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Beyond Mean-Field Description of Bose-Einstein Condensate

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List of Abbreviations

- BEC — Bose-Einstein Condensate.
- CI — Configuration Interaction.
- CISD — CI With Single and Double Substitutions.
- ENPT — Epstein-Nesbet Perturbation Theory.
- GP — Gross-Pitaevskii.
- HF — Hartree-Fock.
- HO — Harmonic Oscillator.
- LHY — Lee-Huang-Yang.
- MBPT — Many-Body Perturbation Theory.
- MF — Mean Field.
- PT — Perturbation Theory.
- RSPT — Rayleigh-Schrödinger Perturbation Theory.
- QCISD — Quadratic CISD.

Abstract

This thesis work is on the theoretical description of dilute Bose-Einstein condensates (BEC) that are non-uniform, meaning that more than one single-particle state is occupied. This phenomenon is usually called quantum depletion. A common model for the ground state of a dilute and weakly interacting BEC is the mean-field (MF) approximation leading to the Gross-Pitaevskii (GP) equation. However, for more strongly correlated systems, a beyond MF method is required.

We propose a method for finding the energies of BECs through deriving the expressions up to fourth order in many-body perturbation theory using the GP equation in both Rayleigh-Schrödinger perturbation theory (RSPT) and Epstein-Nesbet perturbation theory (ENPT). The two perturbation theories are similar in terms of computational cost and a comparison of the accuracy of the two is thus of interest.

We implement RSPT and ENPT computationally and apply these methods in the analysis of a one-dimensional quantum ring system using contact interaction. The outputs of the two methods are benchmarked against Configuration Interaction in the low particle-number regime. Excellent agreement was found for both RSPT and ENPT for weak interaction strengths. For very high repulsive interaction strengths, RSPT starts to deviate from the correct solution. ENPT, however, continued to show good agreement in this regime.

ENPT is of particular interest for further research since it provides a better description of systems with higher interaction strengths. This method could be analysed using other kinds of systems, for example systems in a harmonic confinement, to see if it continues to provide accurate results.

Contents

Abstract

1. Introduction	1
2. Theory	4
2.1. Bose-Einstein Statistics	4
2.2. Many-Body Theory	4
2.2.1. Second Quantisation	5
2.3. The Mean-Field Approximation	7
2.4. Gross-Pitaevskii	7
2.5. Brillouin's Theorem	9
2.6. Many-Body Perturbation Theory	9
2.6.1. Rayleigh-Schrödinger Perturbation Theory	9
2.6.2. Epstein-Nesbet Perturbation Theory	11
3. Analytical Results	13
3.1. Fourth-Order Rayleigh-Schrödinger	13
3.2. Fourth-Order Epstein-Nesbet	17
4. Numerical Results	18
4.1. Quantum Ring System with Contact Interaction	18
4.1.1. Sweep of g	19
4.1.3. Comparison of Single Up to Quadruple Excitations	20
4.1.2. Comparison of Basis Sizes	21
5. Summary	22
6. Outlook	23

Acknowledgements

Appendix:

 More Detailed Derivations

1. Introduction

A Bose-Einstein condensate (BEC) is a state of matter that was first predicted by A. Einstein and S. N. Bose between 1924 and 1925 with the introduction of Bose-Einstein statistics which governs the behaviour of bosonic systems [1, 2]. This condensate may form at temperatures close to absolute zero. Bosons can then collectively occupy the lowest single-particle energy state. Just over seventy years later, in 1995, this non-classical state of matter was experimentally verified in rubidium-87 by E. A. Cornell and C. E. Wieman et al., as well as in sodium atoms shortly thereafter by W. Ketterle et al. [3, 4]. The three scientists mentioned were awarded the Nobel prize for these experimental achievements. Since 1995, BECs have been achieved for many other types of bosonic atoms as well as for larger bosonic structures like molecules [5], but also for photons [6] and quasi-particles [7].

Describing many-body systems is a challenging feat. This holds true no matter if one considers the quantum mechanical system or the classical system. The difficulty stems from the complex behaviour that a given particle has due to its dependence on several other, if not all, particles in the system. Due to this dependency, the Schrödinger equation often cannot be separated into single-particle Hamiltonians, and is thus harder to solve. Because of this difficulty, statistical methods and models are often used for simplification, as was the case in the discovery of BEC.

The statistical model often used to describe many-body problems is based on the mean-field (MF) approximation [8]. The atom-atom interactions are replaced by a potential created by all particles collectively such that all particles experience the same potential. One successful MF method is based on the Gross-Pitaevskii (GP) equation that is used to describe BECs where all atoms occupy the same single-particle orbital. This approach has been found to be accurate in describing dilute and weakly interacting BECs [9]. The MF solution, retrieved from the GP equation, is chosen to minimise the energy of the many-body state. For fermions, the equivalent of the GP equation is called the Hartree-Fock (HF) equation [10, 11], which was an earlier development than GP.

In replacing the atom-atom interactions with a MF, the difference between the interactions and the MF instead becomes a residual term. The exclusion of this term gives an initial estimate of the system. Improving upon this estimate can be done through the expansion of the residual in different orders. Here we can make use of many-body perturbation theory (MBPT), specifically Rayleigh-Schrödinger perturbation theory (RSPT) [12], where the residual is called a perturbation. The inclusion of each new order is generally an improvement upon the initial estimate provided the series converges, but becomes more difficult to derive and more computationally heavy. One may also use a different partitioning of RSPT, called Epstein-Nesbet perturbation theory (ENPT) [13, 14]. Using MBPT in the HF equation is called Møller-Plesset [15], though no equivalent

name exists for GP.

