Title of My Thesis



SUBMITTED BY

Jan-Philipp Anton Konrad Christ

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Jan-Philipp Anton Konrad Christ

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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 $\hat{1} =: 1$
- $: \hat{A} :$ 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}^{\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
- Equality up to second order, i.e. higher order terms are neglected.
- $\hbar = 1$ reduced Planck's constant is set to 1
- +h.c. plus the Hermitian conjugate of the previous term
- \sim approximately proportional to
- $\underline{\underline{E}}_{N}$ $N \times N$ identity matrix

| SUMMARY |
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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 at 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 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

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

vanish in the limit $\lambda \to \infty$. 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

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

 $\hat{\eta}(\lambda)$ 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

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

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 omitted.

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 same) diagonal Hamiltonian $\hat{\mathcal{H}}(\lambda=\infty)=:\hat{\mathcal{H}}^{(\infty)}$ so there is in general more than one good choice for $\hat{\eta}$.

It turns out that in most cases

$$\hat{\eta} = \left[\hat{\mathcal{H}}_{\text{diag.}}, \hat{\mathcal{H}} \right], \tag{2.4}$$

where $\hat{\mathcal{H}}_{diag.}$ 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 $\hat{\mathcal{H}}_{int}$ are neglected. In this case, we can write $\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{int}$ and thus

$$\hat{\eta} = \left[\hat{\mathcal{H}}_0, \hat{\mathcal{H}}_{int} \right]. \tag{2.5}$$

This choice 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:

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

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

$$\operatorname{Tr}\left(\hat{\mathcal{H}}_{0}\hat{\mathcal{H}}_{\mathrm{int}}\right) = \operatorname{Tr}\left(\frac{\mathrm{d}\hat{\mathcal{H}}_{0}}{\mathrm{d}\lambda}\hat{\mathcal{H}}_{\mathrm{int}}\right) = 0 \tag{2.7}$$

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 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

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

Then it follows that

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

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 a operator \hat{O} composed of creation and annihilation operators is defined by the following three rules:

1. c-numbers are unaffected by normal ordering:

$$: 1 := 1$$
 (2.10)

2. Linearity:

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

3. Recurrence relation:

$$\hat{\alpha}_k : \hat{O} :=: \hat{\alpha}_k \hat{O} :+ \sum_l C_{k,l} : \partial_{\hat{\alpha}_l} \hat{O} :$$
(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 $\hat{\mathcal{H}}_{int}$, 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.

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

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

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

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

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

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]. The inclusion of those leads to very good agreement of experiment and theory. 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 aforementioned two-phonon scattering terms are quadratic and are again proportional to the boson-impurity coupling constant:

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

The coefficients c_k and s_k can be obtained from

$$W_k = c_k - s_k \tag{2.18a}$$

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

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

$$\gamma := \frac{m_B g_{BB}}{n_0} \tag{2.19}$$

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

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

$$a_{BB} = -\frac{2}{m_B g_{BB}} \tag{2.20}$$

where

$$m_B = \frac{1}{\sqrt{2c\xi}} \tag{2.21}$$

is the mass of the bosons and the dimensionless parameter

$$\eta := \frac{g_{IB}}{g_{BB}} \tag{2.22}$$

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

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_F + \hat{\mathcal{H}}_{2ph} \tag{2.23}$$

2.2.2 The Lee-Low-Pine (LLP) Transformation

The Lee-Low-Pine (LLP) transformation [8] dramatically simplifies the solving 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

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

and then define

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

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

$$+ \sqrt{\frac{n_0}{2\pi}} g_{IB} \int dk W_k \left(\hat{a}_k + \hat{a}_{-k}^{\dagger} \right) + \frac{g_{IB}}{2\pi} \int dk dk' \left(c_k \hat{a}_k^{\dagger} - s_k \hat{a}_{-k} \right) \left(c_{k'} \hat{a}_{k'} - s_{k'} \hat{a}_{-k'}^{\dagger} \right)$$
(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

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

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

$$W_{p,p'} \sim \exp\left(-(\omega_p + \omega_{p'})^2\right) \xrightarrow{\lambda \to \infty} 0,$$
 (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'. However, 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 $\hat{\mathcal{H}}_{int}$ converge to 0, which is why we waive the explicit evaluation of the conditions 2.7.

3.1.2 Application to the 1D Bose Polaron Model

In the heavy impurity limit $M \to \infty$, the dependence of the occupation numbers in the LLP-Hamiltonian 2.26 vanishes and we almost have a purely quadratic Hamiltonian as discussed in the previous section. Before we discuss the significance of the the linear term in the LLP-Hamiltonian we will address the fact that the integrals in there have to discretized for numerical

treatment.

To this end, we will restrict ourselves to a discrete number of modes k where $0 < \Lambda_{IR} \le |k| \le \Lambda_{UV} < \infty$. 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. The spacing between two adjacent k values will be $\Delta k = \frac{2\pi}{L}$ where L is a constant which describes the size of the system.

This allows us to write integrals as sums according to

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

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

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

and the LLP-Hamiltonian becomes:

$$\hat{\mathcal{H}}_{LLP}^{discr.} = g_{IB} n_0 + \sum_{k} \omega_k \hat{a}_k^{\dagger} \hat{a}_k + \sqrt{\frac{n_0 \Delta k}{2\pi}} g_{IB} \sum_{k} W_k \left(\hat{a}_k + \hat{a}_{-k}^{\dagger} \right)$$

$$+ \frac{g_{IB} \Delta k}{2\pi} \sum_{k,k'} \left(c_k \hat{a}_k^{\dagger} - s_k \hat{a}_{-k} \right) \left(c_{k'} \hat{a}_{k'} - s_{k'} \hat{a}_{-k'}^{\dagger} \right)$$
(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.

This can be avoided because the linear terms $W_k\left(\hat{a}_k+\hat{a}_{-k}^{\dagger}\right)$ can be transformed out by applying the displacement operator

$$\hat{D}(\underline{\alpha}) = \exp\left(\sum_{k} \alpha_{k} \hat{a}_{k}^{\dagger} - \text{h.c.}\right) = \exp\left(-\underline{\alpha}^{\dagger} \underline{\underline{\Omega}} \ \underline{\hat{a}}\right)$$
(3.6)

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

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

and the notation

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

for vectors of creation and annihilation operators as well as

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

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

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

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

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

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

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

$$\hat{D}^{\dagger}(\underline{\alpha})\hat{\mathcal{H}}_{LLP}^{discr.}\hat{D}(\underline{\alpha}) = g_{IB}n_0 + \sum_{k} \omega_k (\hat{a}_k^{\dagger} + \alpha_k^*)(\hat{a}_k + \alpha_k)$$

$$+ \sqrt{\frac{n_0 \Delta k}{2\pi}} g_{IB} \sum_{k} W_k \left(\hat{a}_k + \hat{a}_{-k}^{\dagger} + \alpha_k + \alpha_{-k}^*\right)$$

$$+ \frac{g_{IB} \Delta k}{2\pi} \sum_{k,k'} \left(c_k (\hat{a}_k^{\dagger} + \alpha_k^*) - s_k (\hat{a}_{-k} + \alpha_{-k})\right) \left(c_{k'} (\hat{a}_{k'} + \alpha_{k'}) - s_{k'} (\hat{a}_{-k'}^{\dagger} + \alpha_{-k'}^*)\right)$$

$$(3.12)$$

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:

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

We defined

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

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

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

adopting the notation in the generic quadratic Hamiltonian 3.1.

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

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

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 function from julia's DifferentialEquations.jl library with the Tsit5 integrator, a Runge-Kutta integrator of order 5(4) [10], for its general robustness and versatility.

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.

3.2 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 later:

$$\left[\hat{a}^{\dagger}, \hat{f}(\hat{n})\right] = \hat{a}^{\dagger} \left(\hat{f}(\hat{n}) - \hat{f}(\hat{n}+1)\right) \tag{3.16a}$$

$$\left[\hat{a}, \hat{f}(\hat{n})\right] = \hat{a}\left(\hat{f}(\hat{n}) - \hat{f}(\hat{n} - 1)\right) \tag{3.16b}$$

$$\left[\hat{f}(\hat{n}), \hat{a}^{\dagger}\right] = \left(\hat{f}(\hat{n}) - \hat{f}(\hat{n} - 1)\right)\hat{a}^{\dagger} \tag{3.16c}$$

$$\left[\hat{f}(\hat{n}), \hat{a}\right] = \left(\hat{f}(\hat{n}) - \hat{f}(\hat{n}+1)\right)\hat{a} \tag{3.16d}$$

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

We will write $\hat{f}(\hat{n}_1, \hat{n}_2, ...) =: \hat{f}$ and $\hat{f}(\hat{n}_1, \hat{n}_2, ..., \hat{n}_k \pm 1, \hat{n}_{k+1}, ...) =: \hat{f}(\hat{n}_k \pm 1)$. 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:

$$\begin{aligned}
& \left[\hat{f}(\hat{n}), \hat{a}_{k_1}^{\dagger} \hat{a}_{k_2}^{\dagger} \cdots \hat{a}_{k_{n_1}}^{\dagger} \hat{a}_{k_1} \hat{a}_{k_2} \cdots \hat{a}_{k_{n_2}} \right] \\
&= \left(\hat{f} - \hat{f} \left(\hat{n}_{k_1} - 1, \hat{n}_{k_2} - 1, \dots, \hat{n}_{k_{n_1}}, \hat{n}_{k_1} + 1, \hat{n}_{k_2} + 1 \dots \hat{n}_{k_{n_2}} + 1 \right) \right) \hat{a}_{k_1}^{\dagger} \hat{a}_{k_2}^{\dagger} \cdots \hat{a}_{k_{n_1}}^{\dagger} \hat{a}_{k_1} \hat{a}_{k_2} \cdots \hat{a}_{k_{n_2}} \\
& (3.17)
\end{aligned}$$

