tilde{q},\tilde{q}'}, : \hat{a}^\dagger_p \hat{a}^\dagger_{p'} : \right] : \hat{a}^\dagger_{\tilde{q}} \hat{a}_{\tilde{q}'} \\
&= \sum_{p,p'} \sum_{\tilde{q}\neq\tilde{q}'} \hat{W}_{p,p'} \left(\hat{\theta}_{\tilde{q},\tilde{q}'} - \hat{\theta}_{\tilde{q},\tilde{q}'}(\hat{n}_{p'}, \hat{n}_p - 1) \right) \underbrace{: \hat{a}^\dagger_p \hat{a}^\dagger_{p'} :: \hat{a}^\dagger_{\tilde{q}} \hat{a}_{\tilde{q}'} :}_{=: \hat{a}^\dagger_p \hat{a}^\dagger_{p'} \hat{a}^\dagger_{\tilde{q}} \hat{a}_{\tilde{q}'} :} \overset{②}{=} 0
\end{aligned} \tag{A.33}
$$

A.25c:

$$
\sum_{p,p'} \sum_{\tilde{q}\neq\tilde{q}'} \left[\hat{\theta}_{\tilde{q},\tilde{q}'} : \hat{a}^\dagger_{\tilde{q}} \hat{a}_{\tilde{q}'} :, \hat{W}'_{p,p'} : \hat{a}_p \hat{a}_{p'} : \right]
$$

$$
= \sum_{p,p'} \sum_{\tilde{q}\neq\tilde{q}'} \hat{\theta}_{\tilde{q},\tilde{q}'} \hat{W}'_{p,p'} \left[: \hat{a}^\dagger_{\tilde{q}} \hat{a}_{\tilde{q}'} :, : \hat{a}_p \hat{a}_{p'} : \right] \tag{A.34a}
$$

$$
+ \sum_{p,p'} \sum_{\tilde{q}\neq\tilde{q}'} \hat{\theta}_{\tilde{q},\tilde{q}'} \left[: \hat{a}^\dagger_{\tilde{q}} \hat{a}_{\tilde{q}'} :, \hat{W}'_{p,p'} \right] : \hat{a}_p \hat{a}_{p'} : \tag{A.34b}
$$

$$
+ \sum_{p,p'} \sum_{\tilde{q}\neq\tilde{q}'} \hat{W}'_{p,p'} \left[\hat{\theta}_{\tilde{q},\tilde{q}'}, : \hat{a}_p \hat{a}_{p'} : \right] : \hat{a}^\dagger_{\tilde{q}} \hat{a}_{\tilde{q}'} : \tag{A.34c}
$$

We will again start by evaluating A.34a:

$$
\begin{aligned}
&\sum_{p,p'} \sum_{q\neq q'} \hat{\theta}_{q,q'} \hat{W}'_{p,p'} \left[: \hat{a}^\dagger_q \hat{a}_{q'} :, : \hat{a}_p \hat{a}_{p'} : \right] \\
&= \sum_{p,p'} \sum_{q\neq q'} \hat{\theta}_{q,q'} \hat{W}'_{p,p'} \left(\delta_{q,p'} : \hat{a}_p \hat{a}_{q'} : + \delta_{q,p} : \hat{a}_{p'} \hat{a}_{q'} : \right) \\
&= \sum_{p,p'} \sum_{q'} \hat{\theta}_{p',q'} \hat{W}'_{p,p'} : \hat{a}_p \hat{a}_{q'} : + \sum_{p,p'} \sum_{q'} \hat{\theta}_{p,q'} \hat{W}'_{p,p'} : \hat{a}_{p'} \hat{a}_{q'} : \\
&= \sum_{p,p'} \sum_{q} \left(\hat{\theta}_{q,p'} \hat{W}'_{p,q} + \hat{\theta}_{q,p} \hat{W}'_{q,p'} \right) : \hat{a}_p \hat{a}_{p'} :
\end{aligned} \tag{A.35}
$$

A.34b gives no quadratic contribution:

$$
\begin{aligned}
&\sum_{p,p'} \sum_{\tilde{q}\neq\tilde{q}'} \hat{\theta}_{\tilde{q},\tilde{q}'} \left[: \hat{a}^\dagger_{\tilde{q}} \hat{a}_{\tilde{q}'} :, \hat{W}'_{p,p'} \right] : \hat{a}_p \hat{a}_{p'} : \\
&= \sum_{p,p'} \sum_{\tilde{q}\neq\tilde{q}'} \hat{\theta}_{\tilde{q},\tilde{q}'} \left(W'_{p,p'}(\hat{n}_{q'}+1, \hat{n}_q - 1) - W'_{p,p'} \right) \underbrace{: \hat{a}^\dagger_{\tilde{q}} \hat{a}_{\tilde{q}'} :: \hat{a}_p \hat{a}_{p'} :}_{=: \hat{a}^\dagger_{\tilde{q}} \hat{a}_{\tilde{q}'} \hat{a}_p \hat{a}_{p'} :} \overset{②}{=} 0
\end{aligned} \tag{A.36}
$$

A.34c:

$$\sum_{p,p'}\sum_{q\neq q'}\hat{W}'_{p,p'}\left[\hat{\theta}_{q,q'},:\hat{a}_p\hat{a}_{p'}:\right]:\hat{a}_q^\dagger\hat{a}_{q'}:$$

$$=\sum_{p,p'}\sum_{q\neq q'}\hat{W}'_{p,p'}\left(\hat{\theta}_{q,q'}-\hat{\theta}_{q,q'}(\hat{n}_{p'}+1,\hat{n}_p+1)\right):\hat{a}_p\hat{a}_{p'}::\hat{a}_q^\dagger\hat{a}_{q'}: \tag{A.37}$$

$$\overset{②}{=}\sum_{p,p'}\sum_{q\neq q'}\hat{W}'_{p,p'}\left(\hat{\theta}_{q,q'}-\hat{\theta}_{q,q'}(\hat{n}_{p'}+1,\hat{n}_p+1)\right)(\delta_{p,q}:\hat{a}_{p'}\hat{a}_{q'}:+\delta_{p',q}:\hat{a}_p\hat{a}_{q'}:)$$