Of interest in this work is going to fourth-order MBPT for bosons using the GP equation. This is preceded by the work of Quantum-Chemists such as J. A. Pople, a Nobel laureate in Chemistry, that did similar work on fermionic systems in and around the 1970s. Specifically, for the fourth-order perturbation theory (PT) in a paper by Pople et al. using the HF equation [16], substitutions of particles occur that allow for single-up to quadruple-particle excitations from the ground-state. This is also the case in the GP equation due to the shared use of the same kind of PT. Compared to third order, fourth order introduces matrix elements containing single, triple and quadruple excitations. Third order is restricted to matrix elements containing double excitations. Pople et al. found in that paper that the triple excitation added a computational load that was too high, at that time, in comparison to the added precision of the programmed model, and that removing it did not ruin the size consistency of the system. Thus, they decided not to include it for the numerical treatment in that paper. However, they did go on to include it in later papers [17].

To modify the GP equation to improve the description of the system is also possible, but the accuracy of using what is called extended GP is uncertain. One such extended GP description implements the recent theoretical prediction of self-bound BECs through the Lee-Huang-Yang (LHY) correction term in 2015 [18], which was then experimentally verified a couple of years later [19]. Furthermore, when modelling other BECs with other potentials and stronger interaction strengths, extended GP has provided higher energies than some other MF models [20], causing doubt in the ability to take GP further than the previously mentioned cases.

Other methods going beyond the ordinary MF approximation do exist. One of these is called Configuration Interaction (CI), which has proven itself to be numerically exact. The method involves expanding the state into a many-body basis consisting of correctly symmetrized products of one-body states. This method's downfall is the fast growth of the matrix size with the number of particles which results in a time-complexity for the computation that grows very rapidly. In other words, the time to run the calculations grows at an exponential rate [21]. In most cases, CI can only treat a few particles.

An approximate version of CI that in part rectifies the problem of exponentially increasing time-complexity is called CI with Single and Double Substitutions (CISD). In this method, the basis is truncated, and certain restrictions are imposed such that only one or two particles can be in an excited state. Solving the problem of time-complexity comes at a cost, however. With the imposed restrictions, a size-inconsistency is introduced [22]. This inconsistency means that the error of the model increases with particle number [21]. A further extension that solves both of the above-mentioned problems, is called Quadratic CISD (QCISD) [23].

Following this introduction, Sec. 1, the thesis is organized as follows. Section 2 cov-

1. INTRODUCTION

ers theory and choice of notation, giving the necessary background for the work. Among the things covered are the MF approximation, MBPT and GP. The third section contains derivations for the expressions in RSPT and ENPT. Section 4 describes the system that the MBPT methods were applied to, giving implementation details and presenting the obtained results. The fifth section presents a summary of the work and some of the conclusions that could be made. Finally, the sixth section discusses the potential extensions of the work and its applications. Full derivations with more detailed steps are given in the Appendix.

2. Theory

This chapter gives an overview of the relevant theory for the thesis. This starts with a small section on Bose-Einstein statistics, then goes into some details of many-body theory and second quantisation. The MF approximation is presented, which then leads into the theory pertaining to GP. This is then followed by a description of Brillouin's theorem. Lastly, an overview of MBPT is given. The choices of notation are presented throughout to make subsequent sections more accessible.

2.1. Bose-Einstein Statistics

Bosons are characterised by a symmetric wave function under particle exchange. For example, for a two-particle system the wave function can be written as [8, 24, 25]

$$\Phi(\vec{x}_1, \vec{x}_2) = \frac{1}{\sqrt{2}} [\phi_a(\vec{x}_1)\phi_b(\vec{x}_2) + \phi_b(\vec{x}_1)\phi_a(\vec{x}_2)], \quad (2.1)$$

where ϕ_a and ϕ_b are one-body states. The expected occupation of energy levels in a bosonic system in thermal equilibrium is described by the Bose-Einstein distribution, and has the form [25]

$$\langle n_i \rangle = \frac{1}{\exp\left(\frac{\varepsilon_i - \mu}{k_B T}\right) - 1}, \quad (2.2)$$

where $\langle n_i \rangle$ is the mean occupation number in state i , ε_i is the energy level of state i , μ is the chemical potential, k_B is the Boltzmann constant and T is the temperature. In the extreme low-temperature limit, all bosons collapse to the ground state, forming what is called a BEC.

2.2. Many-Body Theory

Throughout this work, many-body operators are generally written with uppercase letters and single-particle operators with lowercase letters. Only one component, or one species of atom will be treated. The general Hamiltonian is composed of three components. The first is the kinetic energy, the second is an external potential, and the third is the inter-particle interactions of the particles in the system. Writing these as \hat{T} , \hat{U} and $\hat{V}_{\text{int}}^{\text{tot}}$ respectively, where int stands for interaction and tot for total, the full many-body Hamiltonian becomes

$$\hat{H} = \hat{T} + \hat{U} + \hat{V}_{\text{int}}^{\text{tot}}. \quad (2.3)$$

Writing these out fully yields

$$\hat{H} = \sum_{i=0}^N (\hat{t}_i + \hat{u}_i) + \sum_{i<j}^N \hat{V}_{\text{int}}, \quad (2.4)$$