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:

$$\hat{a}_{q}: \hat{O}: =: \hat{O}\hat{a}_{q}: + \sum_{k} : \frac{\partial \hat{O}}{\partial \hat{a}_{k}^{\dagger}}:$$

$$=: \hat{O}\hat{a}_{q}: + \sum_{i=1}^{n_{1}} \delta_{k_{i}, q}: \hat{a}_{k_{1}}^{\dagger} \hat{a}_{k_{2}}^{\dagger} \cdots \hat{a}_{k_{i-1}}^{\dagger} \hat{a}_{k_{i+1}}^{\dagger} \cdots \hat{a}_{k_{n_{1}}}^{\dagger} \hat{a}_{k_{1}} \hat{a}_{k_{2}} \cdots \hat{a}_{k_{n_{2}}}:$$

$$\hat{a}_{q}^{\dagger}: \hat{O}: =: \hat{a}_{q}^{\dagger} \hat{O}:$$
(3.18a)

3.2.2 Deriving the Flow Equations

Following the 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 [11], 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 3.16, 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 $\hat{H} \neq \hat{H}(\hat{n}_p \pm 1, \hat{n}_{p'} \pm 1) \ \forall p, p'$ where we used

$$\hat{H} := \sum_{k} \hat{\omega}_k : \hat{a}_k^{\dagger} \hat{a}_k : +\hat{\epsilon}. \tag{3.19}$$

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

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

$$\hat{\mathcal{H}}_{LLP}^{discr.}(P) = g_{IB}n_0 + \frac{1}{2M} \left(P - \sum_{k} k \hat{a}_{k}^{\dagger} \hat{a}_{k} \right)^2 + \sum_{k} \omega_{k} \hat{a}_{k}^{\dagger} \hat{a}_{k}
+ \sqrt{\frac{n_0 \Delta k}{2\pi}} g_{IB} \sum_{k} W_{k} \left(\hat{a}_{k} + \hat{a}_{-k}^{\dagger} \right) + \frac{g_{IB} \Delta k}{2\pi} \sum_{k,k'} \left(c_{k} \hat{a}_{k}^{\dagger} - s_{k} \hat{a}_{-k} \right) \left(c_{k'} \hat{a}_{k'} - s_{k'} \hat{a}_{-k'}^{\dagger} \right)$$
(3.20)

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

$$\hat{\mathcal{H}}_{LLP}^{discr.}(P) = \hat{H}(P) + \frac{g_{IB}\Delta k}{2\pi} \sum_{k \neq k'} (c_k c_{k'} + s_k s_{k'}) \hat{a}_k^{\dagger} \hat{a}_{k'}
+ \sqrt{\frac{n_0 \Delta k}{2\pi}} g_{IB} \sum_{k} W_k \left(\hat{a}_k + \hat{a}_{-k}^{\dagger} \right) - \frac{g_{IB}\Delta k}{2\pi} \sum_{k,k'} \left(c_k s_{k'} \hat{a}_k^{\dagger} \hat{a}_{k'}^{\dagger} + s_k c_{k'} \hat{a}_k \hat{a}_{k'} \right)$$
(3.21)

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

$$\hat{H}(P) := g_{IB}n_0 + \frac{g_{IB}}{2\pi}\Delta k \sum_k s_k^2 + \frac{1}{2M} \left(P - \sum_k k \hat{n}_k \right)^2 + \sum_k \omega_k \hat{n}_k + \frac{g_{IB}\Delta k}{2\pi} \sum_k (c_k^2 + s_k^2) \hat{n}_k \quad (3.22)$$

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

$$\hat{H}(P, \hat{n}_{q} - 1, \hat{n}_{q'} + 1) - \hat{H}(P) = \frac{1}{2M} \left(P + q - q' - \sum_{k} k \hat{n}_{k} \right)^{2} - \frac{1}{2M} \left(P - \sum_{k} k \hat{n}_{k} \right)^{2} + \omega_{q'} - \omega_{q} + \frac{g_{IB} \Delta k}{2\pi} (c_{q'}^{2} + s_{q'}^{2} - c_{q}^{2} - s_{q}^{2})$$

$$= \frac{q - q'}{2M} \left(2P - 2 \sum_{k} k \hat{n}_{k} + q - q' \right) + \omega_{q'} - \omega_{q} + \frac{g_{IB} \Delta k}{2\pi} (c_{q'}^{2} + s_{q'}^{2} - c_{q}^{2} - s_{q}^{2})$$

$$(3.23)$$

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 $\lambda \to \infty$. 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*.
- 4. The resulting system of coupled ODEs can then be solved as in the heavy impurity limit.

SECTION 4______RESULTS

4.1 1D Bose Polaron in the Heavy Impurity Limit

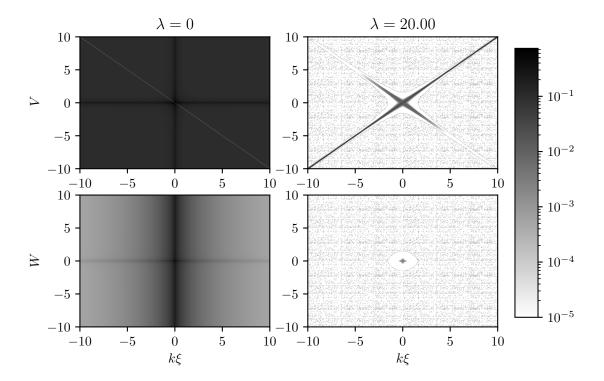


Figure 4.1: Visualization of how the flow progresses for $\eta=10$ by shading larger absolute values for $V_{k,k'}, W_{k,k'}$ darker. We see that good suppression occurs for all $W_{k,k'}$, with slower convergence for smaller |k|, |k'|. Meanwhile, the matrix elements near the diagonal $V_{k,k}$ decay significantly slower than most off-diagonal elements. Also, matrix elements $V_{k,-k}$ converge, but to a value different from zero.

As seen in figure 4.1

| SECTION 5 | | |
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| | CONCLUSION AND OUTLOOK | |
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DETAILED CALCULATIONS

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

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

$$\hat{\eta} := \hat{\eta}(\lambda) := \left[\hat{\mathcal{H}}_{0}, \hat{\mathcal{H}}_{int}\right] = \left[\sum_{k} \omega_{k} \hat{a}_{k}^{\dagger} \hat{a}_{k}, \sum_{q \neq q'} V_{q,q'} \hat{a}_{q}^{\dagger} \hat{a}_{q'} + \sum_{p,p'} \left(W_{p,p'} \hat{a}_{p}^{\dagger} \hat{a}_{p'}^{\dagger} + W_{p,p'}^{*} \hat{a}_{p} \hat{a}_{p'}\right)\right] \quad (A.1)$$

$$= \sum_{k} \sum_{q,q'} \omega_{k} V_{q,q'} \left[\hat{a}_{k}^{\dagger} \hat{a}_{k}, \hat{a}_{q}^{\dagger} \hat{a}_{q'}\right] + \sum_{k} \sum_{p,p'} \left(\omega_{k} W_{p,p'} \left[\hat{a}_{k}^{\dagger} \hat{a}_{k}, \hat{a}_{p}^{\dagger} \hat{a}_{p'}\right] + \omega_{k} W_{p,p'}^{*} \left[\hat{a}_{k}^{\dagger} \hat{a}_{k}, \hat{a}_{p} \hat{a}_{p'}\right]\right)$$

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

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

$$= \sum_{q \neq q'} V_{q,q'} (\omega_{q} - \omega_{q'}) \hat{a}_{q}^{\dagger} \hat{a}_{q'} + \sum_{p,p'} \left(W_{p,p'} (\omega_{p} + \omega_{p'}) \hat{a}_{p}^{\dagger} \hat{a}_{p'} - W_{p,p'}^{*} (\omega_{p} + \omega_{p'}) \hat{a}_{p} \hat{a}_{p'}\right)$$

$$(A.2)$$

Since $\hat{\eta}$ has the same form as $\hat{\mathcal{H}}_{int}$, $\left[\hat{\eta}, \hat{\mathcal{H}}_{0}\right]$ follows by inspection of A.2:

(A.8)