$$=\sum_{p,p'}\sum_{q'}\hat{W}'_{p,p'}\left(\hat{\theta}_{p,q'}-\hat{\theta}_{p,q'}(\hat{n}_{p'}+1,\hat{n}_p+1)\right):\hat{a}_{p'}\hat{a}_{q'}: \tag{A.38}$$

$$+\sum_{p,p'}\sum_{q'}\hat{W}'_{p,p'}\left(\hat{\theta}_{p',q'}-\hat{\theta}_{p',q'}(\hat{n}_{p'}+1,\hat{n}_p+1)\right):\hat{a}_p\hat{a}_{q'}:$$

$$=\sum_{p,p'}\sum_{q}\hat{W}'_{q,p'}\left(\hat{\theta}_{q,p}-\hat{\theta}_{q,p}(\hat{n}_{p'}+1,\hat{n}_q+1)\right):\hat{a}_p\hat{a}_{p'}: \tag{A.39}$$

$$+\sum_{p,p'}\sum_{q}\hat{W}'_{p,q}\left(\hat{\theta}_{q,p'}-\hat{\theta}_{q,p'}(\hat{n}_q+1,\hat{n}_p+1)\right):\hat{a}_p\hat{a}_{p'}:$$

$$=\sum_{p,p'}\sum_{q}\left(\hat{W}'_{q,p'}+\hat{W}'_{p',q}\right)\left(\hat{\theta}_{q,p}-\hat{\theta}_{q,p}(\hat{n}_{p'}+1,\hat{n}_q+1)\right):\hat{a}_p\hat{a}_{p'}: \tag{A.40}$$

A.25d: Follows immediately from the calculations already done for A.25b:

$$\sum_{q\neq q'}\sum_{\tilde{p},\tilde{p}'}\left[\hat{\phi}_{\tilde{p},\tilde{p}'}:\hat{a}_{\tilde{p}}^\dagger\hat{a}_{\tilde{p}'}^\dagger:,\hat{V}_{q,q'}:\hat{a}_q^\dagger\hat{a}_{q'}:\right] \tag{A.41a}$$

$$=-\sum_{q\neq q'}\sum_{p,p'}\left[\hat{V}_{q,q'}:\hat{a}_q^\dagger\hat{a}_{q'}:,\hat{\phi}_{p,p'}:\hat{a}_p^\dagger\hat{a}_{p'}^\dagger:\right] \tag{A.41b}$$

$$=-\sum_{p,p'}\sum_{q}\left(\hat{V}_{p',q}\hat{\phi}_{p,q}+\hat{V}_{p,q}\hat{\phi}_{q,p'}\right):\hat{a}_p^\dagger\hat{a}_{p'}^\dagger: \tag{A.41c}$$

$$-\sum_{p,p'}\sum_{q}\hat{V}_{p,q}\left(\hat{\phi}_{q,p'}(\hat{n}_q+1,\hat{n}_p-1)-\hat{\phi}_{q,p'}\right):\hat{a}_p^\dagger\hat{a}_{p'}^\dagger:$$

$$-\sum_{p,p'}\sum_{q}\hat{V}_{p',q}\left(\hat{\phi}_{p,q}(\hat{n}_q+1,\hat{n}_{p'}-1)-\hat{\phi}_{p,q}\right):\hat{a}_p^\dagger\hat{a}_{p'}^\dagger:$$

A.25e:

$$\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\left[\hat{\phi}_{\tilde{p},\tilde{p}'}:\hat{a}_{\tilde{p}}^\dagger\hat{a}_{\tilde{p}'}^\dagger:,\hat{W}_{p,p'}:\hat{a}_p^\dagger\hat{a}_{p'}^\dagger:\right]$$

$$=\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\hat{\phi}_{\tilde{p},\tilde{p}'}\left[:\hat{a}_{\tilde{p}}^\dagger\hat{a}_{\tilde{p}'}^\dagger:,\hat{W}_{p,p'}\right]:\hat{a}_p^\dagger\hat{a}_{p'}^\dagger: \tag{A.42a}$$

$$+\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\hat{W}_{p,p'}\left[\hat{\phi}_{\tilde{p},\tilde{p}'},:\hat{a}_p^\dagger\hat{a}_{p'}^\dagger:\right]:\hat{a}_{\tilde{p}}^\dagger\hat{a}_{\tilde{p}'}^\dagger: \tag{A.42b}$$

A.42a will be analyzed first:

$$\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\hat{\phi}_{\tilde{p},\tilde{p}'}\left[:\hat{a}_{\tilde{p}}^\dagger\hat{a}_{\tilde{p}'}^\dagger:,\hat{W}_{p,p'}\right]:\hat{a}_p^\dagger\hat{a}_{p'}^\dagger:$$

$$=\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\hat{\phi}_{\tilde{p},\tilde{p}'}\left(\hat{W}_{p,p'}(\hat{n}_{\tilde{p}}+1,\hat{n}_{\tilde{p}'}+1)-\hat{W}_{p,p'}\right):\hat{a}_{\tilde{p}}^\dagger\hat{a}_{\tilde{p}'}^\dagger::\hat{a}_p^\dagger\hat{a}_{p'}^\dagger:\overset{②}{=}0 \tag{A.43}$$

Similiarly, A.42b also gives no quadratic contribution.

A.25f

$$
\begin{aligned}
&\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\left[\hat{\phi}_{\tilde{p},\tilde{p}'}:\hat{a}^\dagger_{\tilde{p}}\hat{a}^\dagger_{\tilde{p}'}:,\hat{W}'_{p,p'}:\hat{a}_p\hat{a}_{p'}:\right]\\
&=\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\hat{\phi}_{\tilde{p},\tilde{p}'}\hat{W}'_{p,p'}\left[:\hat{a}^\dagger_{\tilde{p}}\hat{a}^\dagger_{\tilde{p}'}:,:\hat{a}_p\hat{a}_{p'}:\right] &\text{(A.44a)}\\
&+\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\hat{\phi}_{\tilde{p},\tilde{p}'}\left[:\hat{a}^\dagger_{\tilde{p}}\hat{a}^\dagger_{\tilde{p}'}:,\hat{W}'_{p,p'}\right]:\hat{a}_p\hat{a}_{p'}: &\text{(A.44b)}\\
&+\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\hat{W}'_{p,p'}\left[\hat{\phi}_{\tilde{p},\tilde{p}'},:\hat{a}_p\hat{a}_{p'}:\right]:\hat{a}^\dagger_{\tilde{p}}\hat{a}^\dagger_{\tilde{p}'}: &\text{(A.44c)}
\end{aligned}
$$