2. THEORY

where \hat{t}_i is the kinetic energy and \hat{u}_i the potential energy of particle i . We can group the kinetic and potential terms to form a single-particle Hamiltonian according to

$$\hat{H}_0 = \sum_{i=0}^N \hat{h}_i = \sum_{i=0}^N (\hat{t}_i + \hat{u}_i), \quad (2.5)$$

where $\hat{h}_i = \hat{t}_i + \hat{u}_i$. Consequently, we may rewrite the full many-body Hamiltonian as

$$\hat{H} = \sum_{i=0}^N \hat{h}_i + \sum_{i<j}^N \hat{V}_{\text{int}}. \quad (2.6)$$

The reason for the strict inequality in the second sum is to prevent counting interactions twice. A common choice of interaction because of its simplicity, is called contact interaction. For dilute gases at very low temperatures, the interaction between atoms may be modeled by an effective interaction potential in the form of a delta function $\delta(\hat{x}_i - \hat{x}_j)$ and a coupling strength g . With this choice, the Hamiltonian in Eq. (2.6) becomes

$$\hat{H} = \sum_{i=0}^N \hat{h}_i + \sum_{i<j}^N g\delta(\hat{x}_i - \hat{x}_j). \quad (2.7)$$

2.2.1. Second Quantisation

Annihilation and creation operators are mappings between many-body Hilbert spaces $\mathcal{H}(N)$ with different particle numbers N [8]. Instead of seeing these operators as mappings between Hilbert spaces, we can construct what is called a Fock space, $\mathcal{F}(\mathcal{H})$ where these operators instead act on the space $\mathcal{F}(\mathcal{H})$. Specifically for bosons, we require a symmetric Fock space $\mathcal{F}^+(\mathcal{H})$. No details on the construction of this space will be provided here, the reader is instead referred to [8]. In second quantization, occupation number representation is used, meaning that a state is written in terms of occupancy of different single-particle states. The annihilation operator in this representation is defined as

$$\hat{a}_i |\dots, n_i, \dots\rangle \equiv \sqrt{n_i} |\dots, n_i - 1, \dots\rangle, \quad (2.8)$$

where n_i is the number of bosons in $\phi_i \in \mathcal{H}(1)$, which is the wave function of a single-particle state i of a one-dimensional system. The creation operator is defined as

$$\hat{a}_i^\dagger |\dots, n_i, \dots\rangle \equiv \sqrt{n_i + 1} |\dots, n_i + 1, \dots\rangle. \quad (2.9)$$

The number operator gives the total number of particles in the system as its eigenvalue. It is defined as the sum of pairs of annihilation and creation operators acting on a state i in the system as

$$\hat{N} \equiv \sum_{i=0}^{\infty} \hat{a}_i^\dagger \hat{a}_i. \quad (2.10)$$

Any pair of operators obey certain commutation relations. In the case of bosons, the annihilation and creation operators obey the following commutation relations

$$[\hat{a}_i, \hat{a}_j^\dagger] = -[\hat{a}_j^\dagger, \hat{a}_i] = \hat{a}_i \hat{a}_j^\dagger - \hat{a}_j^\dagger \hat{a}_i = \delta_{i,j}, \quad (2.11)$$

$$[\hat{a}_i, \hat{a}_j] = [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0. \quad (2.12)$$

Using these two operators, we can rewrite the many-body Hamiltonian. In particular, a single-particle operator such as \hat{H}_0 becomes

$$\hat{H}_0 = \sum_{i,j} \hat{a}_i^\dagger \hat{a}_j \langle i | \hat{h} | j \rangle, \quad (2.13)$$

where

$$\langle i | \hat{h} | j \rangle = \int \phi_i^*(x) \hat{h} \phi_j(x) dx. \quad (2.14)$$

In the same way, the representation of a double-particle operator such as $\hat{V}_{\text{int}}^{\text{tot}}$ is

$$\hat{V}_{\text{int}}^{\text{tot}} = \frac{1}{2} \sum_{i,j,k,l} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k \langle ij | \hat{V}_{\text{int}} | kl \rangle, \quad (2.15)$$

where

$$\langle ij | \hat{V}_{\text{int}} | kl \rangle \equiv \iint \phi_i^*(x) \phi_j^*(x') \hat{V}_{\text{int}}(x, x') \phi_k(x) \phi_l(x') dx dx'. \quad (2.16)$$

We would now like to adapt the occupation number representation to the case of BECs. As a first step we choose to write the ground state as

$$|\Phi\rangle = |N, 0, 0, \dots\rangle, \quad (2.17)$$

with all N particles occupying the ground state ϕ_0 . Single excitations can then be written as

$$|\Phi_0^r\rangle = |N - 1, \dots, 1_r, \dots\rangle. \quad (2.18)$$

Continuing along the same lines, we can write a double excitation as

$$|\Phi_{00}^{rs}\rangle = |N - 2, \dots, 1_r, \dots, 1_s, \dots\rangle, \quad (2.19)$$

and so on. Here, "..." denotes all unoccupied states, represented by 0, in between the occupied states. The subscript for Φ denotes the vacancies in the ground state and the superscript denotes occupied higher-energy orbitals. Having a zero in the subscript and the superscript would then represent a particle taken from the ground state and placed back in the ground state, which has accomplished nothing and the zeros can be removed as follows

$$|\Phi\rangle = |\Phi_0^0\rangle. \quad (2.20)$$

Also useful is the introduction of a short-hand notation which we define as

$$\langle ij || kl \rangle \equiv \frac{1}{2} [\langle ij | \hat{V}_{\text{int}} | kl \rangle + \langle ji | \hat{V}_{\text{int}} | kl \rangle]. \quad (2.21)$$