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

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{bmatrix}
\sum_{q \neq q'} V_{q,q'}(\omega_{q} - \omega_{q'}) \hat{a}_{q}^{\dagger} \hat{a}_{q'}, \sum_{\bar{q} \neq \bar{q}'} V_{\bar{q},\bar{q}'} \hat{a}_{\bar{q}}^{\dagger} \hat{a}_{\bar{q}'} \\
= \sum_{q \neq q'} \sum_{\bar{q} \neq \bar{q}'} V_{\bar{q},\bar{q}'} V_{q,q'}(\omega_{q} - \omega_{q'}) \left[\hat{a}_{q}^{\dagger} \hat{a}_{q'}, \hat{a}_{\bar{q}}^{\dagger} \hat{a}_{\bar{q}'} \right] \\
= \sum_{q \neq q'} \sum_{\bar{q} \neq \bar{q}'} V_{\bar{q},\bar{q}'} V_{q,q'}(\omega_{q} - \omega_{q'}) \left(\hat{a}_{q}^{\dagger} \hat{a}_{\bar{q}'} \delta_{q',\bar{q}} - \hat{a}_{\bar{q}}^{\dagger} \hat{a}_{q'} \delta_{q,\bar{q}'} \right) \\
= \sum_{q \neq q'} \sum_{\bar{q}'} V_{q',\bar{q}'} V_{q,q'}(\omega_{q} - \omega_{q'}) \hat{a}_{q}^{\dagger} \hat{a}_{\bar{q}'} - \sum_{q \neq q'} \sum_{\bar{q}} V_{\bar{q},q} V_{q,q'}(\omega_{q} - \omega_{q'}) \hat{a}_{\bar{q}}^{\dagger} \hat{a}_{q'} \\
= \sum_{q,q'} \sum_{\bar{q}'} V_{q',\bar{q}'} V_{q,q'}(\omega_{q} - \omega_{q'}) \hat{a}_{q}^{\dagger} \hat{a}_{\bar{q}'} - \sum_{q,q'} \sum_{\bar{q}} V_{\bar{q},q} V_{q,q'}(\omega_{q} - \omega_{q'}) \hat{a}_{\bar{q}}^{\dagger} \hat{a}_{q'} \\
= \sum_{q,q'} \sum_{\bar{q}} V_{\bar{q},q'} V_{q,\bar{q}}(\omega_{q} - \omega_{\bar{q}}) \hat{a}_{q}^{\dagger} \hat{a}_{q'} - \sum_{q,q'} \sum_{\bar{q}} V_{q,\bar{q}} V_{\bar{q},q'}(\omega_{\bar{q}} - \omega_{q'}) \hat{a}_{q}^{\dagger} \hat{a}_{q'} \\
= \sum_{q \neq q'} \sum_{\bar{q}} V_{\bar{q},q'} V_{q,\bar{q}}(\omega_{q} - \omega_{\bar{q}}) \hat{a}_{q}^{\dagger} \hat{a}_{q'} - \sum_{q \neq q'} \sum_{\bar{q}} V_{q,\bar{q}} V_{\bar{q},q'}(\omega_{\bar{q}} - \omega_{q'}) \hat{a}_{q}^{\dagger} \hat{a}_{q'} \\
+ \sum_{k} \sum_{\bar{q}} V_{\bar{q},k} V_{k,\bar{q}}(\omega_{k} - \omega_{\bar{q}}) \hat{a}_{k}^{\dagger} \hat{a}_{k} - \sum_{q \neq q'} \sum_{\bar{q}} V_{q,\bar{q}} V_{\bar{q},q'}(\omega_{\bar{q}} - \omega_{q'}) \hat{a}_{q}^{\dagger} \hat{a}_{q'} \\
+ \sum_{k} \sum_{\bar{q}} V_{\bar{q},q'} V_{q,\bar{q}}(\omega_{q} - \omega_{\bar{q}}) \hat{a}_{q}^{\dagger} \hat{a}_{q'} - \sum_{q \neq q'} \sum_{\bar{q}} V_{q,\bar{q}} V_{\bar{q},q'}(\omega_{\bar{q}} - \omega_{q'}) \hat{a}_{q}^{\dagger} \hat{a}_{q'} \\
+ \sum_{k} \sum_{\bar{q}} V_{\bar{q},q'} V_{q,\bar{q}}(\omega_{q} - \omega_{\bar{q}}) \hat{a}_{q}^{\dagger} \hat{a}_{q'} - \sum_{q \neq q'} \sum_{\bar{q}} V_{q,\bar{q}} V_{\bar{q},q'}(\omega_{\bar{q}} - \omega_{q'}) \hat{a}_{q}^{\dagger} \hat{a}_{q'} \\
+ \sum_{k} \sum_{\bar{q}} 2 V_{\bar{q},k} V_{k,\bar{q}}(\omega_{k} - \omega_{\bar{q}}) \hat{a}_{k}^{\dagger} \hat{a}_{k}$$
(A.9)

A.6:

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

$$+\sum_{p,p'}\sum_{q}V_{q,p}(\omega_{p}-\omega_{q})(W_{q,p'}^{*}+W_{p',q}^{*})\hat{a}_{p}\hat{a}_{p'}$$
(A.10)

A.7:

$$\begin{split} & \left[\sum_{p,p'} \left(W_{p,p'}(\omega_{p} + \omega_{p'}) \hat{a}_{p}^{\dagger} \hat{a}_{p'}^{\dagger} - W_{p,p'}^{*}(\omega_{p} + \omega_{p'}) \hat{a}_{p} \hat{a}_{p'} \right), \sum_{\bar{q} \neq \bar{q}'} V_{\bar{q},\bar{q}'} \hat{a}_{\bar{q}}^{\dagger} \hat{a}_{\bar{q}'} \right] \\ & = \sum_{p,p'} \sum_{\bar{q} \neq \bar{q}'} V_{\bar{q},\bar{q}'}(\omega_{p} + \omega_{p'}) \left(W_{p,p'} \left[\hat{a}_{p}^{\dagger} \hat{a}_{p'}^{\dagger}, \hat{a}_{\bar{q}}^{\dagger} \hat{a}_{\bar{q}'} \right] - W_{p,p'}^{*} \left[\hat{a}_{p} \hat{a}_{p'}, \hat{a}_{\bar{q}}^{\dagger} \hat{a}_{\bar{q}'} \right] \right) \\ & = -\sum_{p,p'} \sum_{q \neq q'} V_{q,q'}(\omega_{p} + \omega_{p'}) W_{p,p'} \left(\hat{a}_{q}^{\dagger} \hat{a}_{p}^{\dagger} \delta_{q',p'} + \hat{a}_{q}^{\dagger} \hat{a}_{p'}^{\dagger} \delta_{q',p} \right) \\ & - \sum_{p,p'} \sum_{q \neq q'} V_{q,q'}(\omega_{p} + \omega_{p'}) W_{p,p'}^{*} \left(\hat{a}_{p} \hat{a}_{q'} \delta_{q,p'} + \hat{a}_{p'} \hat{a}_{q'} \delta_{q,p} \right) \\ & = -\sum_{p,p'} \sum_{q} V_{q,p'}(\omega_{p} + \omega_{p'}) W_{p,p'}^{*} \hat{a}_{q}^{\dagger} \hat{a}_{p}^{\dagger} - \sum_{p,p'} \sum_{q} V_{q,p}(\omega_{p} + \omega_{p'}) W_{p,p'}^{*} \hat{a}_{q}^{\dagger} \hat{a}_{p'} \\ & - \sum_{p,p'} \sum_{q'} V_{p',q'}(\omega_{p} + \omega_{p'}) W_{p,q'}^{*} \hat{a}_{p}^{\dagger} \hat{a}_{p'} - \sum_{p,p'} \sum_{q'} V_{p,q'}(\omega_{p} + \omega_{p'}) W_{p,p'}^{*} \hat{a}_{p}^{\dagger} \hat{a}_{p'} \\ & - \sum_{p,p'} \sum_{q'} V_{p',q}(\omega_{p} + \omega_{q'}) W_{p,q'}^{*} \hat{a}_{p}^{\dagger} \hat{a}_{p'} - \sum_{p,p'} \sum_{q'} V_{p,q}(\omega_{q} + \omega_{p'}) W_{q',p'}^{*} \hat{a}_{p}^{\dagger} \hat{a}_{p'} \\ & - \sum_{p,p'} \sum_{q'} V_{p,q}(\omega_{q} + \omega_{p'}) (W_{p',q}^{*} + W_{q,p'}^{*}) \hat{a}_{p}^{\dagger} \hat{a}_{p'}^{\dagger} \\ & - \sum_{p,p'} \sum_{q} V_{p,q}(\omega_{q} + \omega_{p'}) (W_{p',q}^{*} + W_{q,p'}^{*}) \hat{a}_{p}^{\dagger} \hat{a}_{p'} \end{aligned} \tag{A.11}$$

A.8:

$$\begin{split} & \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_{\bar{p},\bar{p}'} \left(W_{\bar{p},\bar{p}'} \hat{a}_{\bar{p}}^{\dagger} \hat{a}_{\bar{p}'}^{\dagger} + W_{\bar{p},\bar{p}'}^{*} \hat{a}_{\bar{p}} \hat{a}_{\bar{p}'} \right) \right] \\ & = \sum_{p,p'} \sum_{\bar{p},\bar{p}'} W_{p,p'}(\omega_{p} + \omega_{p'}) W_{\bar{p},\bar{p}'}^{*} \left[\hat{a}_{p}^{\dagger} \hat{a}_{p'}^{\dagger}, \hat{a}_{\bar{p}} \hat{a}_{\bar{p}'} \right] - \sum_{p,p'} \sum_{\bar{p},\bar{p}'} W_{p,p'}^{*}(\omega_{p} + \omega_{p'}) \left[\hat{a}_{p} \hat{a}_{p'}, \hat{a}_{\bar{p}}^{\dagger} \hat{a}_{\bar{p}'} \right] \\ & = - \sum_{p,p'} \sum_{\bar{p},\bar{p}'} W_{p,p'}(\omega_{p} + \omega_{p'} + \omega_{\bar{p}} + \omega_{\bar{p}'}) W_{\bar{p},\bar{p}'}^{*} \hat{a}_{\bar{p}} \hat{a}_{\bar{p}}^{\dagger} \right] \\ & = - \sum_{p,p'} \sum_{\bar{p},\bar{p}'} W_{p,p'}(\omega_{p} + \omega_{p'} + \omega_{\bar{p}} + \omega_{\bar{p}'}) W_{\bar{p},\bar{p}'}^{*} \hat{a}_{\bar{p}} \hat{a}_{\bar{p}'}^{\dagger} \delta_{\bar{p}',p'} \\ & - \sum_{p,p'} \sum_{\bar{p},\bar{p}'} W_{p,p'}(\omega_{p} + \omega_{p'} + \omega_{\bar{p}} + \omega_{\bar{p}'}) W_{\bar{p},\bar{p}'}^{*} \hat{a}_{\bar{p}} \hat{a}_{\bar{p}'}^{\dagger} \delta_{\bar{p}',p'} \\ & - \sum_{p,p'} \sum_{\bar{p},\bar{p}'} W_{p,p'}(\omega_{p} + \omega_{p'} + \omega_{\bar{p}} + \omega_{\bar{p}'}) W_{\bar{p},\bar{p}'}^{*} \hat{a}_{\bar{p}} \hat{a}_{\bar{p}'} \delta_{\bar{p},p'} \\ & - \sum_{p,p'} \sum_{\bar{p},\bar{p}'} W_{p,p'}(\omega_{p} + \omega_{p'} + \omega_{\bar{p}}) W_{\bar{p},p'}^{*} \hat{a}_{\bar{p}} \hat{a}_{\bar{p}'} \delta_{\bar{p}',p'} \\ & - \sum_{p,p'} \sum_{\bar{p}} W_{p,p'}(\omega_{p} + 2\omega_{p'} + \omega_{\bar{p}'}) W_{\bar{p}',\bar{p}'}^{*} \hat{a}_{\bar{p}} \hat{a}_{\bar{p}'} - \sum_{p,p'} \sum_{\bar{p}} W_{p,p'}(2\omega_{p} + \omega_{p'} + \omega_{\bar{p}}) W_{\bar{p},\bar{p}}^{*} \hat{a}_{\bar{p}} \hat{a}_{\bar{p}'} \\ & - \sum_{p,p'} \sum_{\bar{p}'} W_{p,p'}(\omega_{p} + 2\omega_{p'} + \omega_{\bar{p}'}) W_{p',\bar{p}'}^{*} \hat{a}_{\bar{p}} \hat{a}_{\bar{p}'} - \sum_{p,p'} \sum_{\bar{p}'} W_{p,p'}(2\omega_{p} + \omega_{p'} + \omega_{\bar{p}'}) W_{p,\bar{p}'}^{*} \hat{a}_{\bar{p}'} \hat{a}_{\bar{p}'} \\ & - \sum_{p,p'} \sum_{\bar{p}'} W_{p,p'}(\omega_{p} + 2\omega_{p'} + \omega_{\bar{p}'}) W_{p',\bar{p}'}^{*} \hat{a}_{\bar{p}} \hat{a}_{\bar{p}'} - \sum_{p,p'} \sum_{\bar{p}'} W_{p,p'}(2\omega_{p} + \omega_{p'} + \omega_{\bar{p}'}) W_{p,\bar{p}'}^{*} \hat{a}_{\bar{p}'}^{\dagger} \hat{a}_{\bar{p}'} \\ & - \sum_{p,p'} \sum_{\bar{p}'} W_{p,p'}(\omega_{p} + 2\omega_{p'} + \omega_{\bar{p}'}) W_{p',\bar{p}'}^{*} \hat{a}_{\bar{p}'} \hat{a}_{\bar{p}'} - \sum_{p,p'} \sum_{\bar{p}'} W_{p,p'}(2\omega_{p} + \omega_{p'} + \omega_{\bar{p}'}) W_{p',\bar{p}'}^{*} \hat{a}_{\bar{p}'}^{\dagger} \hat{a}_{\bar{p}'} - \sum_{p,p'} \sum_{\bar{p}'} W_{p,p'}(2\omega_{p} + \omega_{p'} + \omega_{\bar{p}'})$$

$$\begin{split} &-\sum_{p,p'}\sum_{\tilde{p}'}W_{p,\tilde{p}'}(\omega_{p}+2\omega_{\tilde{p}'}+\omega_{p'})W_{\tilde{p}',p'}^{*}\hat{a}_{p}^{\dagger}\hat{a}_{p'}-\sum_{p,p'}\sum_{\tilde{p}'}W_{\tilde{p}',p}(2\omega_{\tilde{p}'}+\omega_{p}+\omega_{p'})W_{\tilde{p}',p'}^{*}\hat{a}_{p}^{\dagger}\hat{a}_{p'}\\ &=-\sum_{p,p'}\sum_{\tilde{p}}(W_{p,\tilde{p}}+W_{\tilde{p},p})(\omega_{p}+2\omega_{\tilde{p}}+\omega_{p'})W_{p',\tilde{p}}^{*}\hat{a}_{p'}\hat{a}_{p}^{\dagger}\\ &-\sum_{p,p'}\sum_{\tilde{p}'}(W_{p,\tilde{p}'}+W_{\tilde{p}',p})(\omega_{p}+2\omega_{\tilde{p}'}+\omega_{p'})W_{p',\tilde{p}}^{*}(\hat{a}_{p}^{\dagger}\hat{a}_{p'}\\ &=-\sum_{p,p'}\sum_{\tilde{p}}(W_{p,\tilde{p}}+W_{\tilde{p},p})(\omega_{p}+2\omega_{\tilde{p}}+\omega_{p'})W_{p',\tilde{p}}^{*}(\delta_{p,p'}+\hat{a}_{p}^{\dagger}\hat{a}_{p'})\\ &-\sum_{p,p'}\sum_{\tilde{p}}(W_{p,\tilde{p}}+W_{\tilde{p},p})(\omega_{p}+2\omega_{\tilde{p}}+\omega_{p'})W_{\tilde{p},p'}^{*}\hat{a}_{p}^{\dagger}\hat{a}_{p'}\\ &=-\sum_{p,p'}\sum_{\tilde{p}}(W_{p,\tilde{p}}+W_{\tilde{p},p})(\omega_{p}+2\omega_{\tilde{p}}+\omega_{p'})(W_{\tilde{p},p'}^{*}+W_{p',\tilde{p}}^{*})\hat{a}_{p}^{\dagger}\hat{a}_{p'}\\ &-2\sum_{k}\sum_{\tilde{p}}(W_{k,\tilde{p}}+W_{\tilde{p},k})(\omega_{k}+\omega_{\tilde{p}})W_{k,\tilde{p}}^{*}\\ &=-\sum_{q\neq q'}\sum_{\tilde{p}}(W_{q,\tilde{p}}+W_{\tilde{p},k})(\omega_{q}+2\omega_{\tilde{p}}+\omega_{q'})(W_{\tilde{p},q'}^{*}+W_{q',\tilde{p}}^{*})\hat{a}_{q}^{\dagger}\hat{a}_{q'}\\ &-2\sum_{k}\sum_{\tilde{p}}(W_{k,\tilde{p}}+W_{\tilde{p},k})(\omega_{k}+\omega_{\tilde{p}})(W_{\tilde{p},k}^{*}+W_{k,\tilde{p}}^{*})\hat{a}_{k}^{\dagger}\hat{a}_{k}\\ &-2\sum_{k}\sum_{\tilde{p}}(W_{k,\tilde{p}}+W_{\tilde{p},k})(\omega_{k}+\omega_{\tilde{p}})(W_{k,\tilde{p}}^{*}+W_{k,\tilde{p}}^{*})\hat{a}_{k}^{\dagger}\hat{a}_{k} \end{split}$$

$$(A.12)$$

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

$$\hat{\mathcal{H}}(\lambda) = \sum_{k} \omega_{k}(\lambda) \hat{a}_{k}^{\dagger} \hat{a}_{k} + \sum_{q \neq q'} V_{q,q'}(\lambda) \hat{a}_{q}^{\dagger} \hat{a}_{q'} + \sum_{p,p'} \left(W_{p,p'}(\lambda) \hat{a}_{p}^{\dagger} \hat{a}_{p'}^{\dagger} + W_{p,p'}^{*}(\lambda) \hat{a}_{p} \hat{a}_{p'} \right) + \epsilon(\lambda) \quad (A.13)$$

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 $\hat{\mathcal{H}}_{int}$ 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 $q \neq q'$:

$$\partial_{\lambda}\omega_{k} = \sum_{\tilde{q}} 2V_{\tilde{q},k}V_{k,\tilde{q}}(\omega_{k} - \omega_{\tilde{q}}) - 2\sum_{\tilde{p}} (W_{k,\tilde{p}} + W_{\tilde{p},k})(\omega_{k} + \omega_{\tilde{p}})(W_{\tilde{p},k}^{*} + W_{k,\tilde{p}}^{*})$$

$$(A.14a)$$

$$\partial_{\lambda}V_{q,q'} = -V_{q,q'}(\omega_{q} - \omega_{q'})^{2} - \sum_{\tilde{p}} (W_{q,\tilde{p}} + W_{\tilde{p},q})(\omega_{q} + \omega_{q'} + 2\omega_{\tilde{p}})(W_{\tilde{p},q'}^{*} + W_{q',\tilde{p}}^{*})$$

$$+ \sum_{\tilde{q}} V_{\tilde{q},q'}V_{q,\tilde{q}}(\omega_{q} + \omega_{q'} - 2\omega_{\tilde{q}})$$

$$(A.14b)$$

$$\partial_{\lambda}W_{p,p'} = -W_{p,p'}(\omega_{p} + \omega_{p'})^{2} - \sum_{q} V_{p,q}(\omega_{q} + \omega_{p'})(W_{p',q} + W_{q,p'})$$

$$+ \sum_{q} V_{p,q}(\omega_{p} - \omega_{q})(W_{q,p'} + W_{p',q})$$

$$(A.14c)$$

$$\partial_{\lambda}W_{p,p'}^{*} = -W_{p,p'}^{*}(\omega_{p} + \omega_{p'})^{2} - \sum_{q} V_{q,p}(\omega_{q} + \omega_{p'})(W_{p',q}^{*} + W_{q,p'}^{*})$$

$$+ \sum_{q} V_{q,p}(\omega_{p} - \omega_{q})(W_{q,p'}^{*} + W_{p',q}^{*})$$

$$(A.14d)$$

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

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

A.2 Deriving the Flow Equations with n-dependence

A.2.1 The Canonical Generator

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

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

Upon realizing that $\sum_{k} \hat{\omega}_{k} : \hat{a}_{k}^{\dagger} \hat{a}_{k}$: is also just a function of the number operators, we can consider $\hat{\mathcal{H}}_{0} := \hat{H} := \sum_{k} \hat{\omega}_{k} : \hat{a}_{k}^{\dagger} \hat{a}_{k} : +\hat{\epsilon}$ as the diagonal part of $\hat{\mathcal{H}}$.