A.44a:

$$
\begin{aligned}
&\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\hat{\phi}_{\tilde{p},\tilde{p}'}\hat{W}'_{p,p'}\left(\delta_{p',\tilde{p}'}\hat{a}_p\hat{a}^\dagger_{\tilde{p}}+\delta_{p',\tilde{p}}\hat{a}_p\hat{a}^\dagger_{\tilde{p}'}+\delta_{p,\tilde{p}'}\hat{a}^\dagger_{\tilde{p}}\hat{a}_{p'}+\delta_{p,\tilde{p}}\hat{a}^\dagger_{\tilde{p}'}\hat{a}_{p'}\right)\\
&=-\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\hat{\phi}_{\tilde{p},\tilde{p}'}\hat{W}'_{p,p'}\delta_{p',\tilde{p}'}\left(:\hat{a}^\dagger_{\tilde{p}}\hat{a}_p:+\delta_{p,\tilde{p}}\right) &\text{(A.45)}\\
&-\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\hat{\phi}_{\tilde{p},\tilde{p}'}\hat{W}'_{p,p'}\delta_{p',\tilde{p}}\left(:\hat{a}^\dagger_{\tilde{p}'}\hat{a}_p:+\delta_{\tilde{p}',p}\right)\\
&-\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\hat{\phi}_{\tilde{p},\tilde{p}'}\hat{W}'_{p,p'}\delta_{p,\tilde{p}'}:\hat{a}^\dagger_{\tilde{p}}\hat{a}_{p'}:\\
&-\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\hat{\phi}_{\tilde{p},\tilde{p}'}\hat{W}'_{p,p'}\delta_{p,\tilde{p}}:\hat{a}^\dagger_{\tilde{p}'}\hat{a}_{p'}:\\
&=-\sum_{p,p'}\sum_{\tilde{p}}\hat{\phi}_{\tilde{p},p'}\hat{W}'_{p,p'}:\hat{a}^\dagger_{\tilde{p}}\hat{a}_p: &\text{(A.46)}\\
&-\sum_{p,p'}\sum_{\tilde{p}'}\hat{\phi}_{p',\tilde{p}'}\hat{W}'_{p,p'}:\hat{a}^\dagger_{\tilde{p}'}\hat{a}_p:\\
&-\sum_{p,p'}\sum_{\tilde{p}}\hat{\phi}_{\tilde{p},p}\hat{W}'_{p,p'}:\hat{a}^\dagger_{\tilde{p}}\hat{a}_{p'}:\\
&-\sum_{p,p'}\sum_{\tilde{p}'}\hat{\phi}_{p,\tilde{p}'}\hat{W}'_{p,p'}:\hat{a}^\dagger_{\tilde{p}'}\hat{a}_{p'}:\\
&-\sum_{p,p'}\left(\hat{\phi}_{p,p'}\hat{W}'_{p,p'}+\hat{\phi}_{p',p}\hat{W}'_{p,p'}\right)\\
&=-\sum_{p,p'}\sum_{\tilde{p}}\hat{\phi}_{p,\tilde{p}}\hat{W}'_{p',\tilde{p}}:\hat{a}^\dagger_{p}\hat{a}_{p'}: &\text{(A.47)}\\
&-\sum_{p,p'}\sum_{\tilde{p}}\hat{\phi}_{\tilde{p},p}\hat{W}'_{p',\tilde{p}}:\hat{a}^\dagger_{p}\hat{a}_{p'}:\\
&-\sum_{p,p'}\sum_{\tilde{p}}\hat{\phi}_{p,\tilde{p}}\hat{W}'_{\tilde{p},p'}:\hat{a}^\dagger_{p}\hat{a}_{p'}:\\
&-\sum_{p,p'}\sum_{\tilde{p}}\hat{\phi}_{\tilde{p},p}\hat{W}'_{\tilde{p},p'}:\hat{a}^\dagger_{p}\hat{a}_{p'}:\\
&-\sum_{p,p'}\left(\hat{\phi}_{p,p'}\hat{W}'_{p,p'}+\hat{\phi}_{p',p}\hat{W}'_{p,p'}\right)\\
&=-\sum_{p,p'}\sum_{\tilde{p}}\left(\hat{\phi}_{p,\tilde{p}}\hat{W}'_{p',\tilde{p}}+\hat{\phi}_{\tilde{p},p}\hat{W}'_{p',\tilde{p}}+\hat{\phi}_{p,\tilde{p}}\hat{W}'_{\tilde{p},p'}+\hat{\phi}_{\tilde{p},p}\hat{W}'_{\tilde{p},p'}\right):\hat{a}^\dagger_{p}\hat{a}_{p'}: &\text{(A.48)}\\
&-\sum_{p,p'}\left(\hat{\phi}_{p,p'}\hat{W}'_{p,p'}+\hat{\phi}_{p',p}\hat{W}'_{p,p'}\right)
\end{aligned}
$$

A.44b gives no quadratic contribution:

$$\begin{aligned}
&\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\hat{\phi}_{\tilde{p},\tilde{p}'}\left[:\hat{a}^\dagger_{\tilde{p}}\hat{a}^\dagger_{\tilde{p}'}:,\hat{W}'_{p,p'}\right]:\hat{a}_p\hat{a}_{p'}:\\
&=\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\hat{\phi}_{\tilde{p},\tilde{p}'}\left(\hat{W}'_{p,p'}(\hat{n}_p-1,\hat{n}_{p'}-1)-\hat{W}'_{p,p'}\right):\hat{a}^\dagger_{\tilde{p}}\hat{a}^\dagger_{\tilde{p}'}::\hat{a}_p\hat{a}_{p'}:\\
&=\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\hat{\phi}_{\tilde{p},\tilde{p}'}\left(\hat{W}'_{p,p'}(\hat{n}_p-1,\hat{n}_{p'}-1)-\hat{W}'_{p,p'}\right):\hat{a}^\dagger_{\tilde{p}}\hat{a}^\dagger_{\tilde{p}'}\hat{a}_p\hat{a}_{p'}:\overset{②}{=}0
\end{aligned}\tag{A.49}$$

