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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 which does not commute with every other operator
1	indicates $1 \in \mathbb{N}$ or the identity operator $\hat{1} =: \mathbb{1}$
$: \hat{A} :$	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}
$\{\hat{A}, \hat{B}\}$	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
∂_x	partial derivative $\frac{\partial}{\partial x}$ w.r.t. x
$\stackrel{\textcircled{2}}{=}$	Equality up to second order, i.e. higher order terms are neglected.
$\hbar = 1$	reduced Planck's constant is set to 1
$+\text{h.c.}$	plus the Hermitian conjugate of the previous term
\sim	approximately proportional to
$\underline{\underline{E}}_N$	$N \times N$ identity matrix
$\text{sgn}(\cdot)$	signum function
\mathcal{O}	Landau Big O
\gtrsim	greater than an approximate value

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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].

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 coefficients depend on (bosonic) occupation numbers.

The first case occurs, for example, in the BEC polaron problem in the limit of an infinite impurity mass. The dependence on occupation numbers comes into play when this impurity is not fixed, that is, when it has a finite mass.

This thesis is organized 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-Pine (LLP) Transformation. The flow equations both for 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 in Appendix A. The flow equations for the purely quadratic case will be tested on a one dimensional Bose polaron model in Section 4 and compared to the findings of Grusdt *et al.*[4]. We then close with a conclusion and an outlook in Section 5.

SECTION 2

THEORETICAL BACKGROUND

2.1 The Flow Equation Approach

This section is intended to be a concise and rather operational overview of the flow equation approach. S. Kehrein provides an excellent in-depth introduction [5] on which most of the discussion in this section is based.

2.1.1 General Mechanism

We start with a Hamiltonian $\hat{\mathcal{H}}$ and our goal is to continuously transform $\hat{\mathcal{H}}$ into an unitarily equivalent diagonal Hamiltonian. This transformation \hat{U} is a function of a flow parameter λ with $[\lambda] = \text{Energy}^{-2}$ and will be chosen such that the off-diagonal elements in

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

vanish in the limit $\lambda \rightarrow \infty$. Stone's theorem on one-parameter unitary groups guarantees the existence of $\hat{\eta}(\lambda)$ which is anti-hermitian, i.e. $\hat{\eta}(\lambda) = -\hat{\eta}^\dagger(\lambda)$, and fulfills

$$\hat{U}(\lambda) = e^{\hat{\eta}(\lambda)}. \quad (2.2)$$

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

$$\frac{d\hat{\mathcal{H}}(\lambda)}{d\lambda} = [\hat{\eta}(\lambda), \hat{\mathcal{H}}(\lambda)]. \quad (2.3)$$

This is what we will refer to as the flow equation for the Hamiltonian $\hat{\mathcal{H}}(\lambda)$. From now on, the λ -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 transformations 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

$$\hat{\eta} = [\hat{\mathcal{H}}_{\text{diag.}}, \hat{\mathcal{H}}], \quad (2.4)$$

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

$$\hat{\eta} = [\hat{\mathcal{H}}_0, \hat{\mathcal{H}}_{\text{int}}]. \quad (2.5)$$

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 trace of its square becomes smaller in the flow:

$$\frac{d}{d\lambda} \text{Tr} \left(\hat{\mathcal{H}}_{\text{int}}^2 \right) \leq 0 \quad (2.6)$$

It can be proved [5, pp. 27-28] that this is always the case iff

$$\text{Tr} \left(\hat{\mathcal{H}}_0 \hat{\mathcal{H}}_{\text{int}} \right) = \text{Tr} \left(\frac{d\hat{\mathcal{H}}_0}{d\lambda} \hat{\mathcal{H}}_{\text{int}} \right) = 0 \quad (2.7)$$

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 [5, 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

$$C_{k,l} := \langle \psi_{NO} | \hat{\alpha}_k \hat{\alpha}_l | \psi_{NO} \rangle. \quad (2.8)$$

Then it follows that

$$[\hat{\alpha}_k, \hat{\alpha}_l] = C_{k,l} - C_{l,k} \quad (2.9)$$

which can be proved readily by applying the canonical commutation relations to equation 2.8 and by using the normalization of $|\psi_{NO}\rangle$. 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:

$$: 1 := 1 \quad (2.10)$$

2. Linearity:

$$: c \hat{O}_1 + \hat{O}_2 := c : \hat{O}_1 : + : \hat{O}_2 : \quad \forall c \in \mathbb{C} \quad (2.11)$$

3. Recurrence relation:

$$\hat{\alpha}_k : \hat{O} := \hat{\alpha}_k \hat{O} : + \sum_l C_{k,l} : \partial_{\hat{\alpha}_l} \hat{O} : \quad (2.12)$$

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, if 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 2.5 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. Without normal ordering, fourth-order terms could also contribute to second-order terms. 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 2.8 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.

$$|GS(\lambda)\rangle = \hat{U}(\lambda)\hat{U}^\dagger(\lambda = \infty)|GS\rangle. \quad (2.13)$$

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, 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 good 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 or a Bose-Einstein condensate (BEC). It was introduced by Herbert Fröhlich in 1954 to study the effect of electron-phonon coupling on the electrical conductivity of polar crystals [6]. The Fröhlich Hamiltonian can also be used to describe the interaction of an impurity with the Bogoliubov phonons of an BEC, which leads to the formation of a quasiparticle called the Bose polaron because the impurity atom becomes “dressed” in a cloud of phonons. This dressing changes important properties of the impurity, such as its effective mass and mobility.

We follow [4] and write the Fröhlich Hamiltonian in one dimension in the following form:

$$\hat{\mathcal{H}}_F = g_{IB}n_0 + \frac{\hat{p}^2}{2M} + \int dk \omega_k \hat{a}_k^\dagger \hat{a}_k + \sqrt{\frac{n_0}{2\pi}} g_{IB} \int dk W_k e^{ik\hat{x}} (\hat{a}_k + \hat{a}_{-k}^\dagger) \quad (2.14)$$

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

$$w_k = ck \sqrt{1 + \frac{1}{2}\xi^2 k^2} \quad (2.15)$$

where we introduced ξ as the healing length of the Bose condensate and c as the speed of sound in the condensate. 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

$$W_k = \left(\frac{(\xi k)^2}{2 + (\xi k)^2} \right)^{1/4} \quad (2.16)$$

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 [4]. 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 [7]. 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 [4].

The aforementioned two-phonon scattering terms are quadratic and are again proportional to the boson-impurity coupling constant:

$$\hat{\mathcal{H}}_{2\text{ph}} = \frac{g_{IB}}{2\pi} \int dk dk' (c_k \hat{a}_k^\dagger - s_k \hat{a}_{-k}) (c_{k'} \hat{a}_{k'} - s_{k'} \hat{a}_{-k'}^\dagger) e^{i(k-k')x} \quad (2.17)$$

The coefficients c_k and s_k can be obtained from

$$W_k = c_k - s_k \quad (2.18a)$$

$$W_k^{-1} = c_k + s_k \quad (2.18b)$$

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

$$\gamma := \frac{m_B g_{BB}}{n_0} \quad (2.19)$$

is large. Because this regime will not be considered in this thesis, $\hat{\mathcal{H}}_F$ and $\hat{\mathcal{H}}_{2\text{ph}}$ model the polaron problem well for our purposes.

For future reference, we will now also introduce the 1D boson-boson s-wave scattering length

$$a_{BB} = -\frac{2}{m_B g_{BB}} \quad (2.20)$$

where

$$m_B = \frac{1}{\sqrt{2c\xi}} \quad (2.21)$$

is the mass of the bosons and the dimensionless parameter

$$\eta := \frac{g_{IB}}{g_{BB}} \quad (2.22)$$

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

For small η , the Fröhlich Hamiltonian describes the physics of the impurity accurately. For strong coupling, however, two-phonon terms must be included and our full Hamiltonian reads

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_F + \hat{\mathcal{H}}_{2\text{ph}} \quad (2.23)$$

2.2.2 The Lee-Low-Pine (LLP) Transformation

The Lee-Low-Pine (LLP) transformation [8] dramatically simplifies the solving of the full Hamiltonian 2.23. 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.

We take advantage of the fact that the total momentum operator is

$$\hat{P}_{\text{tot}} = \int dk k \hat{a}_k^\dagger \hat{a}_k + \hat{p} \quad (2.24)$$

and then define

$$\hat{U}_{\text{LLP}} := \exp \left(-i\hat{x} \cdot \left(\hat{P} - \int dk k \hat{a}_k^\dagger \hat{a}_k \right) \right) \quad (2.25)$$

This is the desired transformation because \hat{p} is the generator of (infinitesimal) translations of the impurity and \hat{x} generates translations of the impurity in momentum space.

The transformed Hamiltonian as a function of the total conserved system momentum P then reads:

$$\begin{aligned} \hat{U}_{\text{LLP}}^\dagger \hat{\mathcal{H}} \hat{U}_{\text{LLP}} &:= \hat{\mathcal{H}}_{\text{LLP}}(P) = g_{IB} n_0 + \frac{1}{2M} \left(P - \int dk k \hat{a}_k^\dagger \hat{a}_k \right)^2 + \int dk \omega_k \hat{a}_k^\dagger \hat{a}_k \\ &+ \sqrt{\frac{n_0}{2\pi}} g_{IB} \int dk W_k \left(\hat{a}_k + \hat{a}_{-k}^\dagger \right) + \frac{g_{IB}}{2\pi} \int dk dk' \left(c_k \hat{a}_k^\dagger - s_k \hat{a}_{-k} \right) \left(c_{k'} \hat{a}_{k'} - s_{k'} \hat{a}_{-k'}^\dagger \right) \end{aligned} \quad (2.26)$$

SECTION 3

DETERMINING THE FLOW EQUATIONS

3.1 Purely Quadratic Case

3.1.1 Deriving the Flow Equations

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

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

and no truncation scheme as discussed in Section 2.1.3 has to be employed. For details of the calculations consult section A.1.

There we followed precisely the recipe described in Section 2.1.1: First the canonical generator 2.4 is calculated. Then the derivative of the flow Hamiltonian is calculated via the commutator of the generator and the Hamiltonian in equation 2.3. The flow equations then follow by a simple comparison of coefficients from the quadratic Hamiltonian (plus a constant energy ϵ) ansatz for the flow Hamiltonian.

Note that the 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

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

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

assuming that there are no degeneracies present. If there were, it would mean that $(\omega_q - \omega_{q'})^2 = 0$ for some pair q, q' . But even the occurrence of (near-)degeneracies does not necessarily imply that the corresponding matrix elements do not decay [9]. This is because the second order terms coupling the ODEs for the different matrix elements are non-trivial and might, depending on the initial condition, even sufficiently suppress degenerate matrix elements.

Consequently, applying the equations to a concrete problem provides the best test of their performance and convergence properties.

Checking the condition 2.6 is a strong indicator for good convergence properties but does not necessarily imply that all elements in $\hat{\mathcal{H}}_{\text{int}}$ converge to 0, which is why we waive the explicit evaluation of the conditions 2.7 which imply 2.6.

3.1.2 Application to the 1D Bose Polaron Model

In the heavy impurity limit $M \rightarrow \infty$, the dependence of the occupation numbers in the LLP-Hamiltonian 2.26 vanishes and we almost have a purely quadratic Hamiltonian 3.1 as discussed in the previous section. Before we discuss the significance of the linear term in the LLP-Hamiltonian we will address the fact that the integrals in there have to be 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 $\Lambda_{UV}\xi = 10^1$.

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. Typical values are of order $\Delta k \sim 10^{-1}\xi$.

This allows us to approximate integrals by sums

$$\int dk \rightarrow \Delta k \sum_k. \quad (3.3)$$

The commutation relations of the creation and annihilation operators in $\hat{\mathcal{H}}_{\text{LLP}}$ are $[\hat{a}_k, \hat{a}_{k'}^\dagger] = \delta(k-k')$. 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

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

and the LLP-Hamiltonian becomes:

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

It would be possible to expand 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 $W_k (\hat{a}_k + \hat{a}_{-k}^\dagger)$ can be transformed out by applying the displacement operator

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

to the Hamiltonian 3.5. Here we introduced the symplectic $2N \times 2N$ matrix

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

and the notation

$$\hat{\underline{a}} = (\hat{a}_{k_1}, \dots, \hat{a}_{k_N}, \hat{a}_{k_1}^\dagger, \dots, \hat{a}_{k_N}^\dagger)^T \quad (3.8)$$

for vectors of creation and annihilation operators as well as

$$\underline{\alpha} = (\alpha_{k_1}, \dots, \alpha_{k_N}, \alpha_{k_1}^*, \dots, \alpha_{k_N}^*)^T \in \mathbb{C}^{2N} \quad (3.9)$$

for vectors of c-numbers. In this context N is equal to the number of modes on our discrete grid.