The first step in the calculating the flow equations is again to calculate the canonical commutator $\hat{\eta} := \left[\hat{\mathcal{H}}_0, \hat{\mathcal{H}}_{int}\right]$:

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

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

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

A.16a

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

A.16b

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

A.16c

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

This gives the canonical generator as:

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

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

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

$$=: \sum_{q \neq q'} \hat{\theta}_{q,q'} : \hat{a}_q^{\dagger} \hat{a}_{q'} : + \sum_{p,p'} \left(\hat{\phi}_{p,p'} : \hat{a}_p^{\dagger} \hat{a}_{p'}^{\dagger} : + \hat{\psi}_{p,p'} : \hat{a}_p \hat{a}_{p'} : \right)$$
(A.22)

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

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

$$\left[\eta^{(2)}, \hat{\mathcal{H}}_{0}\right] = -\sum_{q \neq q'} \hat{\theta}_{q,q'} \left(\hat{H} - \hat{H}(\hat{n}_{q} - 1, \hat{n}_{q'} + 1)\right) : \hat{a}_{q}^{\dagger} \hat{a}_{q'} :$$

$$-\sum_{p,p'} \hat{\phi}_{p,p'} \left(\hat{H} - \hat{H}(\hat{n}_{p'} - 1, \hat{n}_{p} - 1)\right) : \hat{a}_{p}^{\dagger} \hat{a}_{p'}^{\dagger} :$$

$$-\sum_{p,p'} \hat{\psi}_{p,p'} \left(\hat{H} - \hat{H}(\hat{n}_{p'} + 1, \hat{n}_{p} + 1)\right) : \hat{a}_{p} \hat{a}_{p'} :$$

$$= -\sum_{q \neq q'} \hat{V}_{q,q'} \left(\hat{H} - \hat{H}(\hat{n}_{q} - 1, \hat{n}_{q'} + 1)\right)^{2} : \hat{a}_{q}^{\dagger} \hat{a}_{q'} :$$

$$-\sum_{p,p'} \hat{W}_{p,p'} \left(\hat{H} - \hat{H}(\hat{n}_{p'} - 1, \hat{n}_{p} - 1)\right)^{2} : \hat{a}_{p}^{\dagger} \hat{a}_{p'}^{\dagger} :$$

$$-\sum_{p,p'} \hat{W}_{p,p'}^{\dagger} \left(\hat{H} - \hat{H}(\hat{n}_{p'} + 1, \hat{n}_{p} + 1)\right)^{2} : \hat{a}_{p} \hat{a}_{p'} :$$

$$-\sum_{p,p'} \hat{W}_{p,p'}^{\dagger} \left(\hat{H} - \hat{H}(\hat{n}_{p'} + 1, \hat{n}_{p} + 1)\right)^{2} : \hat{a}_{p} \hat{a}_{p'} :$$

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

$$\begin{split} \left[\eta^{(2)}, \hat{\mathcal{H}}_{\text{int}} \right] &= \sum_{q \neq q'} \sum_{\tilde{q} \neq \tilde{q}'} \left[\hat{\theta}_{\tilde{q}, \tilde{q}'} : \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{\tilde{q}'} :, \hat{V}_{q, q'} : \hat{a}_{q}^{\dagger} \hat{a}_{q'} : \right] \\ &+ \sum_{p, p'} \sum_{\tilde{q} \neq \tilde{q}'} \left[\hat{\theta}_{\tilde{q}, \tilde{q}'} : \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{\tilde{q}'} :, \hat{W}_{p, p'} : \hat{a}_{p}^{\dagger} \hat{a}_{p'}^{\dagger} : \right] \\ &+ \sum_{p, p'} \sum_{\tilde{q} \neq \tilde{q}'} \left[\hat{\theta}_{\tilde{q}, \tilde{q}'} : \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{\tilde{q}'} :, \hat{W}_{p, p'}^{\dagger} : \hat{a}_{p} \hat{a}_{p'} : \right] \\ &+ \sum_{q \neq q'} \sum_{\tilde{p}, \tilde{p}'} \left[\hat{\phi}_{\tilde{p}, \tilde{p}'} : \hat{a}_{\tilde{p}}^{\dagger} \hat{a}_{\tilde{p}'}^{\dagger} :, \hat{V}_{q, q'} : \hat{a}_{q}^{\dagger} \hat{a}_{q'} : \right] \\ &+ \sum_{q \neq q'} \sum_{\tilde{p}, \tilde{p}'} \left[\hat{\phi}_{\tilde{p}, \tilde{p}'} : \hat{a}_{\tilde{p}}^{\dagger} \hat{a}_{\tilde{p}'}^{\dagger} :, \hat{W}_{p, p'} : \hat{a}_{p}^{\dagger} \hat{a}_{p'}^{\dagger} : \right] \\ &+ \sum_{q \neq q'} \sum_{\tilde{p}, \tilde{p}'} \left[\hat{\phi}_{\tilde{p}, \tilde{p}'} : \hat{a}_{\tilde{p}}^{\dagger} \hat{a}_{\tilde{p}'}^{\dagger} :, \hat{W}_{p, p'} : \hat{a}_{p}^{\dagger} \hat{a}_{p'}^{\dagger} : \right] \end{aligned} \tag{A.25e}$$

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

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

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

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

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

A.25a:

$$\begin{split} \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}_{\tilde{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}_{\tilde{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}_{q'} :] : \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{\tilde{q}'} : \right] \\ &+ \sum_{q \neq q'} \sum_{\tilde{q} \neq \tilde{q}'} \hat{\theta}_{\tilde{q},\tilde{q}'} \hat{V}_{q,q'} \left[\hat{b}_{\tilde{q},\tilde{q}'} : \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{q'} :] : \hat{a}_{\tilde{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{b}_{\tilde{q}',q} : \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{q} : - \delta_{\tilde{q},q'} : \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{q'} : \right) \\ &+ \sum_{q \neq q'} \sum_{\tilde{q} \neq \tilde{q}'} \hat{\theta}_{q,q'} \left[\hat{V}_{\tilde{q},\tilde{q}'} : \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{q'} : \right] : \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{q'} : \\ &= \sum_{q \neq q'} \sum_{\tilde{q} \neq \tilde{q}'} \hat{\theta}_{q,q'} \left[\hat{V}_{\tilde{q},\tilde{q}'} : \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{q'} : \right] : \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{q'} : \\ &= \sum_{q \neq q'} \sum_{\tilde{q} \neq \tilde{q}'} \hat{\theta}_{q,q'} \left[\hat{V}_{\tilde{q},\tilde{q}'} : \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{q'} : \right] : \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{q'} : \\ &= \sum_{q \neq q'} \sum_{\tilde{q} \neq \tilde{q}'} \hat{\theta}_{q,q'} \left[\hat{V}_{\tilde{q},\tilde{q}'} : \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{q'} : \right] : \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{q'} : \\ &= \sum_{q \neq q'} \sum_{\tilde{q} \neq \tilde{q}'} \hat{\theta}_{q,q'} \left[\hat{V}_{\tilde{q},\tilde{q}'} : \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{q'} : \right] : \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{q'} : \\ &= \sum_{q,q'} \sum_{\tilde{q} \neq \tilde{q}'} \hat{\theta}_{q,q'} \left[\hat{V}_{\tilde{q},\tilde{q}'} : \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{q'} : -\hat{\theta}_{\tilde{q},q'} \hat{V}_{q,\tilde{q}} : \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{q'} : \right) \\ &= \sum_{q,q'} \sum_{\tilde{q} \neq \tilde{q}'} \hat{\theta}_{q,q'} \left[\hat{V}_{\tilde{q},q'} : \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{q'} : -\hat{\theta}_{\tilde{q},q'} \hat{V}_{q,\tilde{q}} : \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{q'} : \right) \\ &= \sum_{q,q'} \sum_{\tilde{q} \neq \tilde{q}'} \hat{\theta}_{q,q'} \left[\hat{V}_{\tilde{q},q'} : \hat{a}_{\tilde{q},q'} : \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{q'} : -\hat{\theta}_{\tilde{q},q'} \hat{V}_{q,\tilde{q}} : \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{q'} : \right) \\ &= \sum_{q,q'} \sum_{\tilde{q} \neq \tilde{q}'} \hat{\theta}_{q,q'} \left[\hat{V}_{\tilde{q},q'} : \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{q'} : \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{q'} : \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{q'} : \right) \\ &= \sum_{q,q'} \sum_{\tilde{q} \neq \tilde{q}'} \hat{\theta}_{q,q'} \left[\hat{V}_{\tilde{q},q'} : \hat$$

$$\begin{split} & + \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}_{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_{k} \sum_{\tilde{q}} \hat{V}_{q,\tilde{q}} \left(\hat{\theta}_{\tilde{q},q'} - \hat{\theta}_{\tilde{q},q'} (\hat{n}_{\tilde{q}} + 1, \hat{n}_{q} - 1) \right) : \hat{a}_{q}^{\dagger} \hat{a}_{q'} : \\ & + \sum_{k} \sum_{\tilde{q}} \hat{V}_{k,\tilde{q}} \left(\hat{\theta}_{\tilde{q},k} - \hat{\theta}_{\tilde{q},k} (\hat{n}_{\tilde{q}} + 1, \hat{n}_{k} - 1) \right) : \hat{a}_{k}^{\dagger} \hat{a}_{k} : \\ & - \sum_{q \neq q'} \sum_{\tilde{q}} \hat{\theta}_{q,\tilde{q}} \left(\hat{V}_{\tilde{q},q'} - \hat{V}_{\tilde{q},q'} (\hat{n}_{\tilde{q}} + 1, \hat{n}_{q} - 1) \right) : \hat{a}_{q}^{\dagger} \hat{a}_{q'} : \\ & - \sum_{k} \sum_{\tilde{q}} \hat{\theta}_{k,\tilde{q}} \left(\hat{V}_{\tilde{q},k} - \hat{V}_{\tilde{q},k} (\hat{n}_{\tilde{q}} + 1, \hat{n}_{k} - 1) \right) : \hat{a}_{k}^{\dagger} \hat{a}_{k} : \end{split}$$