A.44c:

$$\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\hat{W}'_{p,p'}\left[\hat{\phi}_{\tilde{p},\tilde{p}'},:\hat{a}_p\hat{a}_{p'}:\right]:\hat{a}^\dagger_{\tilde{p}}\hat{a}^\dagger_{\tilde{p}'}:$$

$$=\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\hat{W}'_{p,p'}\left(\hat{\phi}_{\tilde{p},\tilde{p}'}-\hat{\phi}_{\tilde{p},\tilde{p}'}(\hat{n}_p+1,\hat{n}_{p'}+1)\right):\hat{a}_p\hat{a}_{p'}::\hat{a}^\dagger_{\tilde{p}}\hat{a}^\dagger_{\tilde{p}'}:\tag{A.50}$$

$$\overset{②}{=}\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\hat{W}'_{p,p'}\left(\hat{\phi}_{\tilde{p},\tilde{p}'}-\hat{\phi}_{\tilde{p},\tilde{p}'}(\hat{n}_p+1,\hat{n}_{p'}+1)\right)\delta_{p,\tilde{p}}:\hat{a}^\dagger_{\tilde{p}'}\hat{a}_{p'}:\tag{A.51}$$

$$\begin{aligned}
&+\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\hat{W}'_{p,p'}\left(\hat{\phi}_{\tilde{p},\tilde{p}'}-\hat{\phi}_{\tilde{p},\tilde{p}'}(\hat{n}_p+1,\hat{n}_{p'}+1)\right)\delta_{p,\tilde{p}'}:\hat{a}^\dagger_{\tilde{p}}\hat{a}_{p'}:\\
&+\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\hat{W}'_{p,p'}\left(\hat{\phi}_{\tilde{p},\tilde{p}'}-\hat{\phi}_{\tilde{p},\tilde{p}'}(\hat{n}_p+1,\hat{n}_{p'}+1)\right)\delta_{p',\tilde{p}}:\hat{a}^\dagger_{\tilde{p}'}\hat{a}_{p}:\\
&+\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\hat{W}'_{p,p'}\left(\hat{\phi}_{\tilde{p},\tilde{p}'}-\hat{\phi}_{\tilde{p},\tilde{p}'}(\hat{n}_p+1,\hat{n}_{p'}+1)\right)\delta_{p',\tilde{p}'}:\hat{a}^\dagger_{\tilde{p}}\hat{a}_{p}:\\
&+\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\hat{W}'_{p,p'}\left(\hat{\phi}_{\tilde{p},\tilde{p}'}-\hat{\phi}_{\tilde{p},\tilde{p}'}(\hat{n}_p+1,\hat{n}_{p'}+1)\right)\delta_{p',\tilde{p}}\delta_{p,\tilde{p}'}\\
&+\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\hat{W}'_{p,p'}\left(\hat{\phi}_{\tilde{p},\tilde{p}'}-\hat{\phi}_{\tilde{p},\tilde{p}'}(\hat{n}_p+1,\hat{n}_{p'}+1)\right)\delta_{p',\tilde{p}'}\delta_{p,\tilde{p}}
\end{aligned}$$

$$=\sum_{p,p'}\sum_{\tilde{p}'}\hat{W}'_{p,p'}\left(\hat{\phi}_{p,\tilde{p}'}-\hat{\phi}_{p,\tilde{p}'}(\hat{n}_p+1,\hat{n}_{p'}+1)\right):\hat{a}^\dagger_{\tilde{p}'}\hat{a}_{p'}:\tag{A.52}$$

$$\begin{aligned}
&+\sum_{p,p'}\sum_{\tilde{p}}\hat{W}'_{p,p'}\left(\hat{\phi}_{\tilde{p},p}-\hat{\phi}_{\tilde{p},p}(\hat{n}_p+1,\hat{n}_{p'}+1)\right):\hat{a}^\dagger_{\tilde{p}}\hat{a}_{p'}:\\
&+\sum_{p,p'}\sum_{\tilde{p}'}\hat{W}'_{p,p'}\left(\hat{\phi}_{p',\tilde{p}'}-\hat{\phi}_{p',\tilde{p}'}(\hat{n}_p+1,\hat{n}_{p'}+1)\right):\hat{a}^\dagger_{\tilde{p}'}\hat{a}_{p}:\\
&+\sum_{p,p'}\sum_{\tilde{p}}\hat{W}'_{p,p'}\left(\hat{\phi}_{\tilde{p},p'}-\hat{\phi}_{\tilde{p},p'}(\hat{n}_p+1,\hat{n}_{p'}+1)\right):\hat{a}^\dagger_{\tilde{p}}\hat{a}_{p}:\\
&+\sum_{p,p'}\hat{W}'_{p,p'}\left(\hat{\phi}_{p',p}-\hat{\phi}_{p',p}(\hat{n}_p+1,\hat{n}_{p'}+1)\right)\\
&+\sum_{p,p'}\hat{W}'_{p,p'}\left(\hat{\phi}_{p,p'}-\hat{\phi}_{p,p'}(\hat{n}_p+1,\hat{n}_{p'}+1)\right)
\end{aligned}$$

$$=\sum_{p,p'}\sum_{\tilde{p}}\hat{W}'_{\tilde{p},p'}\left(\hat{\phi}_{\tilde{p},p}-\hat{\phi}_{\tilde{p},p}(\hat{n}_{\tilde{p}}+1,\hat{n}_{p'}+1)\right):\hat{a}^\dagger_{p}\hat{a}_{p'}:\tag{A.53}$$

$$\begin{aligned}
&+\sum_{p,p'}\sum_{\tilde{p}}\hat{W}'_{\tilde{p},p'}\left(\hat{\phi}_{p,\tilde{p}}-\hat{\phi}_{p,\tilde{p}}(\hat{n}_{\tilde{p}}+1,\hat{n}_{p'}+1)\right):\hat{a}^\dagger_{p}\hat{a}_{p'}:\\
&+\sum_{p,p'}\sum_{\tilde{p}}\hat{W}'_{p',\tilde{p}}\left(\hat{\phi}_{\tilde{p},p}-\hat{\phi}_{\tilde{p},p}(\hat{n}_{p'}+1,\hat{n}_{\tilde{p}}+1)\right):\hat{a}^\dagger_{p}\hat{a}_{p'}:\\
&+\sum_{p,p'}\sum_{\tilde{p}}\hat{W}'_{p',\tilde{p}}\left(\hat{\phi}_{p,\tilde{p}}-\hat{\phi}_{p,\tilde{p}}(\hat{n}_{p'}+1,\hat{n}_{\tilde{p}}+1)\right):\hat{a}^\dagger_{p}\hat{a}_{p'}:
\end{aligned}$$