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

$$\hat{D}^\dagger(\underline{\alpha})\hat{a}_{k_i}\hat{D}(\underline{\alpha}) = \hat{a}_{k_i} + \alpha_{k_i} \quad (3.10a)$$

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

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

$$\hat{D}(\underline{\alpha})\hat{a}_{k_i}\hat{D}^\dagger(\underline{\alpha}) = \hat{a}_{k_i} - \alpha_{k_i} \quad (3.11a)$$

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

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:

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

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

$$\forall k : 0 \stackrel{!}{=} \omega_k\alpha_k^* + \tilde{W}_k^{(0)} + \sum_{k'} V_{k',k}^{(0)}\alpha_{k'}^* + \sum_{k'} \alpha_{k'} \left(W_{k,k'}^{(0)} + W_{k',k}^{(0)} \right) \quad (3.13)$$

We defined

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

$$V_{k,k'}^{(0)} := \frac{g_{IB}}{2\pi} \Delta k (c_k c_{k'} + s_k s_{k'}) \quad (3.14b)$$

$$W_{k,k'}^{(0)} := -\frac{g_{IB}}{2\pi} \Delta k s_k c_{k'} \quad (3.14c)$$

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 then be substituted into the Hamiltonian which is then of purely quadratic form: ^[1]

$$\hat{\mathcal{H}}_{\text{LLP}}^{\text{quadr.}} = \sum_k (\omega_k + V_{k,k}^{(0)})\hat{a}_k^\dagger\hat{a}_k + \sum_{q \neq q'} V_{q,q'}^{(0)}\hat{a}_q^\dagger\hat{a}_{q'} + \sum_{p,p'} \left(W_{p,p'}^{(0)}\hat{a}_p^\dagger\hat{a}_{p'}^\dagger + \text{h.c.} \right) + g_{IB}n_0 + \frac{g_{IB}}{2\pi} \Delta k \sum_k s_k^2 \quad (3.15)$$

^[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>.

The flow equations A.14a-A.14e for $\hat{\mathcal{H}}_{\text{LLP}}^{\text{quadr.}}$ 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` functionality from `julia`'s `DifferentialEquations.jl` library in combination with the `Tsit5` integrator, a Runge-Kutta integrator of order 5(4) [10], 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. $c = \xi = 1$ [4, 7]. 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 [11, 12]. Using the short hand notations 3.8 and 3.9 as well as 3.7, our quadratic Hamiltonian can be written in the form:

$$\hat{\mathcal{H}} = E_0 + \sum_{k,k'} \hat{a}_k^\dagger A_{k,k'} \hat{a}_{k'} + \frac{1}{2} \sum_{k,k'} (\hat{a}_k^\dagger B_{k,k'} \hat{a}_{k'}^\dagger + \text{h.c.}) \quad (3.16)$$

$$= E_0 - \frac{1}{2} \sum_k A_{k,k} + \frac{1}{2} \hat{a}^\dagger \begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \hat{a} \quad (3.17)$$

$$= E_0 - \frac{1}{2} \sum_k A_{k,k} + \frac{1}{2} \hat{a}^\dagger \underline{\underline{\Omega}} \underline{\underline{\mathcal{H}}} \hat{a} \quad (3.18)$$

where we introduced

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

and

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

Hermiticity of the Hamiltonian requires $A^\dagger = A$ and B can and must always be chosen s.t. $B^T = B$. This is because $[\hat{a}_k^\dagger, \hat{a}_{k'}^\dagger] = [\hat{a}_k, \hat{a}_{k'}] = 0$, so if we start with a non-symmetric B we can always symmetrize by the transition $B \rightarrow \frac{1}{2}(B + B^T)$.

As shown in [11], the Bogoliubov Transformation

$$\hat{a} \mapsto \underline{\underline{U_B}} \hat{a} \quad (3.21)$$

defined by the matrix

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

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

$$\underline{\underline{U_B}} \underline{\underline{\Omega}} \underline{\underline{U_B}}^\dagger = \underline{\underline{\Omega}}. \quad (3.23)$$

It can be shown that there exists $\underline{\underline{U_B}}$ s.t.

$$\underline{\underline{U_B}}^\dagger \underline{\underline{\Omega}} \underline{\underline{\mathcal{H}}} \underline{\underline{U_B}} = \text{diag}(\lambda_1, \dots, \lambda_N, \lambda_1^*, \dots, \lambda_N^*) \quad (3.24)$$

^[2] For the numerics we again refer to the source code "Solve_Flow_Equations.jl" in <https://github.com/SufficientlySmooth/Bachelor-Thesis-Numerics>

The values $\{\lambda_j^{(*)}\}_{j=1,\dots,N}$ can be obtained by solving the eigenvalue problem of $\underline{\mathcal{H}}$. The eigenvectors then constitute the columns \underline{U}_B .

Additionally, 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

$$\underline{\vartheta} : \mathbb{C}^{2N} \rightarrow \mathbb{C}^{2N}, \begin{pmatrix} \underline{u} \\ \underline{v} \end{pmatrix} \mapsto \begin{pmatrix} \underline{v}^* \\ \underline{u}^* \end{pmatrix} \text{ where } \underline{u}, \underline{v} \in \mathbb{C}^N. \quad (3.25)$$

The relations

$$\{\underline{\vartheta}, \underline{\Omega}\} = 0 \quad (3.26)$$

and

$$[\underline{\Omega}, \underline{\mathcal{H}}, \underline{\vartheta}] = 0 \quad (3.27)$$

imply that if \underline{x} is an eigenvector of $\underline{\Omega} \underline{\mathcal{H}}$ corresponding to the eigenvalue λ , then $\underline{\vartheta} \underline{x}$ 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:

$$\underline{w}_j^\dagger \underline{\Omega} \underline{w}_j > 0 \quad (3.28)$$

The corresponding eigenvector to $-\lambda_j^*$ always has a negative matrix element. It is necessary to classify the eigenvalues in this way, because only then the symplectic condition 3.22 holds.

The symplectic 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 and is (dynamically) unstable. If at least one real eigenvalue is strictly negative, this indicates that the system is not in its lowest energy state, i.e. not in equilibrium. This is called a thermodynamic instability. 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 number operator $\hat{n} = \hat{a}^\dagger \hat{a}$. The following relations will be used when deriving the flow equations:

$$[\hat{a}^\dagger, \hat{f}(\hat{n})] = \hat{a}^\dagger (\hat{f}(\hat{n}) - \hat{f}(\hat{n} + 1)) \quad (3.29a)$$

$$[\hat{a}, \hat{f}(\hat{n})] = \hat{a} (\hat{f}(\hat{n}) - \hat{f}(\hat{n} - 1)) \quad (3.29b)$$

$$[\hat{f}(\hat{n}), \hat{a}^\dagger] = (\hat{f}(\hat{n}) - \hat{f}(\hat{n} - 1)) \hat{a}^\dagger \quad (3.29c)$$

$$[\hat{f}(\hat{n}), \hat{a}] = (\hat{f}(\hat{n}) - \hat{f}(\hat{n} + 1)) \hat{a} \quad (3.29d)$$

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 3.29 are still valid for functions depending on $\{\hat{n}_k\}_k$, because all \hat{n}_k pairwise commute.

We will write $\hat{f}(\hat{n}_1, \hat{n}_2, \dots) =: \hat{f}$ and $\hat{f}(\hat{n}_1, \hat{n}_2, \dots, \hat{n}_k \pm 1, \hat{n}_{k+1}, \dots) =: \hat{f}(\hat{n}_k \pm 1)$. In this notation it is understood that $\hat{f}(\hat{n}_k \pm 1, \hat{n}_k \pm 1) =: \hat{f}(\hat{n}_k \pm 2)$.

Using this notation, it is evident that a simple induction for $n_1, n_2 \in \mathbb{N}_0$ yields the following relation:

$$[\hat{f}(\hat{n}), \hat{a}_{k_1}^\dagger \hat{a}_{k_2}^\dagger \cdots \hat{a}_{k_{n_1}}^\dagger \hat{a}_{k_1} \hat{a}_{k_2} \cdots \hat{a}_{k_{n_2}}]$$

$$= \left(\hat{f} - \hat{f} \left(\hat{n}_{k_1} - 1, \hat{n}_{k_2} - 1, \dots, \hat{n}_{k_{n_1}}, \hat{n}_{k_1} + 1, \hat{n}_{k_2} + 1, \dots, \hat{n}_{k_{n_2}} + 1 \right) \right) \hat{a}_{k_1}^\dagger \hat{a}_{k_2}^\dagger \cdots \hat{a}_{k_{n_1}}^\dagger \hat{a}_{k_1} \hat{a}_{k_2} \cdots \hat{a}_{k_{n_2}} \quad (3.30)$$

Furthermore, applying the recurrence relation 2.12 can be used to successively normal order operators. Let $\hat{O} := \hat{a}_{k_1}^\dagger \hat{a}_{k_2}^\dagger \cdots \hat{a}_{k_{n_1}}^\dagger \hat{a}_{k_1} \hat{a}_{k_2} \cdots \hat{a}_{k_{n_2}}$. Then normal ordering w.r.t. the vacuum yields:

$$\begin{aligned} \hat{a}_q : \hat{O} : &= \hat{O} \hat{a}_q : + \sum_k : \frac{\partial \hat{O}}{\partial \hat{a}_k^\dagger} : \\ &= \hat{O} \hat{a}_q : + \sum_{i=1}^{n_1} \delta_{k_i, q} : \hat{a}_{k_1}^\dagger \hat{a}_{k_2}^\dagger \cdots \hat{a}_{k_{i-1}}^\dagger \hat{a}_{k_{i+1}}^\dagger \cdots \hat{a}_{k_{n_1}}^\dagger \hat{a}_{k_1} \hat{a}_{k_2} \cdots \hat{a}_{k_{n_2}} : \end{aligned} \quad (3.31a)$$

$$\hat{a}_q^\dagger : \hat{O} : = \hat{a}_q^\dagger \hat{O} : \quad (3.31b)$$

3.2.2 Deriving the Flow Equations

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 while the flow Hamiltonian does not. 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 considered expressions 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 [13], 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.