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

A.25b:

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

We start by evaluating A.30a:

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

Next is A.30b:

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

$$= \sum_{p,p'} \sum_{q \neq q'} \hat{\theta}_{q,q'} \left(\hat{W}_{p,p'} (\hat{n}_{q'} + 1, \hat{n}_{q} - 1) - \hat{W}_{p,p'} \right) \underbrace{: \hat{a}_{q}^{\dagger} \hat{a}_{q'} :: \hat{a}_{p}^{\dagger} \hat{a}_{p'}^{\dagger} :}_{\stackrel{@}{=} \delta_{q',p} :: \hat{a}_{p'}^{\dagger} \hat{a}_{q}^{\dagger} :+ \delta_{q',p'} :: \hat{a}_{p}^{\dagger} \hat{a}_{q}^{\dagger} :}$$

$$\stackrel{@}{=} \sum_{p,p'} \sum_{q} \hat{\theta}_{q,p} \left(\hat{W}_{p,p'} (\hat{n}_{p} + 1, \hat{n}_{q} - 1) - \hat{W}_{p,p'} \right) : \hat{a}_{p'}^{\dagger} \hat{a}_{q}^{\dagger} :$$

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

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

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

$$(A.32)$$

A.30c gives no quadratic contribution:

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

$$= \sum_{p,p'} \sum_{\tilde{q} \neq \tilde{q}'} \hat{W}_{p,p'} \left(\hat{\theta}_{\tilde{q},\tilde{q}'} - \hat{\theta}_{\tilde{q},\tilde{q}'} (\hat{n}_{p'}, \hat{n}_{p} - 1) \right) \underbrace{: \hat{a}_{p}^{\dagger} \hat{a}_{p'}^{\dagger} :: \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{\tilde{q}'}}_{=:\hat{a}_{p}^{\dagger} \hat{a}_{q'}^{\dagger} \hat{a}_{\tilde{q}'}} : \underbrace{\overset{@}{=} 0} \tag{A.33}$$

A.25c:

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

We will again start by evaluating A.34a:

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

A.34b gives no quadratic contribution:

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

$$= \sum_{p,p'} \sum_{\tilde{q} \neq \tilde{q}'} \hat{\theta}_{\tilde{q},\tilde{q}'} \left(W_{p,p'}^{\dagger} (\hat{n}_{q'} + 1, \hat{n}_{q} - 1) - W_{p,p'}^{\dagger} \right) \underbrace{: \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{\tilde{q}'} :: \hat{a}_{p} \hat{a}_{p'} :}_{=: \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{\tilde{q}'} \hat{a}_{p} \hat{a}_{p'} :} \underbrace{\overset{2}{=} 0} \tag{A.36}$$

A.34c:

$$\sum_{p,p'} \sum_{q \neq q'} \hat{W}_{p,p'}^{\dagger} \left[\hat{\theta}_{q,q'}, : \hat{a}_{p} \hat{a}_{p'} : \right] : \hat{a}_{q}^{\dagger} \hat{a}_{q'} : \\
= \sum_{p,p'} \sum_{q \neq q'} \hat{W}_{p,p'}^{\dagger} \left(\hat{\theta}_{q,q'} - \hat{\theta}_{q,q'} (\hat{n}_{p'} + 1 \cdot \hat{n}_{p} + 1) \right) : \hat{a}_{p} \hat{a}_{p'} :: \hat{a}_{q}^{\dagger} \hat{a}_{q'} : \\
\stackrel{?}{=} \sum_{p,p'} \sum_{q \neq q'} \hat{W}_{p,p'}^{\dagger} \left(\hat{\theta}_{q,q'} - \hat{\theta}_{q,q'} (\hat{n}_{p'} + 1 \cdot \hat{n}_{p} + 1) \right) (\delta_{p,q} : \hat{a}_{p'} \hat{a}_{q'} : + \delta_{p',q} : \hat{a}_{p} \hat{a}_{q'} :) \\
= \sum_{p,p'} \sum_{q'} \hat{W}_{p,p'}^{\dagger} \left(\hat{\theta}_{p,q'} - \hat{\theta}_{p,q'} (\hat{n}_{p'} + 1 \cdot \hat{n}_{p} + 1) \right) : \hat{a}_{p'} \hat{a}_{q'} : \\
+ \sum_{p,p'} \sum_{q'} \hat{W}_{p,p'}^{\dagger} \left(\hat{\theta}_{p',q'} - \hat{\theta}_{p',q'} (\hat{n}_{p'} + 1 \cdot \hat{n}_{p} + 1) \right) : \hat{a}_{p} \hat{a}_{q'} : \\
= \sum_{p,p'} \sum_{q'} \hat{W}_{q,p'}^{\dagger} \left(\hat{\theta}_{q,p} - \hat{\theta}_{q,p} (\hat{n}_{p'} + 1 \cdot \hat{n}_{q} + 1) \right) : \hat{a}_{p} \hat{a}_{p'} : \\
+ \sum_{p,p'} \sum_{q} \hat{W}_{p,q}^{\dagger} \left(\hat{\theta}_{q,p'} - \hat{\theta}_{q,p'} (\hat{n}_{q} + 1 \cdot \hat{n}_{p} + 1) \right) : \hat{a}_{p} \hat{a}_{p'} : \\
= \sum_{p,p'} \sum_{q} \hat{W}_{p,q'}^{\dagger} \left(\hat{\theta}_{q,p'} - \hat{\theta}_{q,p'} (\hat{n}_{q} + 1 \cdot \hat{n}_{p} + 1) \right) : \hat{a}_{p} \hat{a}_{p'} : \\
= \sum_{p,p'} \sum_{q} \left(\hat{W}_{q,p'}^{\dagger} + \hat{W}_{p',q}^{\dagger} \right) \left(\hat{\theta}_{q,p} - \hat{\theta}_{q,p} (\hat{n}_{p'} + 1 \cdot \hat{n}_{q} + 1) \right) : \hat{a}_{p} \hat{a}_{p'} :$$
(A.40)

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

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

$$= -\sum_{q \neq q'} \sum_{p, p'} \left[\hat{V}_{q, q'} : \hat{a}_{q}^{\dagger} \hat{a}_{q'} :, \hat{\phi}_{p, p'} : \hat{a}_{p}^{\dagger} \hat{a}_{p'}^{\dagger} : \right]$$

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

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

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

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

A.25e:

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

A.42a will be analyzed first:

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

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

A.25f

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

A.44a:

$$\begin{split} \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) \\ &- \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',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} : \hat{a}_{\tilde{p}'}^{\dagger} \hat{a}_{p'} : \\ &- \sum_{p,p'} \sum_{\tilde{p},\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'} \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'} \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',\tilde{p}'}^{\dagger} : \hat{a}_{\tilde{p}'}^{\dagger} \hat{a}_{p'} : \\ &- \sum_{p,p'} \sum_{\tilde{p}'} \hat{\phi}_{\tilde{p},\tilde{p}'} \hat{W}_{p',\tilde{p}'}^{\dagger} : \hat{a}_{\tilde{p}'}^{\dagger} \hat{a}_{p'} : \\ &- \sum_{p,p'} \sum_{\tilde{p}'} \hat{\phi}_{\tilde{p},\tilde{p}'} \hat{W}_{p',\tilde{p}'}^{\dagger} : \hat{a}_{\tilde{p}'}^{\dagger} \hat{a}_{p'} : \\ &- \sum_{p,p'} \sum_{\tilde{p}'} \hat{\phi}_{\tilde{p},\tilde{p}'} \hat{W}_{p',\tilde{p}'}^{\dagger} : \hat{a}_{\tilde{p}'}^{\dagger} \hat{a}_{p'} : \\ &- \sum_{p,p'} \sum_{\tilde{p}'} \hat{\phi}_{\tilde{p},\tilde{p}'} \hat{W}_{p',\tilde{p}'}^{\dagger} : \hat{a}_{\tilde{p}'}^{\dagger} \hat{a}_{p'} : \\ &- \sum_{p,p'} \sum_{\tilde{p}'} \hat{\phi}_{\tilde{p},\tilde{p}'} \hat{W}_{p',\tilde{p}'}^{\dagger} : \hat{a}_{\tilde{p}'}^{\dagger} \hat{a}_{p'} : \\ &- \sum_{p,p'} \sum_{\tilde{p}'} \hat{\phi}_{\tilde{p},\tilde{p}'} \hat{W}_{p',\tilde{p}'}^{\dagger} + \hat{\phi}_{p',p} \hat{W}_{p,p'}^{\dagger} \right) \\ &= - \sum_{p,p'} \sum_{\tilde{p}} \hat{\phi}_{\tilde{p},\tilde{p}'} \hat{W}_{p',\tilde{p}'}^{\dagger} + \hat{\phi}_{p',p} \hat{W}_{p,p'}^{\dagger} \right) \\ &= - \sum_{p,p'} \sum_{\tilde{p}} \hat{\phi}_{\tilde{p},\tilde{p}'} \hat{W}_{p',\tilde{p}'}^{\dagger} + \hat{\phi}_{p',\tilde{p}} \hat{W}_{p',\tilde{p}'}^{\dagger} + \hat{\phi}_{p',\tilde{p}} \hat{W}_{p',\tilde{p}'}^{\dagger} + \hat{\phi}_{p',\tilde{p}} \hat{W}_{p',\tilde{p}'}^{\dagger} + \hat{\phi}_{p',\tilde{p$$