2. THEORY

With Eq. (2.21), we get for example that

$$\langle ii || kl \rangle = \langle ii | \hat{V}_{\text{int}} | kl \rangle. \quad (2.22)$$

In the case of contact interaction we label the interaction potential V_{ijkl}^{cont} and note that the Dirac delta function reduces the integral to

$$\begin{aligned} V_{ijkl}^{\text{cont}} &= \langle ij | g \delta(x - x') | kl \rangle = g \iint \phi_i^*(x) \phi_j^*(x') \delta(x - x') \phi_k(x) \phi_l(x') dx dx' \\ &= g \int \phi_i^*(x) \phi_j^*(x) \phi_k(x) \phi_l(x) dx. \end{aligned} \quad (2.23)$$

2.3. The Mean-Field Approximation

The MF approximation is a method that tries to simplify the complicated interaction terms between particles. The method involves finding a MF potential that best models the interactions of the particles. If one can find a suitable MF potential, the full many-body Hamiltonian can then be expressed as

$$\hat{H} = \hat{H}_{\text{MF}} + \hat{V} = \underbrace{\hat{T} + \hat{U}_{\text{ext}} + \hat{U}_{\text{MF}}}_{\hat{H}_{\text{MF}}} + \underbrace{\hat{V}_{\text{int}}^{\text{tot}} - \hat{U}_{\text{MF}}}_{\hat{V}}, \quad (2.24)$$

where H_{MF} is the MF Hamiltonian and \hat{V} is the perturbation. In many-body theory, with a state $|\Psi_n\rangle \in \mathcal{F}^+(\mathcal{H})$, a good choice of \hat{H}_{MF} can be found through the minimisation of $E_n = \langle \Psi_n | \hat{H} | \Psi_n \rangle$. Minimisation can be performed through variational methods, such as the application of Lagrange multipliers [8]. One very successful application of the MF approximation was to nuclear shell structure (see for example [26]). With the proper choice of MF potential, specifically the Woods-Saxon potential with the inclusion of a term taking spin-orbit coupling into account, the shell structure and magic numbers of the nucleus were accurately predicted. These developments were made by M. G. Mayer and J. H. D. Jensen [27, 28], following previous work of E. Wigner.

2.4. Gross-Pitaevskii

The GP equation is a non-linear differential equation using a MF that optimises the ground state of the system in the same way as in the HF equation for fermions [9] and is often given with the choice of contact interaction as

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + \hat{u} + g(N-1)|\phi|^2 \right) |\phi\rangle = \mu |\phi\rangle, \quad (2.25)$$

where μ is the chemical potential and g is the interaction strength. To generalise this we may replace $g(N-1)|\phi|^2$ with a more general potential \hat{u}_{GP} and write

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + \hat{u} + \hat{u}_{\text{GP}} \right) |\phi\rangle = \mu |\phi\rangle. \quad (2.26)$$

We can now identify the many-body MF Hamiltonian in a similar fashion as in Sec. 2.2

$$\hat{H}_{\text{GP}} = \hat{T} + \hat{U} + \hat{U}_{\text{GP}}, \quad (2.27)$$

or alternatively in the form of the single-particle operator representation given in Eq. (2.13) as

$$\hat{H}_{\text{GP}} = \sum_{i,j} \hat{a}_i^\dagger \hat{a}_j \langle i|\hat{h}|j\rangle + \sum_{i,j} \hat{a}_i^\dagger \hat{a}_j \langle i|\hat{u}_{\text{GP}}|j\rangle, \quad (2.28)$$

where $\langle i|\hat{u}_{\text{GP}}|j\rangle$ is given as [8, 29]

$$\langle i|\hat{u}_{\text{GP}}|j\rangle = \frac{1}{2}(N-1) [\langle 0i|\hat{V}_{\text{int}}|0j\rangle + \langle i0|\hat{V}_{\text{int}}|0j\rangle], \quad (2.29)$$

with a plus sign because of the symmetric wave function of bosons under exchange of particles (see the discussion in connection to Eq. (2.1)). This choice of potential is found from minimising the energy through for example variational methods as mentioned in Sec. 2.3. In the short-hand notation of Eq. (2.21), Eq. (2.29) can also be written as

$$\langle j|\hat{u}_{\text{GP}}|i\rangle = (N-1) \langle 0j || 0i\rangle. \quad (2.30)$$

The next step is to identify the corresponding perturbation. This perturbation will be used to systematically correct the unperturbed solution. Using Eq. (2.24), we identify the perturbation as

$$\hat{V}_{\text{GP}} = \hat{V}_{\text{int}}^{\text{tot}} - \hat{U}_{\text{GP}}, \quad (2.31)$$

or in terms of the representations of single- and double-particle operators given in Eqs. (2.13) and (2.15) as

$$\hat{V}_{\text{GP}} = \hat{V}_{\text{int}}^{\text{tot}} - \hat{U}_{\text{GP}} = \frac{1}{2} \sum_{i,j,l,k} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k \langle ij|\hat{V}_{\text{int}}|kl\rangle - \sum_{i,j} \hat{a}_i^\dagger \hat{a}_j \langle i|\hat{u}_{\text{GP}}|j\rangle. \quad (2.32)$$

We now look at the expectation value of the GP perturbation when a single excitation from the ground state occurs

$$\begin{aligned} \langle \Phi_0^r | \hat{V}_{\text{GP}} | \Phi \rangle &= \frac{1}{2} \sqrt{N} (N-1) [\langle 0r | \hat{V}_{\text{int}} | 00 \rangle + \langle r0 | \hat{V}_{\text{int}} | 00 \rangle] \\ &+ \frac{N-1}{2} \sqrt{N} [\langle 0r | \hat{V}_{\text{int}} | 00 \rangle + \langle r0 | \hat{V}_{\text{int}} | 00 \rangle] = 0. \end{aligned} \quad (2.33)$$

This will greatly simplify the derivation of expressions in Sec. 3.