After evaluating the commutator of $\hat{\eta}$ and the full Hamiltonian where we made frequent use of the equations in 3.29, we end up with 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

$$\hat{H} := \sum_k \hat{\omega}_k : \hat{a}_k^\dagger \hat{a}_k : + \hat{\epsilon}. \quad (3.32)$$

3.2.3 Discussion of the Applicability of the Flow Equations to the Full LLP-Hamiltonian

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

$$\hat{\mathcal{H}}_{\text{LLP}}^{\text{discr.}}(P) = g_{IB} n_0 + \frac{1}{2M} \left(P - \sum_k k \hat{a}_k^\dagger \hat{a}_k \right)^2 + \sum_k \omega_k \hat{a}_k^\dagger \hat{a}_k$$

$$+ \sqrt{\frac{n_0 \Delta k}{2\pi}} g_{IB} \sum_k W_k (\hat{a}_k + \hat{a}_{-k}^\dagger) + \frac{g_{IB} \Delta k}{2\pi} \sum_{k,k'} (c_k \hat{a}_k^\dagger - s_k \hat{a}_{-k}) (c_{k'} \hat{a}_{k'} - s_{k'} \hat{a}_{-k'}^\dagger) \quad (3.33)$$

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

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

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

$$\hat{H}(P) := g_{IB} n_0 + \frac{g_{IB}}{2\pi} \Delta k \sum_k s_k^2 + \frac{1}{2M} \left(P - \sum_k k \hat{n}_k \right)^2 + \sum_k \omega_k \hat{n}_k + \frac{g_{IB} \Delta k}{2\pi} \sum_k (c_k^2 + s_k^2) \hat{n}_k \quad (3.35)$$

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

$$\begin{aligned} \hat{H}(P, \hat{n}_q - 1, \hat{n}_{q'} + 1) - \hat{H}(P) &= \frac{1}{2M} \left(P + q - q' - \sum_k k \hat{n}_k \right)^2 - \frac{1}{2M} \left(P - \sum_k k \hat{n}_k \right)^2 \\ &+ \omega_{q'} - \omega_q + \frac{g_{IB} \Delta k}{2\pi} (c_{q'}^2 + s_{q'}^2 - c_q^2 - s_q^2) \end{aligned} \quad (3.36)$$

$$= \frac{q - q'}{2M} \left(2P - 2 \sum_k k \hat{n}_k + q - q' \right) + \omega_{q'} - \omega_q + \frac{g_{IB} \Delta k}{2\pi} (c_{q'}^2 + s_{q'}^2 - c_q^2 - s_q^2) \quad (3.37)$$

It follows that for fixed q, q' and for fixed expectation values $\langle \hat{n}_k \rangle =: n_k$ there exists one and only one P s.t. $\hat{H}(P, n_q - 1, n_{q'} + 1) - \hat{H}(P) = 0$. For all other values of P , looking at the flow equations in first order, we expect the coefficients in front of $\hat{a}_q^\dagger \hat{a}_{q'}$ to vanish in the limit $\lambda \rightarrow \infty$. By similar reasoning, we can expect that $|\hat{H}(P, \hat{n}_p \pm 1, \hat{n}_{p'} \pm 1) - \hat{H}(P)| > 0$ even for $p = \pm p'$.

This strongly suggests that the flow equations A.59a-A.59d converge to a diagonal Hamiltonian as desired.

Numerically diagonalizing the full LLP-Hamiltonian, which will not be done in this thesis, 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 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 expensive.

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

SECTION 4

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

4.1 In Combination with a Bogoliubov Transformation

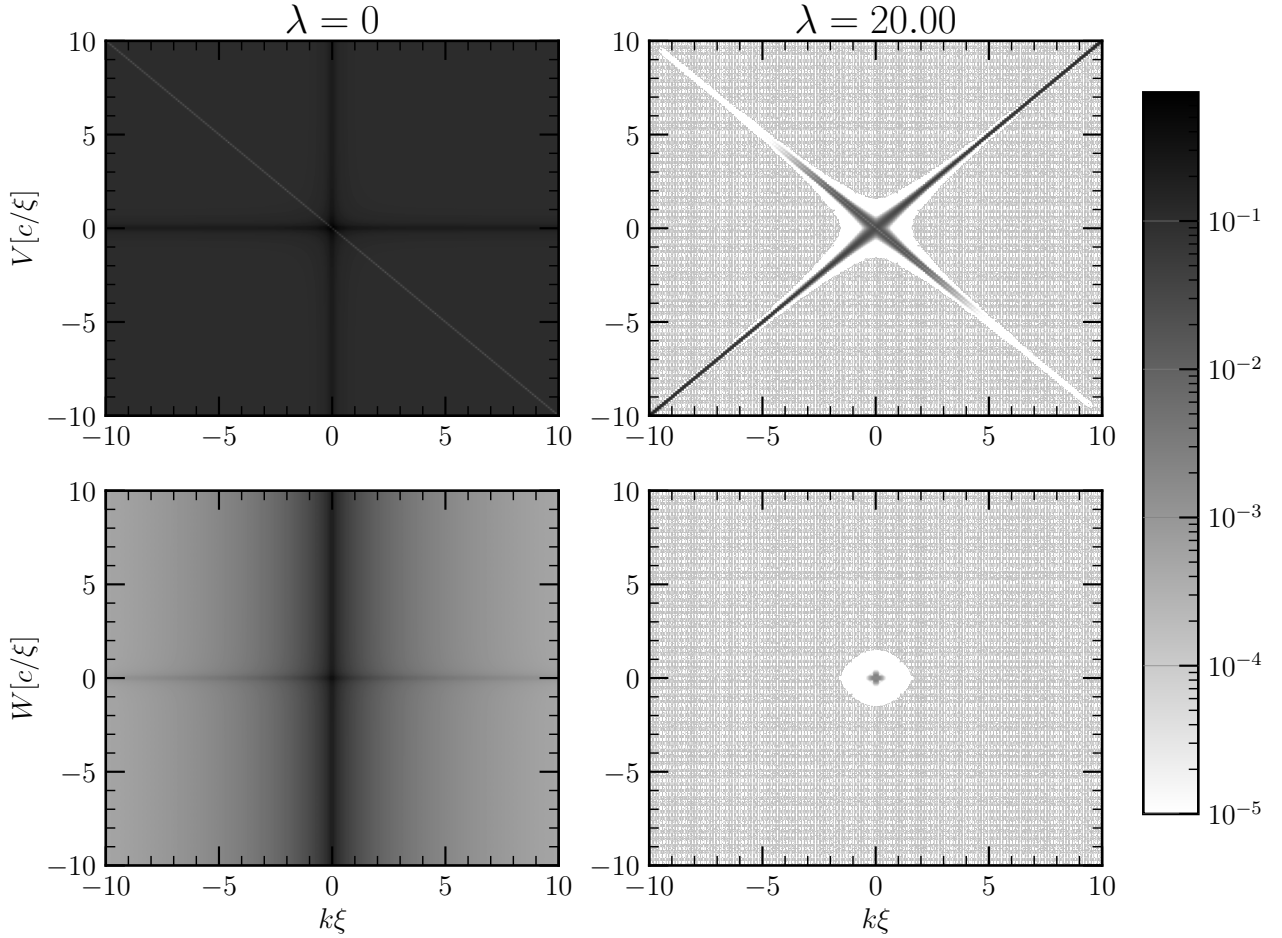


Figure 4.1: Visualization of how the flow progresses for $\eta = 10$ by shading larger absolute values for $V_{k,k'}$, $W_{k,k'}$ darker. It is of note that on the ordinate and abscissa $0 \equiv \pm \lambda_{IR} \xi = \pm 0.1$. We see that good suppression occurs for all $W_{k,k'}$, with slower convergence 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 evaluating if $\text{sgn}(V_{k,k'}) = -\text{sgn}(\partial_\lambda V_{k,k'})$ is fulfilled.

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 $\partial_\lambda V_{k,-k} = \dots$

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

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

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.

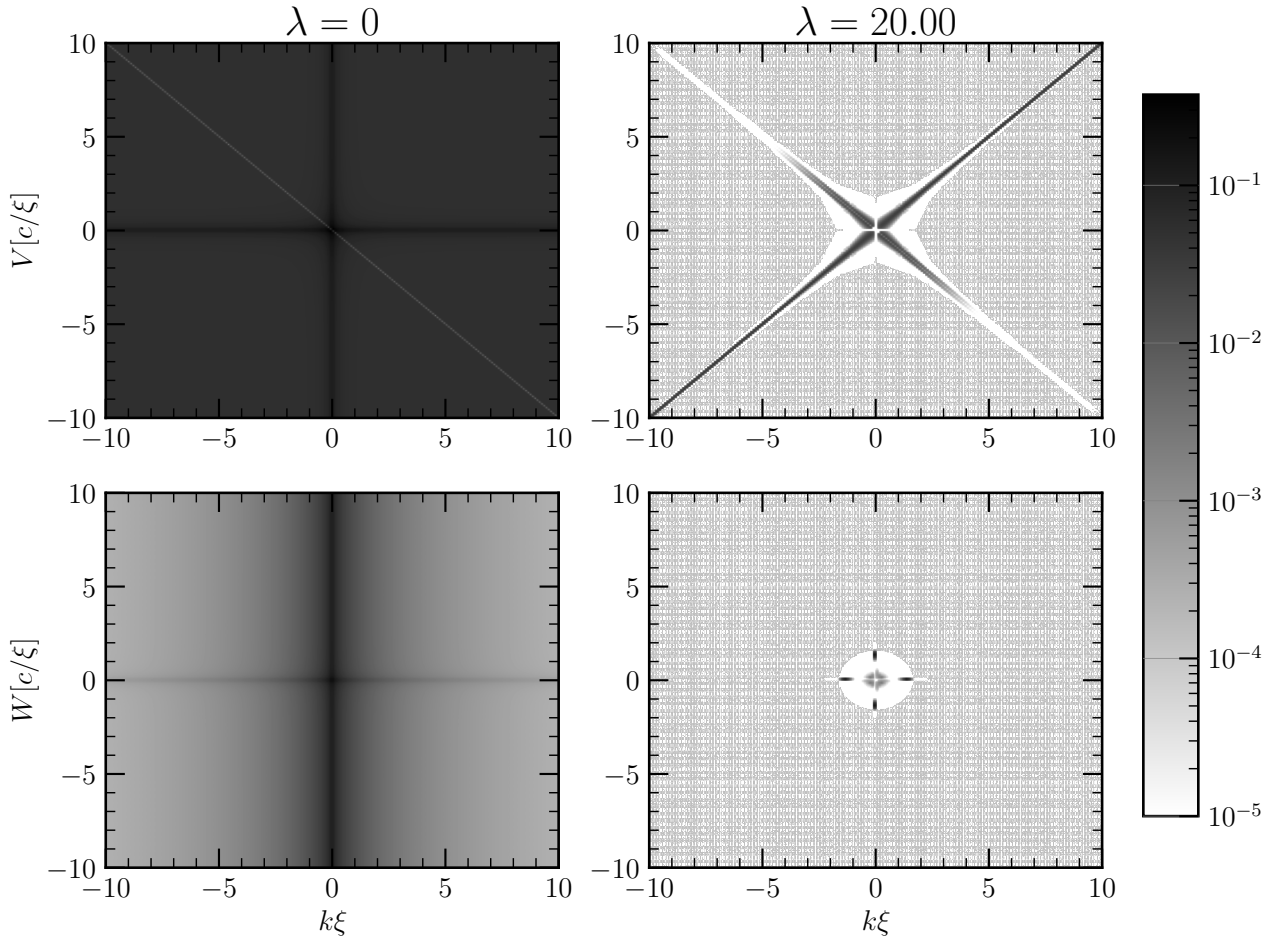


Figure 4.2: Visualization of the flow progression for $\eta = -5.1$ analogous to Figure 4.1. We can see that for this η not all of the $W_{k,k'}$ vanish, which may be related to the fact that we are now observing a system with a thermodynamic instability, as will become clear later on. The entailing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

^[1] For the numerics we again refer to the source code "Bogoliubov_Transformation.py" in <https://github.com/SufficientlySmooth/Bachelor-Thesis-Numerics>

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 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.