$$+\sum_{p,p'}\hat{W}'_{p,p'}\left(\hat{\phi}_{p',p}-\hat{\phi}_{p',p}(\hat{n}_p+1,\hat{n}_{p'}+1)\right)$$
$$+\sum_{p,p'}\hat{W}'_{p,p'}\left(\hat{\phi}_{p,p'}-\hat{\phi}_{p,p'}(\hat{n}_p+1,\hat{n}_{p'}+1)\right)$$

A.25g: Follows immediately from A.25c:

$$\begin{aligned}
&\sum_{q\neq q'}\sum_{\tilde{p},\tilde{p}'}\left[\hat{\psi}_{\tilde{p},\tilde{p}'}:\hat{a}_{\tilde{p}}\hat{a}_{\tilde{p}'}:,\hat{V}_{q,q'}:\hat{a}^\dagger_q\hat{a}_{q'}:\right]\\
&=-\sum_{p,p'}\sum_{\tilde{q}\neq\tilde{q}'}\left[\hat{V}_{\tilde{q},\tilde{q}'}:\hat{a}^\dagger_{\tilde{q}}\hat{a}_{\tilde{q}'}:,\hat{\psi}_{p,p'}:\hat{a}_p\hat{a}_{p'}:\right]\\
&\overset{②}{=}-\sum_{p,p'}\sum_{q}\left(\hat{V}_{q,p'}\hat{\psi}_{p,q}+\hat{\theta}_{q,p}\hat{\psi}_{q,p'}\right):\hat{a}_p\hat{a}_{p'}: \qquad \text{(A.54a)}\\
&-\sum_{p,p'}\sum_{q}\left(\hat{\psi}_{q,p'}+\hat{\psi}_{p',q}\right)\left(\hat{V}_{q,p}-\hat{V}_{q,p}(\hat{n}_{p'}+1,\hat{n}_q+1)\right):\hat{a}_p\hat{a}_{p'}:
\end{aligned}$$

A.25h Follows immediately from A.25f:

$$\begin{aligned}
&\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\left[\hat{\psi}_{\tilde{p},\tilde{p}'}:\hat{a}_{\tilde{p}}\hat{a}_{\tilde{p}'}:,\hat{W}_{p,p'}:\hat{a}^\dagger_p\hat{a}^\dagger_{p'}:\right]\\
&=-\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\left[\hat{W}_{\tilde{p},\tilde{p}'}:\hat{a}^\dagger_{\tilde{p}}\hat{a}^\dagger_{\tilde{p}'}:,\hat{\psi}_{p,p'}:\hat{a}_p\hat{a}_{p'}:\right] \qquad \text{(A.55)}\\
&=\sum_{p,p'}\sum_{\tilde{p}}\left(\hat{W}_{p,\tilde{p}}\hat{\psi}_{p',\tilde{p}}+\hat{W}_{\tilde{p},p}\hat{\psi}_{p',\tilde{p}}+\hat{W}_{p,\tilde{p}}\hat{\psi}_{\tilde{p},p'}+\hat{W}_{\tilde{p},p}\hat{\psi}_{\tilde{p},p'}\right):\hat{a}^\dagger_p\hat{a}_{p'}: \qquad \text{(A.56)}\\
&+\sum_{p,p'}\left(\hat{W}_{p,p'}\hat{\psi}_{p,p'}+\hat{W}_{p',p}\hat{\psi}_{p,p'}\right)\\
&-\sum_{p,p'}\sum_{\tilde{p}}\hat{\psi}_{\tilde{p},p'}\left(\hat{W}_{\tilde{p},p}-\hat{W}_{\tilde{p},p}(\hat{n}_{\tilde{p}}+1,\hat{n}_{p'}+1)\right):\hat{a}^\dagger_p\hat{a}_{p'}:\\
&-\sum_{p,p'}\sum_{\tilde{p}}\hat{\psi}_{\tilde{p},p'}\left(\hat{W}_{p,\tilde{p}}-\hat{W}_{p,\tilde{p}}(\hat{n}_{\tilde{p}}+1,\hat{n}_{p'}+1)\right):\hat{a}^\dagger_p\hat{a}_{p'}:\\
&-\sum_{p,p'}\sum_{\tilde{p}}\hat{\psi}_{p',\tilde{p}}\left(\hat{W}_{\tilde{p},p}-\hat{W}_{\tilde{p},p}(\hat{n}_{p'}+1,\hat{n}_{\tilde{p}}+1)\right):\hat{a}^\dagger_p\hat{a}_{p'}:\\
&-\sum_{p,p'}\sum_{\tilde{p}}\hat{\psi}_{p',\tilde{p}}\left(\hat{W}_{p,\tilde{p}}-\hat{W}_{p,\tilde{p}}(\hat{n}_{p'}+1,\hat{n}_{\tilde{p}}+1)\right):\hat{a}^\dagger_p\hat{a}_{p'}:\\
&-\sum_{p,p'}\hat{\psi}_{p,p'}\left(\hat{W}_{p',p}-\hat{W}_{p',p}(\hat{n}_p+1,\hat{n}_{p'}+1)\right)\\
&-\sum_{p,p'}\hat{\psi}_{p,p'}\left(\hat{W}_{p,p'}-\hat{W}_{p,p'}(\hat{n}_p+1,\hat{n}_{p'}+1)\right)
\end{aligned}$$

A.25i: Similiar to A.25e:

$$\sum_{p,p'}\sum_{\tilde{p},\tilde{p}'}\left[\hat{\psi}_{\tilde{p},\tilde{p}'}:\hat{a}_{\tilde{p}}\hat{a}_{\tilde{p}'}:,\hat{W}'_{p,p'}:\hat{a}_p\hat{a}_{p'}:\right]\overset{②}{=}0 \qquad \text{(A.57)}$$