2.5. Brillouin's Theorem

Brillouin's theorem states that [8, 29]

$$\langle \Phi_0^r | \hat{H} | \Phi \rangle = 0, \quad (2.34)$$

where $|\Phi_0^r\rangle$ is the state with a single excited particle in orbital ϕ_r , and the rest in ϕ_0 .

To show that Brillouin's theorem holds for a BEC, we rewrite $\langle \Phi_0^r | \hat{H} | \Phi \rangle$ using the single- and double-particle operator representations (see Eqs. (2.13,2.15)) as

$$\begin{aligned} \langle \Phi_0^r | \hat{H} | \Phi \rangle &= \sum_{i,j} \langle i | \hat{h} | j \rangle \langle \Phi_0^r | \hat{a}_i^\dagger \hat{a}_j | \Phi \rangle + \frac{1}{2} \sum_{i,j,k,l} \langle ij | \hat{V}_{\text{int}} | kl \rangle \langle \Phi_0^r | \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k | \Phi \rangle \\ &= \sqrt{N} \langle r | \hat{h} | 0 \rangle + \sqrt{N} (N-1) \langle 0r || 00 \rangle. \end{aligned} \quad (2.35)$$

The desired solution in the case of a BEC for the single-particle operator \hat{h} is at the lowest energy eigenstate, $|0\rangle$. In the case of the GP equation, this single-particle operator is $\hat{h}_{\text{GP}} = \hat{h} + \hat{u}_{\text{GP}}$, yielding

$$\langle r | \hat{h}_{\text{GP}} | 0 \rangle = \langle r | (\hat{h} + \hat{u}_{\text{GP}}) | 0 \rangle = \langle r | \hat{h} | 0 \rangle + \langle r | \hat{u}_{\text{GP}} | 0 \rangle = \langle r | \hat{h} | 0 \rangle + (N-1) \langle 0r || 00 \rangle. \quad (2.36)$$

With this we can rewrite Eq. (2.35) to be

$$\langle \Phi_0^r | \hat{H} | \Phi \rangle = \sqrt{N} \langle r | \hat{h}_{\text{GP}} | 0 \rangle = \sqrt{N} \mu_0 \langle r | 0 \rangle = \sqrt{N} \mu_0 \times 0 = 0, \quad (2.37)$$

giving Brillouin's theorem.

Q.E.D.

If E is at a minimum, we have

$$\langle \Phi | \hat{H} | \Phi \rangle = (\langle \Phi | + \eta \langle \Phi_0^r |) \hat{H} (|\Phi\rangle + \eta |\Phi_0^r\rangle), \quad (2.38)$$

where $\eta \in \mathbb{R}$ is a small number. If we expand Eq. (2.38) and neglect terms quadratic in η , we find that $\langle \Phi_0^r | \hat{H} | \Phi \rangle = 0$ minimises the energy.

2.6. Many-Body Perturbation Theory

2.6.1. Rayleigh-Schrödinger Perturbation Theory

RSPT is a general way of treating any perturbation of a Hamiltonian. One example is the perturbation introduced in Eq. (2.24) for the MF approximation. As a starting point, the Schrödinger equation may be written as

$$\hat{H} |\Psi_n\rangle = E_n |\Psi_n\rangle. \quad (2.39)$$

We subsequently introduce a perturbation \hat{V} which is assumed to be linearly separable from the unperturbed Hamiltonian \hat{H}_0 such that

$$\hat{H} = \hat{H}_0 + \lambda\hat{V}, \quad (2.40)$$

where $\lambda \in \mathbb{R}$ can take any value but is set to 1 in the final expressions. Inserting Eq. (2.40) into Eq. (2.39) gives

$$(\hat{H}_0 + \lambda\hat{V}) |\Psi_n\rangle = E_n |\Psi_n\rangle. \quad (2.41)$$

We may expand $|\Psi_n\rangle$ in λ as

$$|\Psi_n\rangle = \sum_{i=0}^{\infty} \lambda^i |\Psi_n^{(i)}\rangle, \quad (2.42)$$

where $|\Psi_n^{(0)}\rangle$ is an eigenstate of \hat{H}_0 and $|\Psi_n^{(i)}\rangle$, $i > 0$, are corrections. Similarly, for the eigenenergy we have

$$E_n = \sum_{j=0}^{\infty} \lambda^j \delta E_n^{(j)}, \quad (2.43)$$

where δ denotes a shift in energy. These expansions can now be inserted into Eq. (2.41), which yields

$$(\hat{H}_0 + \lambda\hat{V}) \sum_{i=0}^{\infty} \lambda^i |\Psi_n^{(i)}\rangle = \sum_{j=0}^{\infty} \lambda^j \delta E_n^{(j)} \sum_{i=0}^{\infty} \lambda^i |\Psi_n^{(i)}\rangle. \quad (2.44)$$

Matching powers of λ then gives different orders for the perturbation correction to the known Hamiltonian \hat{H}_0 . We are interested in going up to fourth order in λ and thus we get the expansion

$$\hat{H}_0 \sum_{i=0}^4 \lambda^i |\Psi_n^{(i)}\rangle + \hat{V} \sum_{i=0}^3 \lambda^{i+1} |\Psi_n^{(i)}\rangle = \sum_{j=0}^4 \lambda^j \delta E_n^{(j)} \sum_{i=0}^4 \lambda^i |\Psi_n^{(i)}\rangle. \quad (2.45)$$