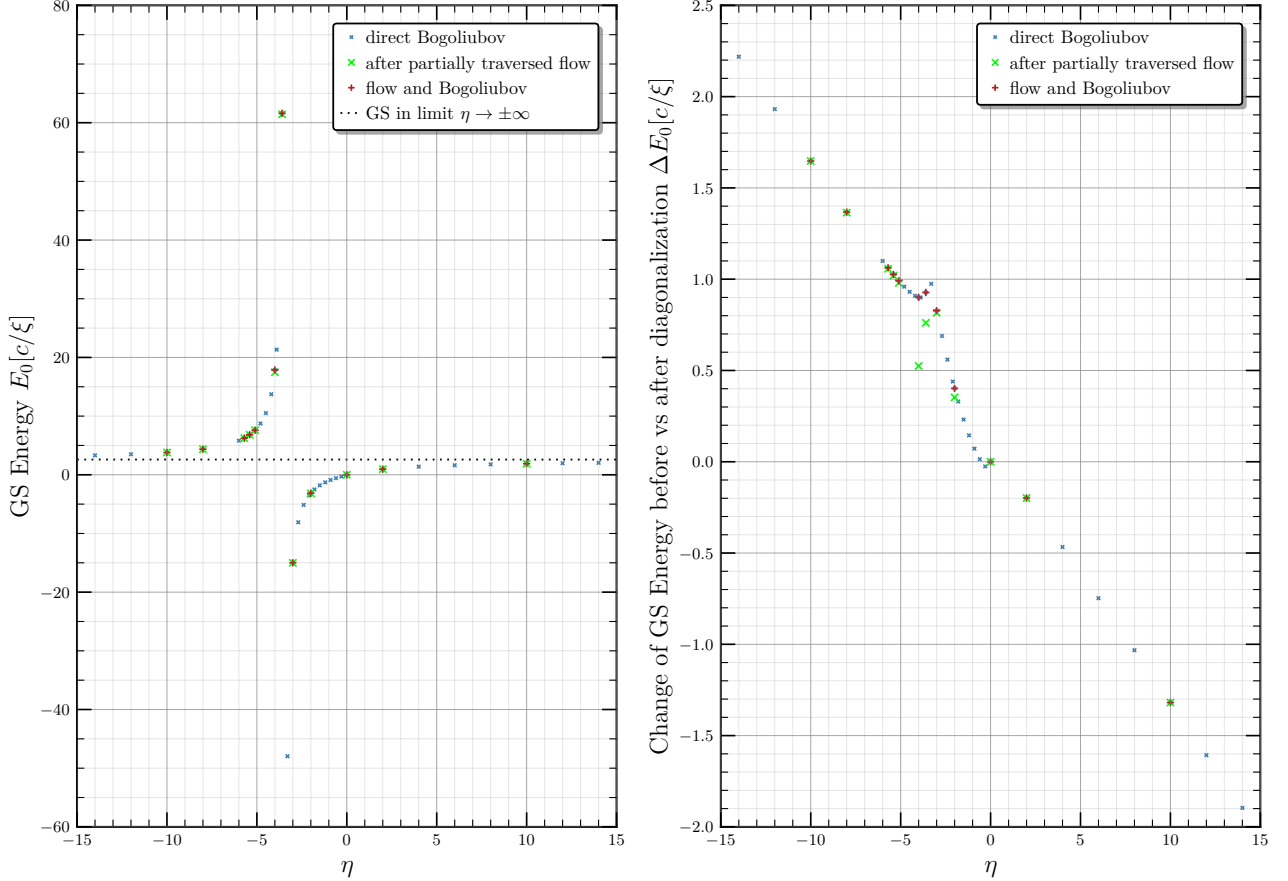


Figure 4.3: The left subplot shows the ground state energy for different η . The results are obtained via three different approaches: First a Bogoliubov transformation is applied directly to the Hamiltonian 3.15. Second, the ground state energy is given by the constant ϵ in the flow Hamiltonian A.13 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 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 surprisingly good behavior of the second method (standalone flow equations) seems plausible when we consider that $\mathcal{O}(N^2)$ flows 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 [11], the prediction for the ground state energy for our system is very accurate. It is noteworthy that the ground state energy in the limit $\eta \rightarrow \pm\infty$ is the same. This is because the two branches are adiabatically connected[4].

But an accurate prediction of the ground state energy does not necessarily imply that all eigenenergies are predicted accurately too.

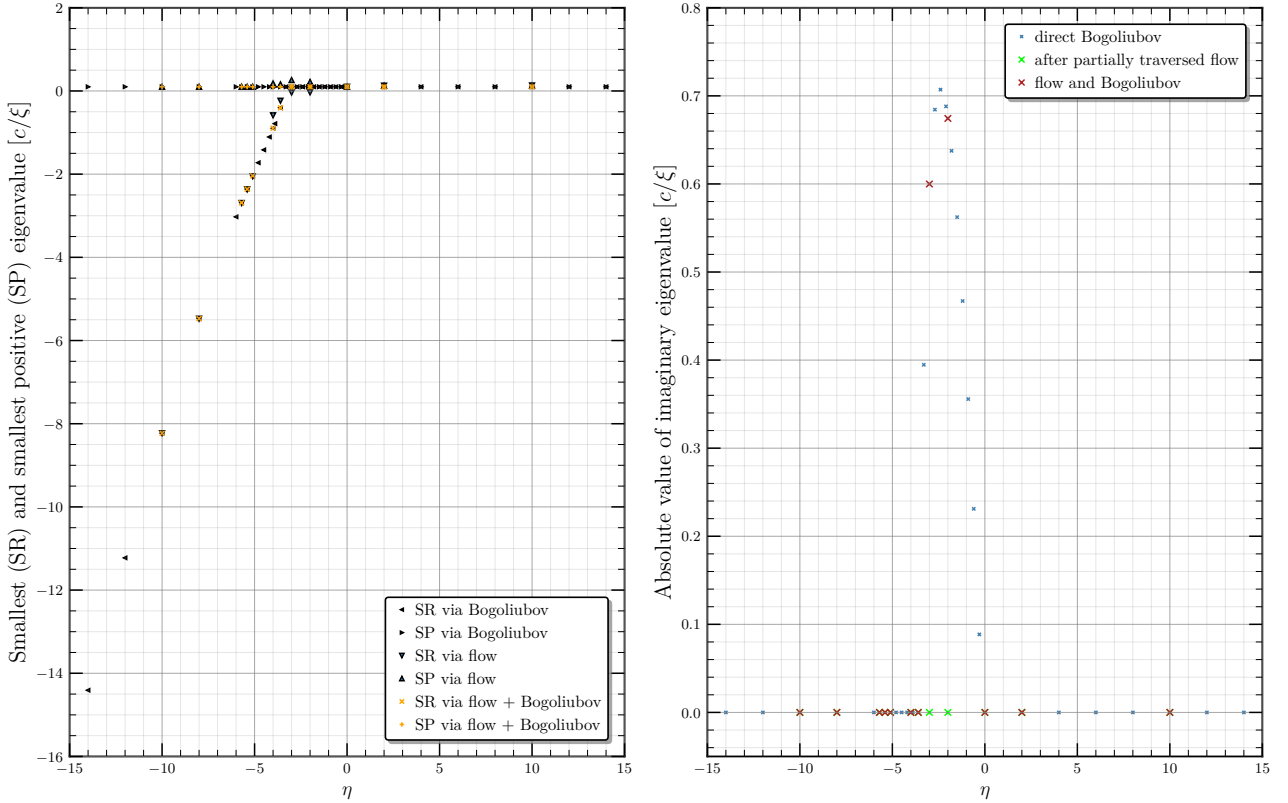


Figure 4.4: The left subplot shows the smallest real (SR) and smallest real positive (SP) eigenvalues of the Hamiltonian for different η . The right subplot illustrates in which regime dynamical instabilities (i.e. imaginary eigenvalues) occur.

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 applied to a Hamiltonian with complex eigenenergies, those will be encoded in behaviour as seen in Figure 4.2 where not all off-diagonal terms vanish.

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 Spectra

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.

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 at that.

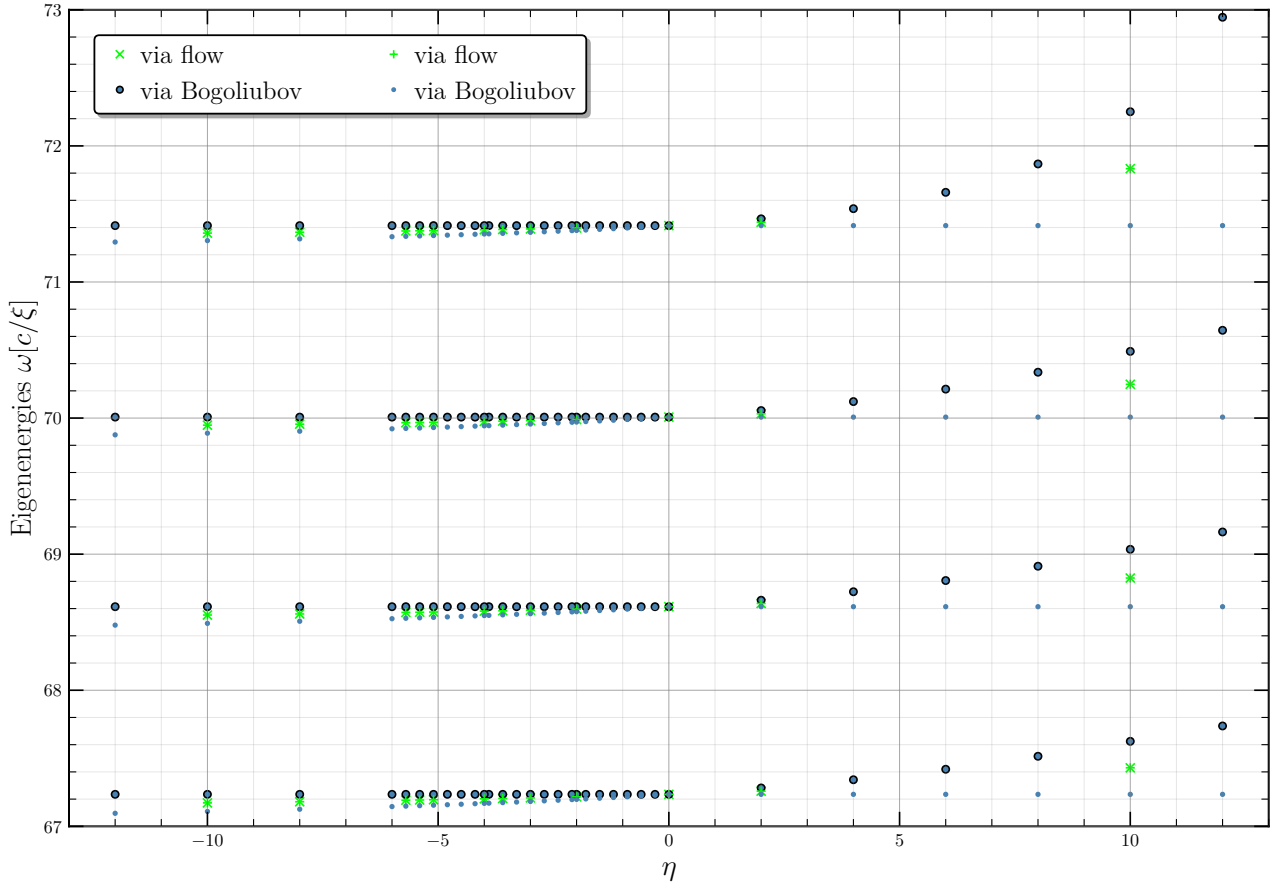


Figure 4.5: This plot shows how the largest eigenvalues change in η . It has been refrained from performing a Bogoliubov transformation after the flow again, since this would only reproduce the values of a direct Bogoliubov transformation anyway due to the unitarity of the flow transformation.

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

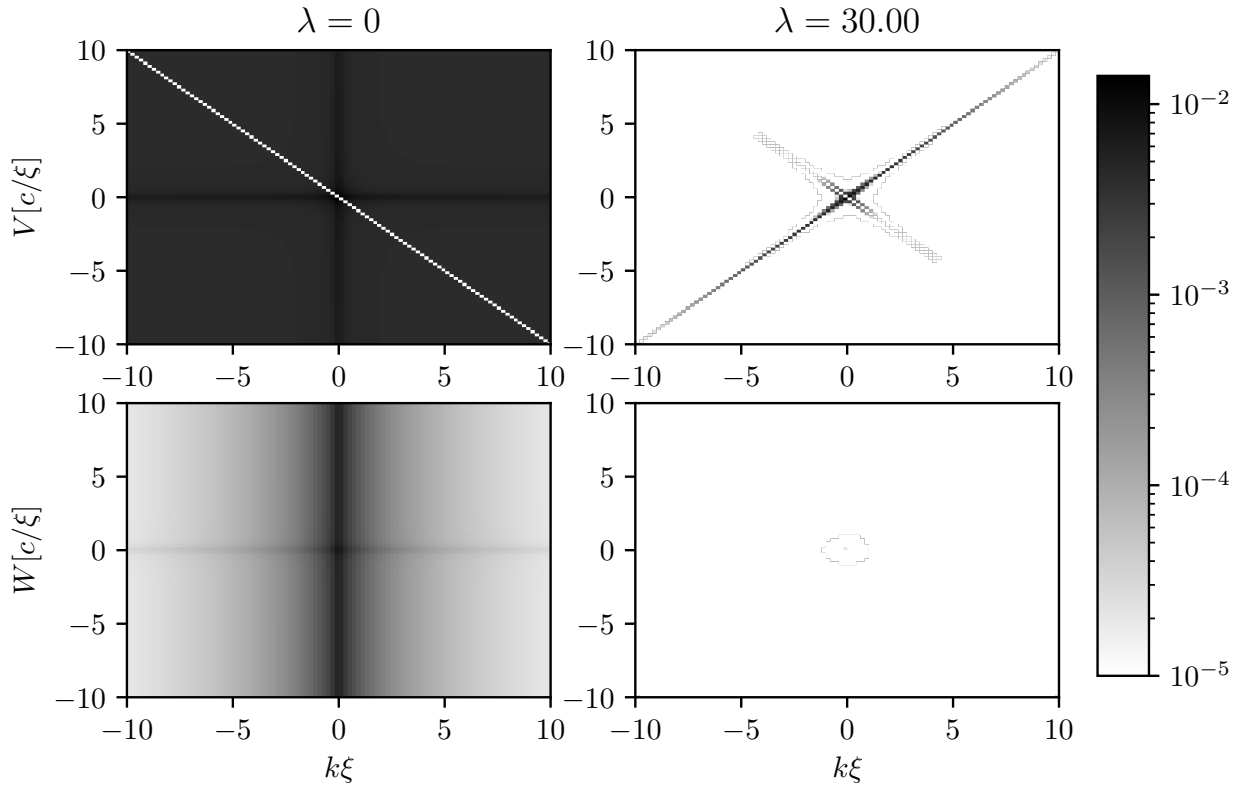


Figure 4.6: Visualization of the flow progression for $\eta = 0.2$ and $\varphi = 1$ analogous to Figure 4.1. We can see that by introducing the symmetry breaking parameter φ , all $V_{k,k'}$ decay from the outside, albeit slowly. Yet, considering the shading scale is logarithmic, many $V_{k,k'}$ can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