A.2.3 The Flow Equations

We conclude that $\hat{\mathcal{H}}(\lambda)$ is of the form

$$\hat{\mathcal{H}}(\lambda)\overset{②}{=}\hat{H}+\sum_{q\neq q'}\hat{V}_{q,q'}(\lambda):\hat{a}^\dagger_q\hat{a}_{q'}: \qquad \text{(A.58)}$$

$$+\sum_{p,p'}\left(\hat{W}_{p,p'}(\lambda):\hat{a}^\dagger_p\hat{a}^\dagger_{p'}:+\hat{W}'_{p,p'}(\lambda):\hat{a}_p\hat{a}_{p'}:\right)$$

where $\hat{\epsilon}(\lambda)$ is an operator which indicates a shift in the energy scale.
Collecting all terms in $\partial_\lambda\hat{\mathcal{H}}(\lambda)=[\hat{\eta}(\lambda),\hat{\mathcal{H}}(\lambda)]$ gives the following flow equations $\forall k,p,p',q,q'$ where $q\neq q'$:

$$\begin{aligned}
\partial_\lambda\hat{V}_{q,q'} \overset{②}{=} &-\hat{V}_{q,q'}\left(\hat{H}-\hat{H}(\hat{n}_q-1,\hat{n}_{q'}+1)\right)^2 \\
&+\sum_{\tilde{q}}\left(\hat{\theta}_{q,q'}\hat{V}_{q',\tilde{q}}-\hat{\theta}_{\tilde{q},q'}\hat{V}_{q,\tilde{q}}\right) \\
&+\sum_{\tilde{q}}\hat{V}_{q,\tilde{q}}\left(\hat{\theta}_{\tilde{q},q'}-\hat{\theta}_{\tilde{q},q'}(\hat{n}_{\tilde{q}}+1,\hat{n}_q-1)\right) \\
&-\sum_{\tilde{q}}\hat{\theta}_{q,\tilde{q}}\left(\hat{V}_{\tilde{q},q'}-\hat{V}_{\tilde{q},q'}(\hat{n}_{\tilde{q}}+1,\hat{n}_q-1)\right) \\
&-\sum_{\tilde{q}}\left(\hat{\phi}_{q,\tilde{q}}\hat{W}'_{q',\tilde{q}}+\hat{\phi}_{\tilde{q},q}\hat{W}'_{q',\tilde{q}}+\hat{\phi}_{q,\tilde{q}}\hat{W}'_{\tilde{q},q'}+\hat{\phi}_{\tilde{q},q}\hat{W}'_{\tilde{q},q'}\right) \\
&+\sum_{\tilde{q}}\hat{W}'_{\tilde{q},q'}\left(\hat{\phi}_{\tilde{q},q}-\hat{\phi}_{\tilde{q},q}(\hat{n}_{\tilde{q}}+1,\hat{n}_{q'}+1)\right) \\
&+\sum_{\tilde{q}}\hat{W}'_{\tilde{q},q'}\left(\hat{\phi}_{q,\tilde{q}}-\hat{\phi}_{q,\tilde{q}}(\hat{n}_{\tilde{q}}+1,\hat{n}_{q'}+1)\right) \\
&+\sum_{\tilde{q}}\hat{W}'_{q',\tilde{q}}\left(\hat{\phi}_{\tilde{q},q}-\hat{\phi}_{\tilde{q},q}(\hat{n}_{q'}+1,\hat{n}_{\tilde{q}}+1)\right) \\
&+\sum_{\tilde{q}}\hat{W}'_{q',\tilde{q}}\left(\hat{\phi}_{q,\tilde{q}}-\hat{\phi}_{q,\tilde{q}}(\hat{n}_{q'}+1,\hat{n}_{\tilde{q}}+1)\right) \\
&+\sum_{\tilde{q}}\left(\hat{W}_{q,\tilde{q}}\hat{\psi}_{q',\tilde{q}}+\hat{W}_{\tilde{q},q}\hat{\psi}_{q',\tilde{q}}+\hat{W}_{q,\tilde{q}}\hat{\psi}_{\tilde{q},q'}+\hat{W}_{\tilde{q},q}\hat{\psi}_{\tilde{q},q'}\right) \\
&-\sum_{\tilde{q}}\hat{\psi}_{\tilde{q},q'}\left(\hat{W}_{\tilde{q},q}-\hat{W}_{\tilde{q},q}(\hat{n}_{\tilde{q}}+1,\hat{n}_{q'}+1)\right) \\
&-\sum_{\tilde{q}}\hat{\psi}_{\tilde{q},q'}\left(\hat{W}_{q,\tilde{q}}-\hat{W}_{q,\tilde{q}}(\hat{n}_{\tilde{q}}+1,\hat{n}_{q'}+1)\right) \\
&-\sum_{\tilde{q}}\hat{\psi}_{q',\tilde{q}}\left(\hat{W}_{\tilde{q},q}-\hat{W}_{\tilde{q},q}(\hat{n}_{q'}+1,\hat{n}_{\tilde{q}}+1)\right) \\
&-\sum_{\tilde{q}}\hat{\psi}_{q',\tilde{q}}\left(\hat{W}_{q,\tilde{q}}-\hat{W}_{q,\tilde{q}}(\hat{n}_{q'}+1,\hat{n}_{\tilde{q}}+1)\right)
\end{aligned} \tag{A.59a}$$

$$\begin{aligned}
\partial_\lambda\hat{W}_{p,p'} \overset{②}{=} &-\hat{W}_{p,p'}\left(\hat{H}-\hat{H}(\hat{n}_{p'}-1,\hat{n}_p-1)\right)^2 \\
&+\sum_q\left(\hat{\theta}_{p',q}\hat{W}_{p,q}+\hat{\theta}_{p,q}\hat{W}_{q,p'}\right) \\
&+\sum_q\hat{\theta}_{p,q}\left(\hat{W}_{q,p'}(\hat{n}_q+1,\hat{n}_p-1)-\hat{W}_{q,p'}\right) \\
&+\sum_q\hat{\theta}_{p',q}\left(\hat{W}_{p,q}(\hat{n}_q+1,\hat{n}_{p'}-1)-\hat{W}_{p,q}\right) \\
&-\sum_q\left(\hat{V}_{p',q}\hat{\phi}_{p,q}+\hat{V}_{p,q}\hat{\phi}_{q,p'}\right) \\
&-\sum_q\hat{V}_{p,q}\left(\hat{\phi}_{q,p'}(\hat{n}_q+1,\hat{n}_p-1)-\hat{\phi}_{q,p'}\right) \\
&-\sum_q\hat{V}_{p',q}\left(\hat{\phi}_{p,q}(\hat{n}_q+1,\hat{n}_{p'}-1)-\hat{\phi}_{p,q}\right)
\end{aligned} \tag{A.59b}$$