The left-hand side of Eq. (2.45) will then become

$$\begin{aligned} & (\hat{H}_0 |\Psi_n^{(0)}\rangle + \hat{H}_0 \lambda |\Psi_n^{(1)}\rangle + \hat{H}_0 \lambda^2 |\Psi_n^{(2)}\rangle + \hat{H}_0 \lambda^3 |\Psi_n^{(3)}\rangle + \hat{H}_0 \lambda^4 |\Psi_n^{(4)}\rangle) \\ & + (\hat{V} \lambda |\Psi_n^{(0)}\rangle + \hat{V} \lambda^2 |\Psi_n^{(1)}\rangle + \hat{V} \lambda^3 |\Psi_n^{(2)}\rangle + \hat{V} \lambda^4 |\Psi_n^{(3)}\rangle), \end{aligned} \quad (2.46)$$

and the right-hand side

$$\begin{aligned} & (\delta E_n^{(0)} + \lambda \delta E_n^{(1)} + \lambda^2 \delta E_n^{(2)} + \lambda^3 \delta E_n^{(3)} + \lambda^4 \delta E_n^{(4)}) \\ & \times (|\Psi_n^{(0)}\rangle + \lambda |\Psi_n^{(1)}\rangle + \lambda^2 |\Psi_n^{(2)}\rangle + \lambda^3 |\Psi_n^{(3)}\rangle + \lambda^4 |\Psi_n^{(4)}\rangle). \end{aligned} \quad (2.47)$$

The zeroth order result, denoted $\mathcal{O}(\lambda^0)$ can be observed to be

$$\delta E_n^{(0)} = \langle \Psi_n^{(0)} | \hat{H}_0 | \Psi_n^{(0)} \rangle. \quad (2.48)$$

This does not involve the perturbation and is the initial solution to the Schrödinger equation. To improve the description of the system, higher order terms need to be

2. THEORY

considered. The expressions for the first three orders in energy can be found in, for example [8, 24, 30] and read in order of $\mathcal{O}(\lambda^i)$ as

$$\mathcal{O}(\lambda) : \delta E_n^{(1)} = \langle \Psi_n^{(0)} | \hat{V} | \Psi_n^{(0)} \rangle, \quad (2.49)$$

$$\mathcal{O}(\lambda^2) : \delta E_n^{(2)} = \sum_{k_1 \neq n}^{\infty} \frac{|\langle \Psi_{k_1}^{(0)} | \hat{V} | \Psi_n^{(0)} \rangle|^2}{E_n^{(0)} - E_{k_1}^{(0)}}, \quad (2.50)$$

$$\begin{aligned} \mathcal{O}(\lambda^3) : \delta E_n^{(3)} &= \sum_{k_2 \neq n}^{\infty} \sum_{k_1 \neq n}^{\infty} \frac{\langle \Psi_n^{(0)} | \hat{V} | \Psi_{k_2}^{(0)} \rangle \langle \Psi_{k_2}^{(0)} | \hat{V} | \Psi_{k_1}^{(0)} \rangle \langle \Psi_{k_1}^{(0)} | \hat{V} | \Psi_n^{(0)} \rangle}{(E_n^{(0)} - E_{k_2}^{(0)}) (E_n^{(0)} - E_{k_1}^{(0)})} \\ &\quad - \langle \Psi_n^{(0)} | \hat{V} | \Psi_n^{(0)} \rangle \sum_{k \neq n}^{\infty} \frac{|\langle \Psi_k^{(0)} | \hat{V} | \Psi_n^{(0)} \rangle|^2}{(E_n^{(0)} - E_k^{(0)})^2}. \end{aligned} \quad (2.51)$$

Finally, the fourth order correction is [16]

$$\begin{aligned} \mathcal{O}(\lambda^4) : \delta E_n^{(4)} &= \sum_{k_1 \neq n}^{\infty} \sum_{k_2 \neq n}^{\infty} \sum_{k_3 \neq n}^{\infty} \frac{\langle \Psi_n^{(0)} | \hat{V} | \Psi_{k_3}^{(0)} \rangle \langle \Psi_{k_3}^{(0)} | \hat{V} | \Psi_{k_2}^{(0)} \rangle \langle \Psi_{k_2}^{(0)} | \hat{V} | \Psi_{k_1}^{(0)} \rangle \langle \Psi_{k_1}^{(0)} | \hat{V} | \Psi_n^{(0)} \rangle}{(E_n^{(0)} - E_{k_3}^{(0)}) (E_n^{(0)} - E_{k_2}^{(0)}) (E_n^{(0)} - E_{k_1}^{(0)})} \\ &\quad - \delta E_n^{(2)} \sum_{k_3 \neq n}^{\infty} \frac{|\langle \Psi_n^{(0)} | \hat{V} | \Psi_{k_3}^{(0)} \rangle|^2}{(E_n^{(0)} - E_{k_3}^{(0)})^2} \\ &\quad - 2 \langle \Psi_n^{(0)} | \hat{V} | \Psi_n^{(0)} \rangle \sum_{k_2 \neq n}^{\infty} \sum_{k_3 \neq n}^{\infty} \frac{\langle \Psi_n^{(0)} | \hat{V} | \Psi_{k_3}^{(0)} \rangle \langle \Psi_{k_3}^{(0)} | \hat{V} | \Psi_{k_2}^{(0)} \rangle \langle \Psi_{k_2}^{(0)} | \hat{V} | \Psi_n^{(0)} \rangle}{(E_n^{(0)} - E_{k_2}^{(0)})^2 (E_n^{(0)} - E_{k_3}^{(0)})} \\ &\quad + \langle \Psi_n^{(0)} | \hat{V} | \Psi_n^{(0)} \rangle^2 \sum_{k_3 \neq n}^{\infty} \frac{|\langle \Psi_n^{(0)} | \hat{V} | \Psi_{k_3}^{(0)} \rangle|^2}{(E_n^{(0)} - E_{k_3}^{(0)})^3}. \end{aligned} \quad (2.52)$$