$$\{\Delta k_n\}_{n \in \mathbb{Z}} \rightarrow \left\{ \Delta k_n + \frac{\varphi}{L} \right\}_{n \in \mathbb{Z}} \quad (4.2)$$

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 $\varphi \rightarrow 0$. This transformation is not merely a mathematically convenient trick but is also physically meaningful. If we consider our BEC in which the impurity is immersed arranged in circular form we expect periodic boundary conditions

$$\psi(x) = \psi(x + L) \quad (4.3)$$

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:

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

It can then be shown [14] that these twisted boundary conditions are equivalent to the shift

$$-i\partial_x \rightarrow -i\partial_x + \frac{\varphi}{L} \quad (4.5)$$

or, after recognizing the momentum operator in position representation,

$$k \rightarrow k + \frac{\varphi}{L}. \quad (4.6)$$

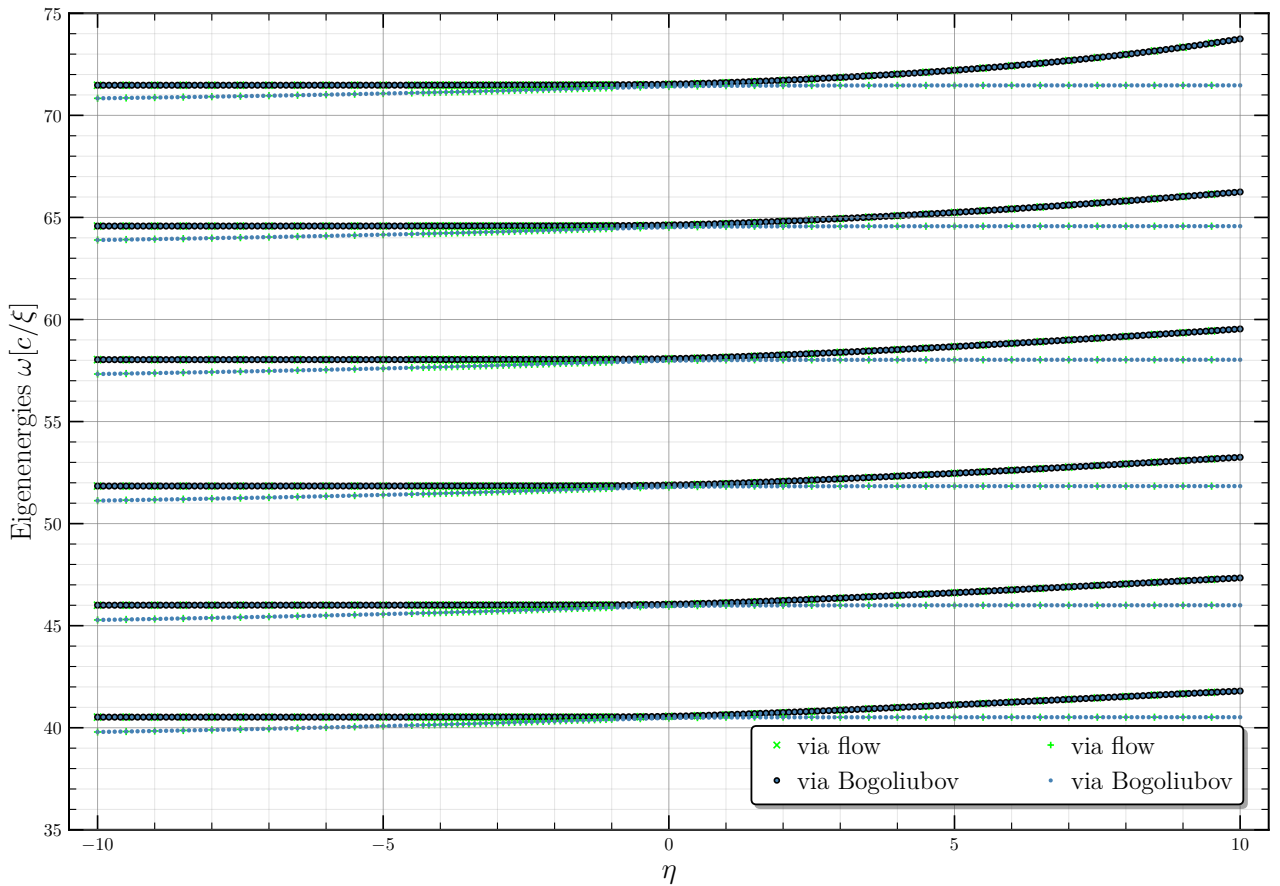


Figure 4.7: This plot shows how the largest eigenvalues change in η analogously to Figure 4.5 when twisted boundary conditions are in place. We can see that the symmetry breaking helps the convergence of the flow equations to the diagonal Hamiltonian.

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 4.7 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.

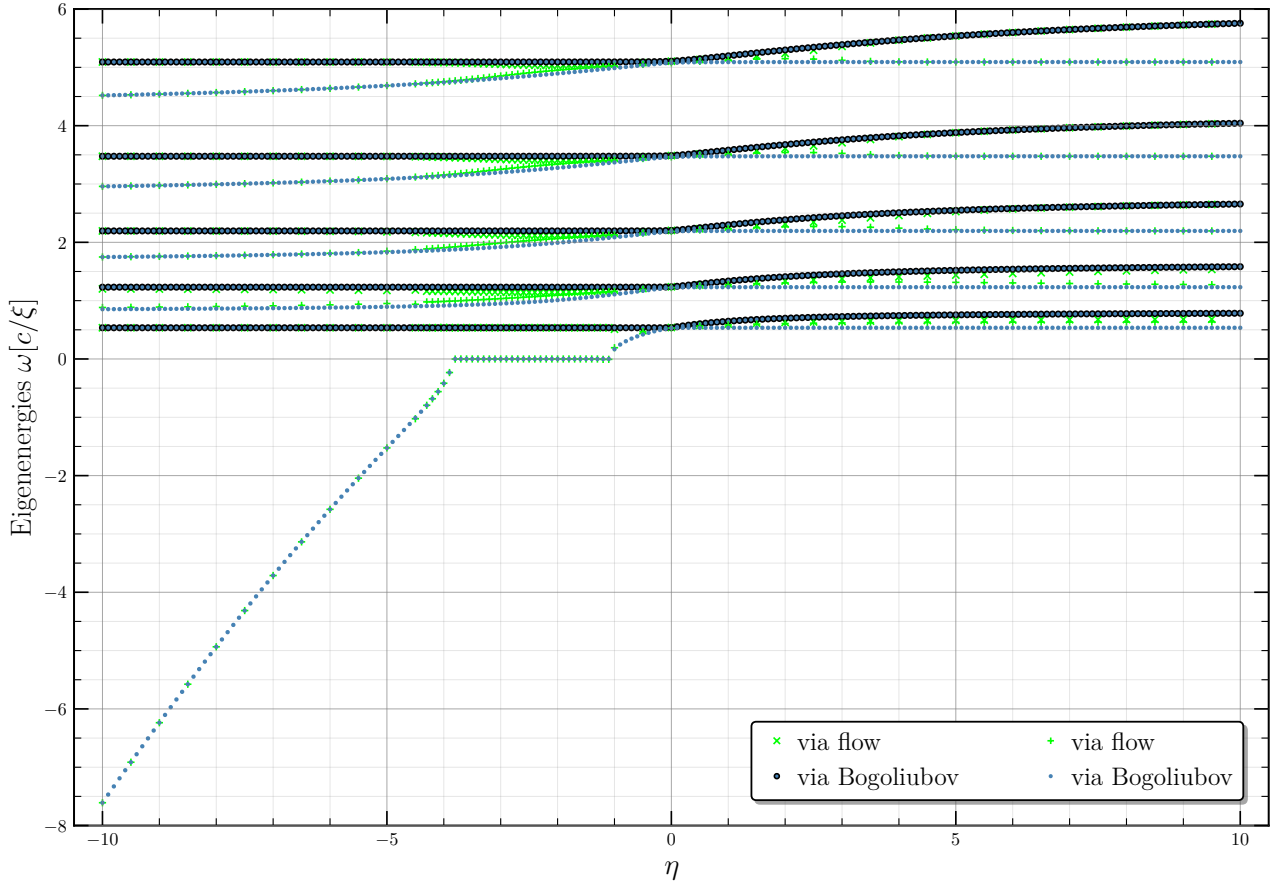


Figure 4.8: This plot shows how the smallest eigenvalues change in η analogously to Figure 4.5 when twisted boundary conditions are in place. We notice a slight discrepancy between the results obtained via Bogoliubov Transformation and via the Flow Equations.

However, it is assumed that these discrepancies 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.

SECTION 5

CONCLUSION AND OUTLOOK

A.1 Deriving the flow equations in the case of no n-dependence

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

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

$$\begin{aligned} &= \sum_k \sum_{q,q'} \omega_k V_{q,q'} [\hat{a}_k^\dagger \hat{a}_k, \hat{a}_q^\dagger \hat{a}_{q'}] + \sum_k \sum_{p,p'} \left(\omega_k W_{p,p'} [\hat{a}_k^\dagger \hat{a}_k, \hat{a}_p^\dagger \hat{a}_{p'}] + \omega_k W_{p,p'}^* [\hat{a}_k^\dagger \hat{a}_k, \hat{a}_p \hat{a}_{p'}] \right) \\ &= \sum_k \sum_{q,q'} \omega_k V_{q,q'} (\hat{a}_k^\dagger \hat{a}_{q'} \delta_{k,q} - \hat{a}_q^\dagger \hat{a}_k \delta_{k,q'}) \\ &+ \sum_k \sum_{p,p'} \left(\omega_k W_{p,p'} (\hat{a}_k^\dagger \hat{a}_p \delta_{k,p'} + \hat{a}_k^\dagger \hat{a}_{p'} \delta_{k,p}) - \omega_k W_{p,p'}^* (\hat{a}_p \hat{a}_k \delta_{k,p'} + \hat{a}_{p'} \hat{a}_k \delta_{k,p}) \right) \\ &= \sum_{q \neq q'} V_{q,q'} (\omega_q - \omega_{q'}) \hat{a}_q^\dagger \hat{a}_{q'} + \sum_{p,p'} \left(W_{p,p'} (\omega_p + \omega_{p'}) \hat{a}_p^\dagger \hat{a}_{p'} - W_{p,p'}^* (\omega_p + \omega_{p'}) \hat{a}_p \hat{a}_{p'} \right) \end{aligned} \quad (\text{A.2})$$