$$
\begin{aligned}
\partial_\lambda \hat{W}'_{p,p'} \overset{\textcircled{2}}{=} & -W'_{p,p'}\left(\hat{H} - \hat{H}(\hat{n}_{p'}+1, \hat{n}_p+1)\right)^2 \\
& + \sum_q \left(\hat{\theta}_{q,p'}\hat{W}'_{p,q} + \hat{\theta}_{q,p}\hat{W}'_{q,p'}\right) \\
& + \sum_q \left(\hat{W}'_{q,p'} + \hat{W}'_{p',q}\right)\left(\hat{\theta}_{q,p} - \hat{\theta}_{q,p}(\hat{n}_{p'}+1, \hat{n}_q+1)\right) \\
& - \sum_q \left(\hat{\psi}_{q,p'} + \hat{\psi}_{p',q}\right)\left(\hat{V}_{q,p} - \hat{V}_{q,p}(\hat{n}_{p'}+1, \hat{n}_q+1)\right) \\
& - \sum_q \left(\hat{V}_{q,p'}\hat{\psi}_{p,q} + \hat{\theta}_{q,p}\hat{\psi}_{q,p'}\right)
\end{aligned}
\tag{A.59c}
$$

$$
\begin{aligned}
\partial_\lambda \hat{H} \overset{\textcircled{2}}{=} & -\sum_{p,p'} \left(\hat{\phi}_{p,p'}\hat{W}'_{p,p'} + \hat{\phi}_{p',p}\hat{W}'_{p,p'}\right) \\
& + \sum_{p,p'} \hat{W}'_{p,p'}\left(\hat{\phi}_{p',p} - \hat{\phi}_{p',p}(\hat{n}_p+1, \hat{n}_{p'}+1)\right) \\
& + \sum_{p,p'} \hat{W}'_{p,p'}\left(\hat{\phi}_{p,p'} - \hat{\phi}_{p,p'}(\hat{n}_p+1, \hat{n}_{p'}+1)\right) \\
& - \sum_q \left(\hat{\psi}_{q,p'} + \hat{\psi}_{p',q}\right)\left(\hat{V}_{q,p} - \hat{V}_{q,p}(\hat{n}_{p'}+1, \hat{n}_q+1)\right) \\
& - \sum_q \left(\hat{V}_{q,p'}\hat{\psi}_{p,q} + \hat{\theta}_{q,p}\hat{\psi}_{q,p'}\right) \\
& - \sum_{p,p'} \hat{\psi}_{p,p'}\left(\hat{W}_{p',p} - \hat{W}_{p',p}(\hat{n}_p+1, \hat{n}_{p'}+1)\right) \\
& - \sum_{p,p'} \hat{\psi}_{p,p'}\left(\hat{W}_{p,p'} - \hat{W}_{p,p'}(\hat{n}_p+1, \hat{n}_{p'}+1)\right) \\
& + \sum_{p,p'} \left(\hat{W}_{p,p'}\hat{\psi}_{p,p'} + \hat{W}_{p',p}\hat{\psi}_{p,p'}\right)
\end{aligned}
\tag{A.59d}
$$

The three operators $\hat{\psi}, \hat{\theta}, \hat{\phi}$ are based on their definition in equation A.22:

$$\hat{\theta}_{q,q'} = \hat{V}_{q,q'}\left(\hat{H} - \hat{H}(\hat{n}_q - 1, \hat{n}_{q'}+1)\right) \tag{A.60}$$

$$\hat{\phi}_{p,p'} = \hat{W}_{p,p'}\left(\hat{H} - \hat{H}(\hat{n}_{p'} - 1, \hat{n}_p - 1)\right) \tag{A.61}$$

$$\hat{\psi}_{p,p'} = \hat{W}'_{p,p'}\left(\hat{H} - \hat{H}(\hat{n}_{p'} + 1, \hat{n}_p + 1)\right) \tag{A.62}$$

A.2.4 Systematically Expanding the Flow Equations in Powers of n

We start by defining quadratic expansion coefficients for $\hat{V}_{q,q'}, \hat{W}_{p,p'}$ and $\hat{H}$:

$$\hat{V}_{q,q'} \approx v^\circ_{q,q'} + \sum_k v^{(k)}_{q,q'}\hat{n}_k + \sum_{k,k'} v^{(k,k')}_{q,q'}\hat{n}_k\hat{n}_{k'} \tag{A.63a}$$

$$\hat{W}_{p,p'} \approx w^\circ_{p,p'} + \sum_k w^{(k)}_{p,p'}\hat{n}_k + \sum_{k,k'} w^{(k,k')}_{p,p'}\hat{n}_k\hat{n}_{k'} \tag{A.63b}$$

$$\hat{H} \approx h^\circ + \sum_k h^{(k)}\hat{n}_k + \sum_{k,k'} h^{(k,k')}\hat{n}_k\hat{n}_{k'} \tag{A.63c}$$

Then, in quadratic order, we get:

$$\hat{V}_{q,q'}\hat{H} \approx v^\circ_{q,q'}\hat{H} + h^\circ V_{q,q'} + \sum_{k,k'} v^{(k)}_{q,q'}h^{(k')}\hat{n}_k\hat{n}_{k'}$$

$$= v^\circ_{q,q'} h^\circ + \sum_k \left(h^\circ v^{(k)}_{q,q'} + v^\circ_{q,q'} h^{(k)} \right) \hat{n}_k + \sum_{k,k'} \left(h^\circ v^{(k,k')}_{q,q'} + v^\circ_{q,q'} h^{(k,k')} + v^{(k)}_{q,q'} h^{(k')} \right) \hat{n}_k \hat{n}_{k'} \tag{A.64a}$$

$$\begin{aligned} \hat{W}_{p,p'} \hat{H} &\approx w^\circ_{p,p'} \hat{H} + h^\circ W_{p,p'} + \sum_{k,k'} w^{(k)}_{p,p'} h^{(k')} \hat{n}_k \hat{n}_{k'} \\ &= w^\circ_{p,p'} h^\circ + \sum_k \left(h^\circ w^{(k)}_{p,p'} + w^\circ_{p,p'} h^{(k)} \right) \hat{n}_k + \sum_{k,k'} \left(h^\circ w^{(k,k')}_{p,p'} + w^\circ_{p,p'} h^{(k,k')} + w^{(k)}_{p,p'} h^{(k')} \right) \hat{n}_k \hat{n}_{k'} \end{aligned} \tag{A.64b}$$