2.6.2. Epstein-Nesbet Perturbation Theory

ENPT is an extension of RSPT utilising a different partitioning [13, 14]. We first note that any orthonormal set of states $\{\Psi_i\}$ forms a basis in symmetric or bosonic Fock space $\mathcal{F}^+(\mathcal{H})$. As such, we may insert two completeness relations in our Hamiltonian in Eq. (2.40) to form

$$\hat{H} = \sum_{i,j} |\Psi_i\rangle \langle \Psi_i | \hat{H} | \Psi_j\rangle \langle \Psi_j |, \quad (2.53)$$

Following similar steps as in Rayleigh-Schrödinger, we divide the Hamiltonian into \hat{H}_0^{EN} (the unperturbed part) and \hat{V}_{EN} (the perturbation). For \hat{H}_0^{EN} we choose the diagonal elements in the matrix representation of \hat{H} in Eq. (2.54) as

$$\hat{H}_0^{\text{EN}} = \sum_i |\Psi_i\rangle \langle \Psi_i | \hat{H} | \Psi_i\rangle \langle \Psi_i |. \quad (2.54)$$

All states $|\Psi_i\rangle$ then become eigenstates of the Hamiltonian, \hat{H}_0^{EN} , from

$$\hat{H}_0^{\text{EN}} |\Psi_i\rangle = \langle \Psi_i | \hat{H} | \Psi_i\rangle |\Psi_i\rangle. \quad (2.55)$$

The eigenvalues of \hat{H}_0^{EN} are thus $\langle \Psi_i | \hat{H} | \Psi_i \rangle$. Since $\hat{H} = \hat{H}_0 + \hat{V}$, we can also find an expression for our perturbation

$$\begin{aligned}
\hat{V}_{\text{EN}} &= \hat{H} - \hat{H}_0^{\text{EN}} = \sum_{j,k} |\Psi_j\rangle \langle \Psi_k| \left(\hat{H} - \sum_i |\Psi_i\rangle \langle \Psi_i| \hat{H} |\Psi_i\rangle \langle \Psi_i| \right) |\Psi_k\rangle \langle \Psi_k| \\
&= \sum_{j,k} |\Psi_j\rangle \langle \Psi_j| \hat{H} |\Psi_k\rangle \langle \Psi_k| - \sum_{i,j,k} |\Psi_j\rangle \langle \Psi_j| \Psi_i\rangle \langle \Psi_i| \hat{H} |\Psi_i\rangle \langle \Psi_i| \Psi_k\rangle \langle \Psi_k| \\
&= \sum_{j,k} |\Psi_j\rangle \langle \Psi_j| \hat{H} |\Psi_k\rangle \langle \Psi_k| - \sum_i |\Psi_i\rangle \langle \Psi_i| \hat{H} |\Psi_i\rangle \langle \Psi_i| \\
&= \sum_{\substack{i,j \\ i \neq j}} |\Psi_j\rangle \langle \Psi_j| \hat{H} |\Psi_i\rangle \langle \Psi_i|. \tag{2.56}
\end{aligned}$$

From Eq. (2.56) we see that all the diagonal matrix elements in the matrix \hat{V} are zero since we subtracted away the diagonal. Alternatively, one could phrase it as only off-diagonal states are allowed to appear in the matrix. If we now in Eq. (2.56) add and subtract the unperturbed Hamiltonian in RSPT, \hat{H}_0 , one can express \hat{V}_{EN} in terms of \hat{V} . To do this, we use that $|\Psi_i\rangle$ is an eigenstate of \hat{H}_0 . Thus, we get

$$\begin{aligned}
\hat{V}_{\text{EN}} &= \sum_{\substack{i,j \\ i \neq j}} |\Psi_j\rangle \langle \Psi_j| \hat{H} |\Psi_i\rangle \langle \Psi_i| = \sum_{\substack{i,j \\ i \neq j}} |\Psi_j\rangle \langle \Psi_j| \hat{H} - \hat{H}_0 + \hat{H}_0 |\Psi_i\rangle \langle \Psi_i| \\
&= \sum_{\substack{i,j \\ i \neq j}} |\Psi_j\rangle \langle \Psi_j| \hat{H} - \hat{H}_0 |\Psi_i\rangle \langle \Psi_i| = \sum_{\substack{i,j \\ i \neq j}} |\Psi_j\rangle \langle \Psi_j| \hat{V} |\Psi_i\rangle \langle \Psi_i|, \tag{2.57}
\end{aligned}$$

with $\hat{V} = \hat{H} - \hat{H}_0$ from Eq. (2.40) with $\lambda = 1$. This means that

$$\langle \Psi_j | \hat{V}_{\text{EN}} | \Psi_i \rangle = \langle \Psi_j | \hat{V} | \Psi_i \rangle, \quad \forall i \neq j, \tag{2.58}$$