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

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

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

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

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

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

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

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

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}_{\tilde{q}} - \sum_k \sum_{\tilde{q}} V_{k,\tilde{q}} V_{\tilde{q},k} (\omega_{\tilde{q}} - \omega_k) \hat{a}_k^\dagger \hat{a}_{\tilde{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}} 2V_{\tilde{q},k} V_{k,\tilde{q}} (\omega_k - \omega_{\tilde{q}}) \hat{a}_k^\dagger \hat{a}_{\tilde{q}} \tag{A.9}
\end{aligned}$$

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

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

A.7:

$$\begin{aligned} & \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}'}^\dagger \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}_p^\dagger\hat{a}_{p'}^\dagger, \hat{a}_{\tilde{q}}^\dagger\hat{a}_{\tilde{q}'}^\dagger \right] - W_{p,p'}^* \left[\hat{a}_p\hat{a}_{p'}, \hat{a}_{\tilde{q}}^\dagger\hat{a}_{\tilde{q}'}^\dagger \right] \right) \\ &= - \sum_{p,p'} \sum_{q \neq q'} V_{q,q'}(\omega_p + \omega_{p'}) W_{p,p'} \left(\hat{a}_q^\dagger\hat{a}_p^\dagger\delta_{q',p'} + \hat{a}_q^\dagger\hat{a}_{p'}^\dagger\delta_{q',p} \right) \\ &\quad - \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}_q^\dagger\hat{a}_p^\dagger - \sum_{p,p'} \sum_q V_{q,p}(\omega_p + \omega_{p'}) W_{p,p'}\hat{a}_q^\dagger\hat{a}_{p'}^\dagger \\ &\quad - \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}_p^\dagger\hat{a}_{p'}^\dagger - \sum_{p,p'} \sum_q V_{p,q}(\omega_q + \omega_{p'}) W_{q,p}\hat{a}_p^\dagger\hat{a}_{p'}^\dagger \\ &\quad - \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}_p^\dagger\hat{a}_{p'}^\dagger \\ &\quad - \sum_{p,p'} \sum_q V_{q,p}(\omega_q + \omega_{p'}) (W_{p',q}^* + W_{q,p'}^*)\hat{a}_p\hat{a}_{p'} \quad (\text{A.11}) \end{aligned}$$

A.8:

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

$$\begin{aligned}
& - \sum_{p,p'} \sum_{\tilde{p}'} W_{p,\tilde{p}'}(\omega_p + 2\omega_{\tilde{p}'} + \omega_{p'}) W_{\tilde{p}',p}^* \hat{a}_p^\dagger \hat{a}_{p'} - \sum_{p,p'} \sum_{\tilde{p}'} W_{\tilde{p}',p}(2\omega_{\tilde{p}'} + \omega_p + \omega_{p'}) W_{\tilde{p}',p'}^* \hat{a}_p^\dagger \hat{a}_{p'} \\
& = - \sum_{p,p'} \sum_{\tilde{p}} (W_{p,\tilde{p}} + W_{\tilde{p},p})(\omega_p + 2\omega_{\tilde{p}} + \omega_{p'}) W_{p',\tilde{p}}^* \hat{a}_{p'}^\dagger \hat{a}_p^\dagger \\
& - \sum_{p,p'} \sum_{\tilde{p}'} (W_{p,\tilde{p}'} + W_{\tilde{p}',p})(\omega_p + 2\omega_{\tilde{p}'} + \omega_{p'}) W_{\tilde{p}',p}^* \hat{a}_p^\dagger \hat{a}_{p'} \\
& = - \sum_{p,p'} \sum_{\tilde{p}} (W_{p,\tilde{p}} + W_{\tilde{p},p})(\omega_p + 2\omega_{\tilde{p}} + \omega_{p'}) W_{p',\tilde{p}}^* (\delta_{p,p'} + \hat{a}_p^\dagger \hat{a}_{p'}) \\
& - \sum_{p,p'} \sum_{\tilde{p}} (W_{p,\tilde{p}} + W_{\tilde{p},p})(\omega_p + 2\omega_{\tilde{p}} + \omega_{p'}) W_{\tilde{p},p'}^* \hat{a}_p^\dagger \hat{a}_{p'} \\
& = - \sum_{p,p'} \sum_{\tilde{p}} (W_{p,\tilde{p}} + W_{\tilde{p},p})(\omega_p + 2\omega_{\tilde{p}} + \omega_{p'}) (W_{\tilde{p},p'}^* + W_{p',\tilde{p}}^*) \hat{a}_p^\dagger \hat{a}_{p'} \\
& - 2 \sum_k \sum_{\tilde{p}} (W_{k,\tilde{p}} + W_{\tilde{p},k})(\omega_k + \omega_{\tilde{p}}) W_{k,\tilde{p}}^* \\
& = - \sum_{q \neq q'} \sum_{\tilde{p}} (W_{q,\tilde{p}} + W_{\tilde{p},q})(\omega_q + 2\omega_{\tilde{p}} + \omega_{q'}) (W_{\tilde{p},q'}^* + W_{q',\tilde{p}}^*) \hat{a}_q^\dagger \hat{a}_{q'} \\
& - 2 \sum_k \sum_{\tilde{p}} (W_{k,\tilde{p}} + W_{\tilde{p},k})(\omega_k + \omega_{\tilde{p}}) (W_{\tilde{p},k}^* + W_{k,\tilde{p}}^*) \hat{a}_k^\dagger \hat{a}_k \\
& - 2 \sum_k \sum_{\tilde{p}} (W_{k,\tilde{p}} + W_{\tilde{p},k})(\omega_k + \omega_{\tilde{p}}) W_{k,\tilde{p}}^* \tag{A.12}
\end{aligned}$$

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

$$\hat{\mathcal{H}}(\lambda) = \sum_k \omega_k(\lambda) \hat{a}_k^\dagger \hat{a}_k + \sum_{q \neq q'} V_{q,q'}(\lambda) \hat{a}_q^\dagger \hat{a}_{q'} + \sum_{p,p'} (W_{p,p'}(\lambda) \hat{a}_p^\dagger \hat{a}_{p'} + W_{p,p'}^*(\lambda) \hat{a}_p \hat{a}_{p'}) + \epsilon(\lambda) \tag{A.13}$$

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 $q \neq q'$:

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

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

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

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

$$\partial_\lambda \epsilon = -2 \sum_{p,p'} (W_{p,p'} + W_{p',p})(\omega_p + \omega_{p'}) W_{p,p'}^* \tag{A.14e}$$

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 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:

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

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 calculating the flow equations is again to calculate the canonical commutator $\hat{\eta} := [\hat{\mathcal{H}}_0, \hat{\mathcal{H}}_{\text{int}}]$:

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

$$+ \sum_{p,p'} [\hat{H}, \hat{W}_{p,p'} : \hat{a}_p^\dagger \hat{a}_{p'}^\dagger :] \quad (\text{A.16b})$$

$$+ \sum_{p,p'} [\hat{H}, \hat{W}_{p,p'}^\dagger : \hat{a}_p \hat{a}_{p'} :] \quad (\text{A.16c})$$

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

A.16a

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

$$(\text{A.18})$$

A.16b

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

A.16c

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

This gives the canonical generator as:

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

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

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

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

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

$$\begin{aligned}
& - \sum_{p,p'} \hat{\phi}_{p,p'} \left(\hat{H} - \hat{H}(\hat{n}_{p'} - 1, \hat{n}_p - 1) \right) : \hat{a}_p^\dagger \hat{a}_{p'}^\dagger : \\
& - \sum_{p,p'} \hat{\psi}_{p,p'} \left(\hat{H} - \hat{H}(\hat{n}_{p'} + 1, \hat{n}_p + 1) \right) : \hat{a}_p \hat{a}_{p'} : \\
& = - \sum_{q \neq q'} \hat{V}_{q,q'} \left(\hat{H} - \hat{H}(\hat{n}_q - 1, \hat{n}_{q'} + 1) \right)^2 : \hat{a}_q^\dagger \hat{a}_{q'} : \\
& - \sum_{p,p'} \hat{W}_{p,p'} \left(\hat{H} - \hat{H}(\hat{n}_{p'} - 1, \hat{n}_p - 1) \right)^2 : \hat{a}_p^\dagger \hat{a}_{p'}^\dagger : \\
& - \sum_{p,p'} \hat{W}_{p,p'}^\dagger \left(\hat{H} - \hat{H}(\hat{n}_{p'} + 1, \hat{n}_p + 1) \right)^2 : \hat{a}_p \hat{a}_{p'} :
\end{aligned} \tag{A.24}$$

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

$$\left[\eta^{(2)}, \hat{\mathcal{H}}_{\text{int}} \right] = \sum_{q \neq q'} \sum_{\tilde{q} \neq \tilde{q}'} \left[\hat{\theta}_{\tilde{q},\tilde{q}'} : \hat{a}_{\tilde{q}}^\dagger \hat{a}_{\tilde{q}'} : , \hat{V}_{q,q'} : \hat{a}_q^\dagger \hat{a}_{q'} : \right] \tag{A.25a}$$

$$+ \sum_{p,p'} \sum_{\tilde{q} \neq \tilde{q}'} \left[\hat{\theta}_{\tilde{q},\tilde{q}'} : \hat{a}_{\tilde{q}}^\dagger \hat{a}_{\tilde{q}'} : , \hat{W}_{p,p'} : \hat{a}_p^\dagger \hat{a}_{p'}^\dagger : \right] \tag{A.25b}$$

$$+ \sum_{p,p'} \sum_{\tilde{q} \neq \tilde{q}'} \left[\hat{\theta}_{\tilde{q},\tilde{q}'} : \hat{a}_{\tilde{q}}^\dagger \hat{a}_{\tilde{q}'} : , \hat{W}_{p,p'}^\dagger : \hat{a}_p \hat{a}_{p'} : \right] \tag{A.25c}$$

$$+ \sum_{q \neq q'} \sum_{\tilde{p},\tilde{p}'} \left[\hat{\phi}_{\tilde{p},\tilde{p}'} : \hat{a}_{\tilde{p}}^\dagger \hat{a}_{\tilde{p}'}^\dagger : , \hat{V}_{q,q'} : \hat{a}_q^\dagger \hat{a}_{q'} : \right] \tag{A.25d}$$

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

$$+ \sum_{p,p'} \sum_{\tilde{p},\tilde{p}'} \left[\hat{\phi}_{\tilde{p},\tilde{p}'} : \hat{a}_{\tilde{p}}^\dagger \hat{a}_{\tilde{p}'}^\dagger :, \hat{W}_{p,p'}^\dagger : \hat{a}_p \hat{a}_{p'} : \right] \quad (\text{A.25f})$$

$$+ \sum_{q \neq q'} \sum_{\tilde{p},\tilde{p}'} \left[\hat{\psi}_{\tilde{p},\tilde{p}'} : \hat{a}_{\tilde{p}} \hat{a}_{\tilde{p}'} :, \hat{V}_{q,q'} : \hat{a}_q^\dagger \hat{a}_{q'} : \right] \quad (\text{A.25g})$$

$$+ \sum_{p,p'} \sum_{\tilde{p},\tilde{p}'} \left[\hat{\psi}_{\tilde{p},\tilde{p}'} : \hat{a}_{\tilde{p}} \hat{a}_{\tilde{p}'} :, \hat{W}_{p,p'}^\dagger : \hat{a}_p^\dagger \hat{a}_{p'}^\dagger : \right] \quad (\text{A.25h})$$

$$+ \sum_{p,p'} \sum_{\tilde{p},\tilde{p}'} \left[\hat{\psi}_{\tilde{p},\tilde{p}'} : \hat{a}_{\tilde{p}} \hat{a}_{\tilde{p}'} :, \hat{W}_{p,p'}^\dagger : \hat{a}_p \hat{a}_{p'} : \right] \quad (\text{A.25i})$$