A.44b gives no quadratic contribution:

$$\sum_{p,p'} \sum_{\tilde{p},\tilde{p}'} \hat{\phi}_{\tilde{p},\tilde{p}'} \left[: \hat{a}_{\tilde{p}}^{\dagger} \hat{a}_{\tilde{p}'}^{\dagger} :, \hat{W}_{p,p'}^{\dagger} \right] : \hat{a}_{p} \hat{a}_{p'} :
= \sum_{p,p'} \sum_{\tilde{p},\tilde{p}'} \hat{\phi}_{\tilde{p},\tilde{p}'} \left(\hat{W}_{p,p'}^{\dagger} (\hat{n}_{p} - 1, \hat{n}_{p'} - 1) - \hat{W}_{p,p'}^{\dagger} \right) : \hat{a}_{\tilde{p}}^{\dagger} \hat{a}_{\tilde{p}'}^{\dagger} :: \hat{a}_{p} \hat{a}_{p'} :
= \sum_{p,p'} \sum_{\tilde{p},\tilde{p}'} \hat{\phi}_{\tilde{p},\tilde{p}'} \left(\hat{W}_{p,p'}^{\dagger} (\hat{n}_{p} - 1, \hat{n}_{p'} - 1) - \hat{W}_{p,p'}^{\dagger} \right) : \hat{a}_{\tilde{p}}^{\dagger} \hat{a}_{\tilde{p}'}^{\dagger} \hat{a}_{p} \hat{a}_{p'} : \stackrel{@}{=} 0$$
(A.49)

A.44c:

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

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

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

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

$$\begin{split} &\sum_{q \neq q'} \sum_{\tilde{p}, \tilde{p}'} \left[\hat{\psi}_{\tilde{p}, \tilde{p}'} : \hat{a}_{\tilde{p}} \hat{a}_{\tilde{p}'} :, \hat{V}_{q, q'} : \hat{a}_{q}^{\dagger} \hat{a}_{q'} : \right] \\ &= -\sum_{p, p'} \sum_{\tilde{q} \neq \tilde{q}'} \left[\hat{V}_{\tilde{q}, \tilde{q}'} : \hat{a}_{\tilde{q}}^{\dagger} \hat{a}_{\tilde{q}'} :, \hat{\psi}_{p, p'} : \hat{a}_{p} \hat{a}_{p'} : \right] \\ &\stackrel{@}{=} -\sum_{p, p'} \sum_{q} \left(\hat{V}_{q, p'} \hat{\psi}_{p, q} + \hat{\theta}_{q, p} \hat{\psi}_{q, p'} \right) : \hat{a}_{p} \hat{a}_{p'} : \\ &- \sum_{p, p'} \sum_{q} \left(\hat{\psi}_{q, p'} + \hat{\psi}_{p', q} \right) \left(\hat{V}_{q, p} - \hat{V}_{q, p} (\hat{n}_{p'} + 1, \hat{n}_{q} + 1) \right) : \hat{a}_{p} \hat{a}_{p'} : \end{split}$$

$$(A.54a)$$

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

$$\begin{split} &\sum_{p,p'} \sum_{\bar{p},\bar{p}'} \left[\hat{\psi}_{\bar{p},\bar{p}'} : \hat{a}_{\bar{p}} \hat{a}_{\bar{p}'} :, \hat{W}_{p,p'} : \hat{a}_{p}^{\dagger} \hat{a}_{p'}^{\dagger} : \right] \\ &= -\sum_{p,p'} \sum_{\bar{p},\bar{p}'} \left[\hat{W}_{\bar{p},\bar{p}'} : \hat{a}_{\bar{p}}^{\dagger} \hat{a}_{\bar{p}'}^{\dagger} :, \hat{\psi}_{p,p'} : \hat{a}_{p} \hat{a}_{p'} : \right] \\ &= \sum_{p,p'} \sum_{\bar{p}} \left(\hat{W}_{p,\bar{p}} \hat{\psi}_{p',\bar{p}} + \hat{W}_{\bar{p},p} \hat{\psi}_{p',\bar{p}} + \hat{W}_{p,\bar{p}} \hat{\psi}_{\bar{p},p'} + \hat{W}_{\bar{p},p} \hat{\psi}_{\bar{p},p'} \right) : \hat{a}_{p}^{\dagger} \hat{a}_{p'} : \\ &+ \sum_{p,p'} \left(\hat{W}_{p,p'} \hat{\psi}_{p,p'} + \hat{W}_{p',p} \hat{\psi}_{p,p'} \right) \\ &- \sum_{p,p'} \sum_{\bar{p}} \hat{\psi}_{\bar{p},p'} \left(\hat{W}_{\bar{p},p} - \hat{W}_{\bar{p},p} (\hat{n}_{\bar{p}} + 1, \hat{n}_{p'} + 1) \right) : \hat{a}_{p}^{\dagger} \hat{a}_{p'} : \\ &- \sum_{p,p'} \sum_{\bar{p}} \hat{\psi}_{p',\bar{p}} \left(\hat{W}_{p,\bar{p}} - \hat{W}_{p,\bar{p}} (\hat{n}_{\bar{p}} + 1, \hat{n}_{p'} + 1) \right) : \hat{a}_{p}^{\dagger} \hat{a}_{p'} : \\ &- \sum_{p,p'} \sum_{\bar{p}} \hat{\psi}_{p',\bar{p}} \left(\hat{W}_{\bar{p},p} - \hat{W}_{\bar{p},p} (\hat{n}_{p'} + 1, \hat{n}_{\bar{p}} + 1) \right) : \hat{a}_{p}^{\dagger} \hat{a}_{p'} : \\ &- \sum_{p,p'} \sum_{\bar{p}} \hat{\psi}_{p',\bar{p}} \left(\hat{W}_{p,\bar{p}} - \hat{W}_{p,\bar{p}} (\hat{n}_{p'} + 1, \hat{n}_{\bar{p}} + 1) \right) : \hat{a}_{p}^{\dagger} \hat{a}_{p'} : \\ &- \sum_{p,p'} \sum_{\bar{p}} \hat{\psi}_{p',\bar{p}} \left(\hat{W}_{p,\bar{p}} - \hat{W}_{p,\bar{p}} (\hat{n}_{p'} + 1, \hat{n}_{\bar{p}} + 1) \right) : \hat{a}_{p}^{\dagger} \hat{a}_{p'} : \\ &- \sum_{p,p'} \hat{\psi}_{p,p'} \left(\hat{W}_{p',p} - \hat{W}_{p',p} (\hat{n}_{p} + 1, \hat{n}_{p'} + 1) \right) \\ &- \sum_{p,p'} \hat{\psi}_{p,p'} \left(\hat{W}_{p,p'} - \hat{W}_{p,p'} (\hat{n}_{p} + 1, \hat{n}_{p'} + 1) \right) \end{split}$$

 $\mathbf{A.25i}$: Similar to A.25e:

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

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 $\partial_{\lambda} \mathcal{H}(\lambda) = [\hat{\eta}(\lambda), \mathcal{H}(\lambda)]$ gives the following flow equations $\forall k, p, p', q, q'$ where $q \neq q'$:

$$\begin{split} \partial_{\lambda} \hat{V}_{q,q'} & \stackrel{\textcircled{\tiny @}}{=} - \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}_{\bar{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},\bar{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}_{q',\bar{q}}^{\dagger} \left(\hat{\phi}_{q,\bar{q}} - \hat{\phi}_{q,\bar{q}} (\hat{n}_{q'} + 1, \hat{n}_{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}} \hat{W}_{q',\bar{q}}^{\dagger} \left(\hat{W}_{q,\bar{q}} - \hat{W}_{q,\bar{q}} (\hat{n}_{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}_{q'} + 1, \hat{n}_{q'} + 1) \right) \\ &- \sum_{\bar{q}} \hat{\psi}_{q',\bar{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}_{q,\bar{q}} - \hat{W}_{q,\bar{q}} (\hat{n}_{q'} + 1, \hat{n}_{\bar{q}} + 1) \right) \\ &+ \sum_{\bar{q}} \hat{\theta}_{p',q} \left(\hat{W}_{q,\bar{q}} - \hat{W}_{q,\bar{q}} (\hat{n}_{q'} + 1, \hat{n}_{\bar{q}} + 1) \right) \\ &+ \sum_{\bar{q}} \hat{\theta}_{p,q} \left(\hat{W}_{q,\bar{q}} - \hat{W}_{q,\bar{q}} (\hat{n}_{q'} + 1, \hat{n}_{\bar{q}} + 1) \right) \\ &+ \sum_{\bar{q}} \hat{\theta}_{p,q} \left(\hat{W}_{q,p'} (\hat{n}_{q} + 1, \hat{n}_{p'} - 1) - \hat{W}_{p,p'} \right) \\ &+ \sum_{\bar{q}} \hat{\theta}_{p,q} \left(\hat{W}_{q,p'} (\hat{n}_{q} + 1, \hat{n}_{p'} - 1) - \hat{W}_{p,q} \right) \\ &- \sum_{\bar{q}} \hat{V}_{p,q} \left(\hat{\phi}_{p,q'} (\hat{n}_{q} + 1, \hat{n}_{p'} - 1) - \hat{\phi}_{p,q} \right) \\ &- \sum_{\bar{q}} \hat{V}_{p,q} \left(\hat{\phi}_{p,q'} (\hat{n}_{q} + 1, \hat{n}_{p'} - 1) - \hat{\phi}_{p,q} \right) \\ &- \sum_{\bar{q}} \hat{V}_{p',q} \left(\hat{\phi}_{p,q'} (\hat{n}_{q} + 1, \hat{n}_{p'} - 1) - \hat{\phi}_{p,q} \right) \\ &- \sum_{\bar{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}$$