Now let $\alpha, \beta \in \{\pm 1\}$:

$$\begin{aligned} \hat{H}_{\tilde{k},\tilde{k}'}(\alpha,\beta) &:= \hat{H} - \hat{H}(\hat{n}_{\tilde{k}} + \alpha, \hat{n}_{\tilde{k}'} + \beta) = -\alpha h^{(\tilde{k})} - \beta h^{(\tilde{k}')} - \left(h^{(\tilde{k},\tilde{k})} + h^{(\tilde{k}',\tilde{k}')} \right) \\ &\quad - \alpha\beta \left(h^{(\tilde{k},\tilde{k}')} + h^{(\tilde{k}',\tilde{k})} \right) - \beta \sum_k (h^{(k,\tilde{k}')} + h^{(\tilde{k}',k)}) \hat{n}_k - \alpha \sum_k (h^{(k,\tilde{k})} + h^{(\tilde{k},k)}) \hat{n}_k \\ &=: h^\circ_{\tilde{k},\tilde{k}'}(\alpha,\beta) + \sum_k h^{(k)}_{\tilde{k},\tilde{k}'}(\alpha,\beta) \hat{n}_k \end{aligned} \tag{A.65}$$

The three operators $\hat{\psi}, \hat{\theta}, \hat{\phi}$ become:

$$\begin{aligned} \hat{\theta}_{q,q'} &= \hat{V}_{q,q'} \left(\hat{H} - \hat{H}(\hat{n}_q - 1, \hat{n}_{q'} + 1) \right) = \hat{V}_{q,q'} \hat{H}_{q,q'}(-,+) \\ &\approx v^\circ_{q,q'} h^\circ_{q,q'}(-,+) + \sum_k \left(h^\circ_{q,q'}(-,+) v^{(k)}_{q,q'} + v^\circ_{q,q'} h^{(k)}_{q,q'}(-,+) \right) \hat{n}_k \\ &\quad + \sum_{k,k'} \left(h^\circ_{q,q'}(-,+) v^{(k,k')}_{q,q'} + v^{(k)}_{q,q'} h^{(k')}_{q,q'}(-,+) \right) \hat{n}_k \hat{n}_{k'} \\ &=: \theta^\circ_{q,q'} + \sum_k \theta^{(k)}_{q,q'} \hat{n}_k + \sum_{k,k'} \theta^{(k,k')}_{q,q'} \hat{n}_k \hat{n}_{k'} \end{aligned} \tag{A.66a}$$

$$\begin{aligned} \hat{\phi}_{p,p'} &= \hat{W}_{p,p'} \left(\hat{H} - \hat{H}(\hat{n}_p - 1, \hat{n}_{p'} + 1) \right) = \hat{W}_{p,p'} \hat{H}_{p,p'}(-,-) \\ &\approx w^\circ_{p,p'} h^\circ_{p,p'}(-,-) + \sum_k \left(h^\circ_{p,p'}(-,-) w^{(k)}_{p,p'} + w^\circ_{p,p'} h^{(k)}_{p,p'}(-,-) \right) \hat{n}_k \\ &\quad + \sum_{k,k'} \left(h^\circ_{p,p'}(-,-) w^{(k,k')}_{p,p'} + w^{(k)}_{p,p'} h^{(k')}_{p,p'}(-,-) \right) \hat{n}_k \hat{n}_{k'} \\ &=: \phi^\circ_{p,p'} + \sum_k \phi^{(k)}_{p,p'} \hat{n}_k + \sum_{k,k'} \phi^{(k,k')}_{p,p'} \hat{n}_k \hat{n}_{k'} \end{aligned} \tag{A.66b}$$

$$\begin{aligned} \hat{\psi}_{p,p'} &= \hat{W}'_{p,p'} \left(\hat{H} - \hat{H}(\hat{n}_p - 1, \hat{n}_{p'} + 1) \right) = \hat{W}_{p,p'} \hat{H}_{p,p'}(+,+) \\ &\approx {w^\circ_{p,p'}}^* h^\circ_{p,p'}(+,+) + \sum_k \left(h^\circ_{p,p'}(+,+) {w^{(k)}_{p,p'}}^* + {w^\circ_{p,p'}}^* h^{(k)}_{p,p'}(+,+) \right) \hat{n}_k \\ &\quad + \sum_{k,k'} \left(h^\circ_{p,p'}(+,+) w^{(k,k')*}_{p,p'} + {w^{(k)}_{p,p'}}^* h^{(k')}_{p,p'}(+,+) \right) \hat{n}_k \hat{n}_{k'} \\ &=: \psi^\circ_{p,p'} + \sum_k \psi^{(k)}_{p,p'} \hat{n}_k + \sum_{k,k'} \psi^{(k,k')}_{p,p'} \hat{n}_k \hat{n}_{k'} \end{aligned} \tag{A.66c}$$

The above expressions for the products of two operators quadratic in n or for the differences of the form $\hat{H} - \hat{H}(\hat{n}_{\tilde{k}} + \alpha, \hat{n}_{\tilde{k}'} + \beta)$ can now be written down completely analogously for arbitrary quadratic operators. The flow equations for the expansion coefficients result from comparing the coefficients in the expressions A.59a-A.59d.

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SELBSTSTÄNDIGKEITSERKLÄRUNG

Hiermit erkläre ich, die vorliegende Arbeit selbständig verfasst zu haben und keine anderen als die in der Arbeit angegebenen Quellen und Hilfsmittel benutzt zu haben.

München, den tba.07.2023

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