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

A.25a:

$$\begin{aligned} & \sum_{q \neq q'} \sum_{\tilde{q} \neq \tilde{q}'} \left[\hat{\theta}_{\tilde{q},\tilde{q}'} : \hat{a}_{\tilde{q}}^\dagger \hat{a}_{\tilde{q}'} :, \hat{V}_{q,q'} : \hat{a}_q^\dagger \hat{a}_{q'} : \right] \\ &= \sum_{q \neq q'} \sum_{\tilde{q} \neq \tilde{q}'} \hat{\theta}_{\tilde{q},\tilde{q}'} \hat{V}_{q,q'} \left[: \hat{a}_{\tilde{q}}^\dagger \hat{a}_{\tilde{q}'} :, : \hat{a}_q^\dagger \hat{a}_{q'} : \right] \\ &+ \sum_{q \neq q'} \sum_{\tilde{q} \neq \tilde{q}'} \hat{V}_{q,q'} \left[\hat{\theta}_{\tilde{q},\tilde{q}'} : \hat{a}_{\tilde{q}}^\dagger \hat{a}_{\tilde{q}'} : \right] : \hat{a}_q^\dagger \hat{a}_{q'} : \\ &+ \sum_{q \neq q'} \sum_{\tilde{q} \neq \tilde{q}'} \hat{\theta}_{\tilde{q},\tilde{q}'} \left[: \hat{a}_{\tilde{q}}^\dagger \hat{a}_{\tilde{q}'} :, \hat{V}_{q,q'} \right] : \hat{a}_q^\dagger \hat{a}_{q'} : \\ &= \sum_{q \neq q'} \sum_{\tilde{q} \neq \tilde{q}'} \hat{\theta}_{\tilde{q},\tilde{q}'} \hat{V}_{q,q'} \left(\delta_{\tilde{q}',q} : \hat{a}_{\tilde{q}}^\dagger \hat{a}_q : - \delta_{\tilde{q},q'} : \hat{a}_q^\dagger \hat{a}_{\tilde{q}'} : \right) \end{aligned} \quad (\text{A.26})$$

$$\begin{aligned} &+ \sum_{q \neq q'} \sum_{\tilde{q} \neq \tilde{q}'} \hat{V}_{q,q'} \left(\hat{\theta}_{\tilde{q},\tilde{q}'} - \hat{\theta}_{\tilde{q},\tilde{q}'} (\hat{n}_{q'} + 1, \hat{n}_q - 1) \right) : \hat{a}_q^\dagger \hat{a}_{q'} : \underbrace{\hat{a}_{\tilde{q}}^\dagger \hat{a}_{\tilde{q}'} :}_{\stackrel{\textcircled{2}}{=} \delta_{q',\tilde{q}} : \hat{a}_q^\dagger \hat{a}_{\tilde{q}'} :} \\ &- \sum_{q \neq q'} \sum_{\tilde{q} \neq \tilde{q}'} \hat{\theta}_{q,q'} \left[\hat{V}_{\tilde{q},\tilde{q}'} : \hat{a}_q^\dagger \hat{a}_{q'} : \right] : \hat{a}_{\tilde{q}}^\dagger \hat{a}_{\tilde{q}'} : \\ &\stackrel{\textcircled{2}}{=} \sum_{q \neq q'} \sum_{\tilde{q}} \left(\hat{\theta}_{\tilde{q},q} \hat{V}_{q,q'} : \hat{a}_{\tilde{q}}^\dagger \hat{a}_q : - \hat{\theta}_{q',\tilde{q}} \hat{V}_{q,q'} : \hat{a}_q^\dagger \hat{a}_{\tilde{q}} : \right) \\ &+ \sum_{q \neq q'} \sum_{\tilde{q}} \hat{V}_{q,q'} \left(\hat{\theta}_{q',\tilde{q}} - \hat{\theta}_{q',\tilde{q}} (\hat{n}_{q'} + 1, \hat{n}_q - 1) \right) : \hat{a}_q^\dagger \hat{a}_{\tilde{q}} : \\ &- \sum_{q \neq q'} \sum_{\tilde{q} \neq \tilde{q}'} \hat{\theta}_{q,q'} \left[\hat{V}_{\tilde{q},\tilde{q}'} : \hat{a}_q^\dagger \hat{a}_{q'} : \right] : \hat{a}_{\tilde{q}}^\dagger \hat{a}_{\tilde{q}'} : \end{aligned}$$

$$\begin{aligned} &= \sum_{q,q'} \sum_{\tilde{q}} \left(\hat{\theta}_{q,q'} \hat{V}_{q',\tilde{q}} : \hat{a}_q^\dagger \hat{a}_{q'} : - \hat{\theta}_{\tilde{q},q'} \hat{V}_{q,\tilde{q}} : \hat{a}_q^\dagger \hat{a}_{q'} : \right) \\ &- \underbrace{\sum_k \sum_{\tilde{q}} \left(\hat{\theta}_{\tilde{q},k} \hat{V}_{k,k} : \hat{a}_{\tilde{q}}^\dagger \hat{a}_k : - \hat{\theta}_{k,\tilde{q}} \hat{V}_{k,k} : \hat{a}_k^\dagger \hat{a}_{\tilde{q}} : \right)}_{=0} \end{aligned} \quad (\text{A.27})$$

$$\begin{aligned} &+ \sum_{q,q'} \sum_{\tilde{q}} \hat{V}_{q,\tilde{q}} \left(\hat{\theta}_{\tilde{q},q'} - \hat{\theta}_{\tilde{q},q'} (\hat{n}_{\tilde{q}} + 1, \hat{n}_q - 1) \right) : \hat{a}_q^\dagger \hat{a}_{q'} : \\ &- \underbrace{\sum_k \sum_{\tilde{q}} \hat{V}_{k,k} \left(\hat{\theta}_{k,\tilde{q}} - \hat{\theta}_{k,\tilde{q}} (\hat{n}_k + 1, \hat{n}_k - 1) \right) : \hat{a}_k^\dagger \hat{a}_{\tilde{q}} :}_{=0} \\ &- \sum_{q \neq q'} \sum_{\tilde{q} \neq \tilde{q}'} \hat{\theta}_{q,q'} \left[\hat{V}_{\tilde{q},\tilde{q}'} : \hat{a}_q^\dagger \hat{a}_{q'} : \right] : \hat{a}_{\tilde{q}}^\dagger \hat{a}_{\tilde{q}'} : \\ &= \sum_{q \neq q'} \sum_{\tilde{q}} \left(\hat{\theta}_{q,q'} \hat{V}_{q',\tilde{q}} : \hat{a}_q^\dagger \hat{a}_{q'} : - \hat{\theta}_{\tilde{q},q'} \hat{V}_{q,\tilde{q}} : \hat{a}_q^\dagger \hat{a}_{q'} : \right) \end{aligned} \quad (\text{A.28})$$

$$\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'} : \\
& + \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,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} \tag{A.29}$$

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

A.25b:

$$\begin{aligned}
& \sum_{p,p'} \sum_{\tilde{q} \neq \tilde{q}'} \left[\hat{\theta}_{\tilde{q},\tilde{q}'} : \hat{a}_{\tilde{q}}^\dagger \hat{a}_{\tilde{q}'} : , \hat{W}_{p,p'} : \hat{a}_p^\dagger \hat{a}_{p'} : \right] \\
& = \sum_{p,p'} \sum_{\tilde{q} \neq \tilde{q}'} \hat{\theta}_{\tilde{q},\tilde{q}'} \hat{W}_{p,p'} \left[: \hat{a}_{\tilde{q}}^\dagger \hat{a}_{\tilde{q}'} : , : \hat{a}_p^\dagger \hat{a}_{p'} : \right]
\end{aligned} \tag{A.30a}$$

$$+ \sum_{p,p'} \sum_{\tilde{q} \neq \tilde{q}'} \hat{\theta}_{\tilde{q},\tilde{q}'} \left[: \hat{a}_{\tilde{q}}^\dagger \hat{a}_{\tilde{q}'} : , \hat{W}_{p,p'} \right] : \hat{a}_p^\dagger \hat{a}_{p'} : \tag{A.30b}$$

$$+ \sum_{p,p'} \sum_{\tilde{q} \neq \tilde{q}'} \hat{W}_{p,p'} \left[\hat{\theta}_{\tilde{q},\tilde{q}'} : \hat{a}_p^\dagger \hat{a}_{p'} : \right] : \hat{a}_{\tilde{q}}^\dagger \hat{a}_{\tilde{q}'} : \tag{A.30c}$$

We start by evaluating A.30a:

$$\begin{aligned}
& \sum_{p,p'} \sum_{\tilde{q} \neq \tilde{q}'} \hat{\theta}_{\tilde{q},\tilde{q}'} \hat{W}_{p,p'} \left[: \hat{a}_{\tilde{q}}^\dagger \hat{a}_{\tilde{q}'} : , : \hat{a}_p^\dagger \hat{a}_{p'} : \right] \\
& = \sum_{p,p'} \sum_{q \neq q'} \hat{\theta}_{q,q'} \hat{W}_{p,p'} \left(\delta_{q',p'} : \hat{a}_q^\dagger \hat{a}_p^\dagger : + \delta_{q',p} : \hat{a}_q^\dagger \hat{a}_{p'}^\dagger : \right) \\
& = \sum_{p,p'} \sum_q \hat{\theta}_{q,p'} \hat{W}_{p,p'} : \hat{a}_q^\dagger \hat{a}_p^\dagger : + \sum_{p,p'} \sum_q \hat{\theta}_{q,p} \hat{W}_{p,p'} : \hat{a}_q^\dagger \hat{a}_{p'}^\dagger : \\
& = \sum_{p,p'} \sum_q \left(\hat{\theta}_{p',q} \hat{W}_{p,q} + \hat{\theta}_{p,q} \hat{W}_{q,p'} \right) : \hat{a}_p^\dagger \hat{a}_{p'}^\dagger :
\end{aligned} \tag{A.31}$$

Next is A.30b:

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

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

A.30c gives no quadratic contribution:

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

A.25c:

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

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

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

We will again start by evaluating A.34a:

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

A.34b gives no quadratic contribution:

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

A.34c:

$$\begin{aligned} & \sum_{p,p'} \sum_{q \neq q'} \hat{W}_{p,p'}^\dagger \left[\hat{\theta}_{q,q'}, : \hat{a}_p \hat{a}_{p'} : \right] : \hat{a}_q^\dagger \hat{a}_{q'} : \\ &= \sum_{p,p'} \sum_{q \neq q'} \hat{W}_{p,p'}^\dagger \left(\hat{\theta}_{q,q'} - \hat{\theta}_{q,q'} (\hat{n}_{p'} + 1, \hat{n}_p + 1) \right) : \hat{a}_p \hat{a}_{p'} : : \hat{a}_q^\dagger \hat{a}_{q'} : \end{aligned} \quad (\text{A.37})$$

$$\begin{aligned} & \stackrel{\textcircled{2}}{=} \sum_{p,p'} \sum_{q \neq q'} \hat{W}_{p,p'}^\dagger \left(\hat{\theta}_{q,q'} - \hat{\theta}_{q,q'} (\hat{n}_{p'} + 1, \hat{n}_p + 1) \right) (\delta_{p,q} : \hat{a}_{p'} \hat{a}_{q'} : + \delta_{p',q} : \hat{a}_p \hat{a}_{q'} :) \\ &= \sum_{p,p'} \sum_{q'} \hat{W}_{p,p'}^\dagger \left(\hat{\theta}_{p,q'} - \hat{\theta}_{p,q'} (\hat{n}_{p'} + 1, \hat{n}_p + 1) \right) : \hat{a}_{p'} \hat{a}_{q'} : \end{aligned} \quad (\text{A.38})$$

$$\begin{aligned} & + \sum_{p,p'} \sum_{q'} \hat{W}_{p,p'}^\dagger \left(\hat{\theta}_{p',q'} - \hat{\theta}_{p',q'} (\hat{n}_{p'} + 1, \hat{n}_p + 1) \right) : \hat{a}_p \hat{a}_{q'} : \\ &= \sum_{p,p'} \sum_q \hat{W}_{q,p'}^\dagger \left(\hat{\theta}_{q,p} - \hat{\theta}_{q,p} (\hat{n}_{p'} + 1, \hat{n}_q + 1) \right) : \hat{a}_p \hat{a}_{p'} : \end{aligned} \quad (\text{A.39})$$

$$\begin{aligned} & + \sum_{p,p'} \sum_q \hat{W}_{p,q}^\dagger \left(\hat{\theta}_{q,p'} - \hat{\theta}_{q,p'} (\hat{n}_q + 1, \hat{n}_p + 1) \right) : \hat{a}_p \hat{a}_{p'} : \\ &= \sum_{p,p'} \sum_q \left(\hat{W}_{q,p'}^\dagger + \hat{W}_{p',q}^\dagger \right) \left(\hat{\theta}_{q,p} - \hat{\theta}_{q,p} (\hat{n}_{p'} + 1, \hat{n}_q + 1) \right) : \hat{a}_p \hat{a}_{p'} : \end{aligned} \quad (\text{A.40})$$