$$\begin{split} \partial_{\lambda} \hat{W}_{p,p'}^{\dagger} & \stackrel{@}{=} -W_{p,p'}^{\dagger} \left(\hat{H} - \hat{H}(\hat{n}_{p'} + 1, \hat{n}_{p} + 1) \right)^{2} \\ &+ \sum_{q} \left(\hat{\theta}_{q,p'} \hat{W}_{p,q}^{\dagger} + \hat{\theta}_{q,p} \hat{W}_{q,p'}^{\dagger} \right) \\ &+ \sum_{q} \left(\hat{W}_{q,p'}^{\dagger} + \hat{W}_{p',q}^{\dagger} \right) \left(\hat{\theta}_{q,p} - \hat{\theta}_{q,p} (\hat{n}_{p'} + 1, \hat{n}_{q} + 1) \right) \\ &- \sum_{q} \left(\hat{\psi}_{q,p'} + \hat{\psi}_{p',q} \right) \left(\hat{V}_{q,p} - \hat{V}_{q,p} (\hat{n}_{p'} + 1, \hat{n}_{q} + 1) \right) \\ &- \sum_{q} \left(\hat{V}_{q,p'} \hat{\psi}_{p,q} + \hat{\theta}_{q,p} \hat{\psi}_{q,p'} \right) \\ \partial_{\lambda} \hat{H} & \stackrel{@}{=} - \sum_{p,p'} \left(\hat{\phi}_{p,p'} \hat{W}_{p,p'}^{\dagger} + \hat{\phi}_{p',p} \hat{W}_{p,p'}^{\dagger} \right) \\ &+ \sum_{p,p'} \hat{W}_{p,p'}^{\dagger} \left(\hat{\phi}_{p',p} - \hat{\phi}_{p',p} (\hat{n}_{p} + 1, \hat{n}_{p'} + 1) \right) \\ &+ \sum_{p,p'} \hat{W}_{p,p'}^{\dagger} \left(\hat{\phi}_{p,p'} - \hat{\phi}_{p,p'} (\hat{n}_{p} + 1, \hat{n}_{p'} + 1) \right) \\ &- \sum_{q} \left(\hat{V}_{q,p'} \hat{\psi}_{p,q} + \hat{\theta}_{q,p} \hat{\psi}_{q,p'} \right) \\ &- \sum_{q} \left(\hat{V}_{q,p'} \hat{\psi}_{p,q} + \hat{\theta}_{q,p} \hat{\psi}_{q,p'} \right) \\ &- \sum_{p,p'} \hat{\psi}_{p,p'} \left(\hat{W}_{p',p} - \hat{W}_{p',p} (\hat{n}_{p} + 1, \hat{n}_{p'} + 1) \right) \\ &- \sum_{p,p'} \hat{\psi}_{p,p'} \left(\hat{W}_{p,p'} - \hat{W}_{p,p'} (\hat{n}_{p} + 1, \hat{n}_{p'} + 1) \right) \\ &+ \sum_{p,p'} \left(\hat{W}_{p,p'} \hat{\psi}_{p,p'} + \hat{W}_{p',p} \hat{\psi}_{p,p'} \right) \end{aligned}$$

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

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

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

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

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

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

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

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

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

Then, in quadratic order, we get:

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

$$= v_{q,q'}^{\circ} h^{\circ} + \sum_{k} \left(h^{\circ} v_{q,q'}^{(k)} + v_{q,q'}^{\circ} h^{(k)} \right) \hat{n}_{k} + \sum_{k,k'} \left(h^{\circ} v_{q,q'}^{(k,k')} + v_{q,q'}^{\circ} h^{(k,k')} + v_{q,q'}^{(k)} h^{(k')} \right) \hat{n}_{k} \hat{n}_{k'}$$

$$(A.64a)$$

$$\hat{W}_{p,p'} \hat{H} \approx w_{p,p'}^{\circ} \hat{H} + h^{\circ} W_{p,p'} + \sum_{k,k'} w_{p,p'}^{(k)} h^{(k')} \hat{n}_{k} \hat{n}_{k'}$$

$$= w_{p,p'}^{\circ} h^{\circ} + \sum_{k} \left(h^{\circ} w_{p,p'}^{(k)} + w_{p,p'}^{\circ} h^{(k)} \right) \hat{n}_{k} + \sum_{k,k'} \left(h^{\circ} w_{p,p'}^{(k,k')} + w_{p,p'}^{\circ} h^{(k,k')} + w_{p,p'}^{(k)} h^{(k')} \right) \hat{n}_{k} \hat{n}_{k'}$$

$$(A.64b)$$

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

$$\hat{H}_{\tilde{k},\tilde{k}'}(\alpha,\beta) := \hat{H} - \hat{H}(\hat{n}_{\tilde{k}} + \alpha, \hat{n}_{\tilde{k}'} + \beta) = -\alpha h^{(\tilde{k})} - \beta h^{(\tilde{k}')} - \left(h^{(\tilde{k},\tilde{k})} + h^{(\tilde{k}',\tilde{k}')}\right) \\
- \alpha\beta \left(h^{(\tilde{k},\tilde{k}')} + h^{(\tilde{k}',\tilde{k})}\right) - \beta \sum_{k} (h^{(k,\tilde{k}')} + h^{(\tilde{k}',k)}) \hat{n}_{k} - \alpha \sum_{k} (h^{(k,\tilde{k})} + h^{(\tilde{k},k)}) \hat{n}_{k} \\
=: h_{\tilde{k},\tilde{k}'}^{\circ}(\alpha,\beta) + \sum_{k} h_{\tilde{k},\tilde{k}'}^{(k)}(\alpha,\beta) \hat{n}_{k} \tag{A.65}$$

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

$$\begin{split} \hat{\theta}_{q,q'} &= \hat{V}_{q,q'} \left(\hat{H} - \hat{H}(\hat{n}_{q} - 1, \hat{n}_{q'} + 1) \right) = \hat{V}_{q,q'} \hat{H}_{q,q'}(-, +) \\ &\approx v_{q,q'}^{\circ} h_{q,q'}^{\circ}(-, +) + \sum_{k} \left(h_{q,q'}^{\circ}(-, +) v_{q,q'}^{(k)} + v_{q,q'}^{\circ} h_{q,q'}^{(k)}(-, +) \right) \hat{n}_{k} \\ &+ \sum_{k,k'} \left(h_{q,q'}^{\circ}(-, +) v_{q,q'}^{(k,k')} + v_{q,q'}^{(k)} h_{q,q'}^{(k)}(-, +) \right) \hat{n}_{k} \hat{n}_{k'} \\ &=: \theta_{q,q'}^{\circ} + \sum_{k} \theta_{q,q'}^{(k)} \hat{n}_{k} + \sum_{k,k'} \theta_{q,q'}^{(k,k')} \hat{n}_{k} \hat{n}_{k'} \\ &\approx w_{p,p'}^{\circ} \left(\hat{H} - \hat{H}(\hat{n}_{p} - 1, \hat{n}_{p'} + 1) \right) = \hat{W}_{p,p'} \hat{H}_{p,p'}(-, -) \\ &\approx w_{p,p'}^{\circ} h_{p,p'}^{\circ}(-, -) + \sum_{k} \left(h_{p,p'}^{\circ}(-, -) w_{p,p'}^{(k)} + w_{p,p'}^{\circ} h_{p,p'}^{(k)}(-, -) \right) \hat{n}_{k} \\ &+ \sum_{k,k'} \left(h_{p,p'}^{\circ}(-, -) w_{p,p'}^{(k,k')} + w_{p,p'}^{(k)} h_{p,p'}^{(k)}(-, -) \right) \hat{n}_{k} \hat{n}_{k'} \\ &=: \phi_{p,p'}^{\circ} + \sum_{k} \phi_{p,p'}^{(k)} \hat{n}_{k} + \sum_{k,k'} \phi_{p,p'}^{(k,k')} \hat{n}_{k} \hat{n}_{k'} \\ &\approx w_{p,p'}^{\circ} * h_{p,p'}^{\circ}(+, +) + \sum_{k} \left(h_{p,p'}^{\circ}(+, +) w_{p,p'}^{(k)} * h_{p,p'}^{(k)}(+, +) \right) \hat{n}_{k} \\ &+ \sum_{k,k'} \left(h_{p,p'}^{\circ}(+, +) w_{p,p'}^{(k,k')} * + w_{p,p'}^{(k)} * h_{p,p'}^{(k)}(+, +) \right) \hat{n}_{k} \hat{n}_{k'} \end{aligned} \tag{A.66c}$$

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Munich, 22.06.2023