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

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

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

$$\begin{aligned} &= - \sum_{p,p'} \sum_q \left(\hat{V}_{p',q} \hat{\phi}_{p,q} + \hat{V}_{p,q} \hat{\phi}_{q,p'} \right) : \hat{a}_p^\dagger \hat{a}_{p'}^\dagger : \\ &- \sum_{p,p'} \sum_q \hat{V}_{p,q} \left(\hat{\phi}_{q,p'} (\hat{n}_q + 1, \hat{n}_p - 1) - \hat{\phi}_{q,p} \right) : \hat{a}_p^\dagger \hat{a}_{p'}^\dagger : \\ &- \sum_{p,p'} \sum_q \hat{V}_{p',q} \left(\hat{\phi}_{p,q} (\hat{n}_q + 1, \hat{n}_{p'} - 1) - \hat{\phi}_{p,q} \right) : \hat{a}_p^\dagger \hat{a}_{p'}^\dagger : \end{aligned} \quad (\text{A.41c})$$

A.25e:

$$\begin{aligned} & \sum_{p,p'} \sum_{\tilde{p}, \tilde{p}'} \left[\hat{\phi}_{\tilde{p}, \tilde{p}'} : \hat{a}_{\tilde{p}}^\dagger \hat{a}_{\tilde{p}'}^\dagger :, \hat{W}_{p,p'} : \hat{a}_p^\dagger \hat{a}_{p'}^\dagger : \right] \\ &= \sum_{p,p'} \sum_{\tilde{p}, \tilde{p}'} \hat{\phi}_{\tilde{p}, \tilde{p}'} \left[: \hat{a}_{\tilde{p}}^\dagger \hat{a}_{\tilde{p}'}^\dagger :, \hat{W}_{p,p'} \right] : \hat{a}_p^\dagger \hat{a}_{p'}^\dagger : \end{aligned} \quad (\text{A.42a})$$

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

A.42a will be analyzed first:

$$\begin{aligned} & \sum_{p,p'} \sum_{\tilde{p}, \tilde{p}'} \hat{\phi}_{\tilde{p}, \tilde{p}'} \left[: \hat{a}_{\tilde{p}}^\dagger \hat{a}_{\tilde{p}'}^\dagger :, \hat{W}_{p,p'} \right] : \hat{a}_p^\dagger \hat{a}_{p'}^\dagger : \\ &= \sum_{p,p'} \sum_{\tilde{p}, \tilde{p}'} \hat{\phi}_{\tilde{p}, \tilde{p}'} \left(\hat{W}_{p,p'} (\hat{n}_{\tilde{p}} + 1, \hat{n}_{\tilde{p}'} + 1) - \hat{W}_{p,p'} \right) : \hat{a}_{\tilde{p}}^\dagger \hat{a}_{\tilde{p}'}^\dagger : : \hat{a}_p^\dagger \hat{a}_{p'}^\dagger : \stackrel{\textcircled{2}}{=} 0 \end{aligned} \quad (\text{A.43})$$

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

A.25f

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

$$+ \sum_{p,p'} \sum_{\tilde{p},\tilde{p}'} \hat{\phi}_{\tilde{p},\tilde{p}'} \left[: \hat{a}_{\tilde{p}}^\dagger \hat{a}_{\tilde{p}'}^\dagger : , \hat{W}_{p,p'}^\dagger \right] : \hat{a}_p \hat{a}_{p'} : \quad (\text{A.44b})$$

$$+ \sum_{p,p'} \sum_{\tilde{p},\tilde{p}'} \hat{W}_{p,p'}^\dagger \left[\hat{\phi}_{\tilde{p},\tilde{p}'} , : \hat{a}_p \hat{a}_{p'} : \right] : \hat{a}_{\tilde{p}}^\dagger \hat{a}_{\tilde{p}'}^\dagger : \quad (\text{A.44c})$$

A.44a:

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

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

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

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

$$- \sum_{p,p'} \left(\hat{\phi}_{p,p'} \hat{W}_{p,p'}^\dagger + \hat{\phi}_{p',p} \hat{W}_{p,p'}^\dagger \right)$$

A.44b gives no quadratic contribution:

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

A.44c:

$$\begin{aligned}
& \sum_{p,p'} \sum_{\tilde{p},\tilde{p}'} \hat{W}_{p,p'}^\dagger \left[\hat{\phi}_{\tilde{p},\tilde{p}'} : \hat{a}_p \hat{a}_{p'} : \right] : \hat{a}_{\tilde{p}}^\dagger \hat{a}_{\tilde{p}'}^\dagger : \\
&= \sum_{p,p'} \sum_{\tilde{p},\tilde{p}'} \hat{W}_{p,p'}^\dagger \left(\hat{\phi}_{\tilde{p},\tilde{p}'} - \hat{\phi}_{\tilde{p},\tilde{p}'} (\hat{n}_p + 1, \hat{n}_{p'} + 1) \right) : \hat{a}_p \hat{a}_{p'} :: \hat{a}_{\tilde{p}}^\dagger \hat{a}_{\tilde{p}'}^\dagger :
\end{aligned} \tag{A.50}$$

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

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

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

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

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

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

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

$$\begin{aligned}
& \sum_{p,p'} \sum_{\tilde{p}, \tilde{p}'} \left[\hat{\psi}_{\tilde{p}, \tilde{p}'} : \hat{a}_{\tilde{p}} \hat{a}_{\tilde{p}'}^\dagger : , \hat{W}_{p,p'} : \hat{a}_p^\dagger \hat{a}_{p'}^\dagger : \right] \\
& = - \sum_{p,p'} \sum_{\tilde{p}, \tilde{p}'} \left[\hat{W}_{\tilde{p}, \tilde{p}'} : \hat{a}_{\tilde{p}}^\dagger \hat{a}_{\tilde{p}'}^\dagger : , \hat{\psi}_{p,p'} : \hat{a}_p \hat{a}_{p'} : \right]
\end{aligned} \tag{A.55}$$

$$\begin{aligned}
& = \sum_{p,p'} \sum_{\tilde{p}} \left(\hat{W}_{p,\tilde{p}} \hat{\psi}_{p',\tilde{p}} + \hat{W}_{\tilde{p},p} \hat{\psi}_{p',\tilde{p}} + \hat{W}_{p,\tilde{p}} \hat{\psi}_{\tilde{p},p'} + \hat{W}_{\tilde{p},p} \hat{\psi}_{\tilde{p},p'} \right) : \hat{a}_p^\dagger \hat{a}_{p'} : \\
& + \sum_{p,p'} \left(\hat{W}_{p,p'} \hat{\psi}_{p,p'} + \hat{W}_{p',p} \hat{\psi}_{p,p'} \right) \\
& - \sum_{p,p'} \sum_{\tilde{p}} \hat{\psi}_{\tilde{p},p'} \left(\hat{W}_{\tilde{p},p} - \hat{W}_{\tilde{p},p}(\hat{n}_{\tilde{p}} + 1, \hat{n}_{p'} + 1) \right) : \hat{a}_p^\dagger \hat{a}_{p'} : \\
& - \sum_{p,p'} \sum_{\tilde{p}} \hat{\psi}_{\tilde{p},p'} \left(\hat{W}_{p,\tilde{p}} - \hat{W}_{p,\tilde{p}}(\hat{n}_{\tilde{p}} + 1, \hat{n}_{p'} + 1) \right) : \hat{a}_p^\dagger \hat{a}_{p'} : \\
& - \sum_{p,p'} \sum_{\tilde{p}} \hat{\psi}_{p',\tilde{p}} \left(\hat{W}_{\tilde{p},p} - \hat{W}_{\tilde{p},p}(\hat{n}_{p'} + 1, \hat{n}_{\tilde{p}} + 1) \right) : \hat{a}_p^\dagger \hat{a}_{p'} : \\
& - \sum_{p,p'} \sum_{\tilde{p}} \hat{\psi}_{p',\tilde{p}} \left(\hat{W}_{p,\tilde{p}} - \hat{W}_{p,\tilde{p}}(\hat{n}_{p'} + 1, \hat{n}_{\tilde{p}} + 1) \right) : \hat{a}_p^\dagger \hat{a}_{p'} : \\
& - \sum_{p,p'} \hat{\psi}_{p,p'} \left(\hat{W}_{p',p} - \hat{W}_{p',p}(\hat{n}_p + 1, \hat{n}_{p'} + 1) \right) \\
& - \sum_{p,p'} \hat{\psi}_{p,p'} \left(\hat{W}_{p,p'} - \hat{W}_{p,p'}(\hat{n}_p + 1, \hat{n}_{p'} + 1) \right)
\end{aligned} \tag{A.56}$$

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

$$\sum_{p,p'} \sum_{\tilde{p}, \tilde{p}'} \left[\hat{\psi}_{\tilde{p}, \tilde{p}'} : \hat{a}_{\tilde{p}} \hat{a}_{\tilde{p}'}^\dagger : , \hat{W}_{p,p'}^\dagger : \hat{a}_p \hat{a}_{p'} : \right] \stackrel{\textcircled{2}}{=} 0 \tag{A.57}$$

A.2.3 The Flow Equations

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

$$\hat{\mathcal{H}}(\lambda) \stackrel{\textcircled{2}}{=} \hat{H} + \sum_{q \neq q'} \hat{V}_{q,q'}(\lambda) : \hat{a}_q^\dagger \hat{a}_{q'} : \tag{A.58}$$

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

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

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

$$\partial_\lambda \hat{W}_{p,p'}^\dagger \stackrel{\textcircled{2}}{=} -W_{p,p'}^\dagger \left(\hat{H} - \hat{H}(\hat{n}_{p'} + 1, \hat{n}_p + 1) \right)^2 \quad (\text{A.59c})$$

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

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

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

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

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

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} :

$$\hat{V}_{q,q'} \approx v_{q,q'}^\circ + \sum_k v_{q,q'}^{(k)} \hat{n}_k + \sum_{k,k'} v_{q,q'}^{(k,k')} \hat{n}_k \hat{n}_{k'} \quad (\text{A.63a})$$

$$\hat{W}_{p,p'} \approx w_{p,p'}^\circ + \sum_k w_{p,p'}^{(k)} \hat{n}_k + \sum_{k,k'} w_{p,p'}^{(k,k')} \hat{n}_k \hat{n}_{k'} \quad (\text{A.63b})$$

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

Then, in quadratic order, we get:

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

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

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

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

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

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

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

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

$$\begin{aligned} \hat{\psi}_{p,p'} &= \hat{W}_{p,p'}^\dagger \left(\hat{H} - \hat{H}(\hat{n}_p - 1, \hat{n}_{p'} + 1) \right) = \hat{W}_{p,p'} \hat{H}_{p,p'}(+, +) \\ &\approx w_{p,p'}^\circ{}^* h_{p,p'}^\circ(+, +) + \sum_k \left(h_{p,p'}^\circ(+, +) w_{p,p'}^{(k)*} + w_{p,p'}^\circ{}^* h_{p,p'}^{(k)}(+, +) \right) \hat{n}_k \\ &\quad + \sum_{k,k'} \left(h_{p,p'}^\circ(+, +) w_{p,p'}^{(k,k')*} + w_{p,p'}^{(k)*} h_{p,p'}^{(k')}(+, +) \right) \hat{n}_k \hat{n}_{k'} \\ &=: \psi_{p,p'}^\circ + \sum_k \psi_{p,p'}^{(k)} \hat{n}_k + \sum_{k,k'} \psi_{p,p'}^{(k,k')} \hat{n}_k \hat{n}_{k'} \end{aligned} \quad (\text{A.66c})$$

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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DECLARATION OF AUTHORSHIP

I hereby declare that I have written this thesis independently and by myself and that I have not used any sources or auxiliary materials other than those indicated in the thesis.

Munich, July 2023

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