and that all diagonal elements $\langle \Psi_i | \hat{V}_{\text{EN}} | \Psi_i \rangle = 0$ when using the perturbation in Eq. (2.58). From Eq. (2.58), we thus make note of the fact that zeroth order ENPT is now

$$\begin{aligned}
\langle \Psi_n | \hat{H}_0^{\text{EN}} | \Psi_n \rangle &= \langle \Psi_n | \hat{H}_0 | \Psi_n \rangle + \sum_i \langle \Psi_n | \Psi_i \rangle \langle \Psi_i | \hat{V} | \Psi_i \rangle \langle \Psi_i | \Psi_n \rangle \\
&= \langle \Psi_n | \hat{H}_0 | \Psi_n \rangle + \langle \Psi_n | \hat{V} | \Psi_n \rangle, \tag{2.59}
\end{aligned}$$

and that corresponding expressions will appear in the denominators of higher orders for other states, as the denominators are given as

$$\langle \Psi_n | \hat{H}_0^{\text{EN}} | \Psi_n \rangle - \langle \Psi_k | \hat{H}_0^{\text{EN}} | \Psi_k \rangle, \tag{2.60}$$

with $|\Psi_n\rangle$ being the ground state and $|\Psi_k\rangle$ being some other state. The specific choice in Eq. (2.54), that the eigenvalues of \hat{H}_0^{EN} are given by $\langle \Psi_i | \hat{H} | \Psi_i \rangle$, is one of many. Instead one may consider what is called generalised Epstein-Nesbet, which we will not discuss here, and instead the reader is referred to [31].

3. Analytical Results

3.1. Fourth-Order Rayleigh-Schrödinger

The fourth-order correction is of main concern and that is where we shall start. We pick \hat{H}_0 to be \hat{H}_{GP} as given in Eq. (2.28). The matrix elements appearing in Eq. (2.52) need to be evaluated when inserting the perturbation \hat{V}_{GP} given in Eq. (2.31), which henceforth will be written simply as \hat{V} . The derived expressions for fourth order can also be used for deriving lower orders and as such, these are instead given at the end of this section. First, we recount the fourth-order expression, now rewritten in the chosen notation of occupation number representation for BECs, to be

$$\begin{aligned}
\delta E_0^{(4)} = & \sum_{r \leq s} \sum_{\varrho \leq \sigma} \sum_{a \leq b < c \leq d} \frac{\langle \Phi | \hat{V} | \Phi_{00}^{\varrho\sigma} \rangle \langle \Phi_{00}^{\varrho\sigma} | \hat{V} | \Phi_{0000}^{abcd} \rangle \langle \Phi_{0000}^{abcd} | \hat{V} | \Phi_{00}^{rs} \rangle \langle \Phi_{00}^{rs} | \hat{V} | \Phi \rangle}{(2\mu_0 - \mu_\varrho - \mu_\sigma)(4\mu_0 - \mu_a - \mu_b - \mu_c - \mu_d)(2\mu_0 - \mu_r - \mu_s)} \\
& - \delta E_0^{(2)} \sum_{r \leq s} \frac{|\langle \Phi | \hat{V} | \Phi_{00}^{rs} \rangle|^2}{(2\mu_0 - \mu_r - \mu_s)^2} \\
& - 2\delta E_0^{(1)} \sum_{r \leq s} \sum_{\varrho \leq \sigma} \frac{\langle \Phi | \hat{V} | \Phi_{00}^{\varrho\sigma} \rangle \langle \Phi_{00}^{\varrho\sigma} | \hat{V} | \Phi_{00}^{rs} \rangle \langle \Phi_{00}^{rs} | \hat{V} | \Phi \rangle}{(2\mu_0 - \mu_\varrho - \mu_\sigma)(2\mu_0 - \mu_r - \mu_s)^2} \\
& + (\delta E_0^{(1)})^2 \sum_{r \leq s} \frac{|\langle \Phi | \hat{V} | \Phi_{00}^{rs} \rangle|^2}{(2\mu_0 - \mu_r - \mu_s)^3}, \tag{3.1}
\end{aligned}$$

with r, s, ϱ, σ and $d > 0$ because of the fact that the sums are over all states except the ground state (see Eq. (2.52)). Here, we introduce two new factors, t^{rs} and τ^{abcd} , to condense the notation. We define them as

$$t^{rs} \equiv \frac{\langle \Phi_{00}^{rs} | \hat{V} | \Phi \rangle}{2\mu_0 - \mu_r - \mu_s} = \begin{cases} \frac{\sqrt{N(N-1)}}{\sqrt{2}(2\mu_0 - \mu_r - \mu_s)} \langle rs | \hat{V}_{\text{int}} | 00 \rangle & r = s \\ \frac{\sqrt{N(N-1)}}{2\mu_0 - \mu_r - \mu_s} \langle rs | \hat{V}_{\text{int}} | 00 \rangle & r \neq s, \end{cases} \tag{3.2}$$

and

$$\tau^{abcd} \equiv \frac{\sum_{r \leq s} \langle \Phi_{0000}^{abcd} | \hat{V}_{\text{int}} | \Phi_{00}^{rs} \rangle t^{rs}}{\sqrt{4\mu_0 - \mu_a - \mu_b - \mu_c - \mu_d}}. \tag{3.3}$$

These factors are self-adjoint since the interaction \hat{V}_{int} is assumed to be real. The first term in Eq. (3.1) is

$$\sum_{r \leq s} \sum_{\varrho \leq \sigma} \sum_{a \leq b < c \leq d} \frac{\langle \Phi | \hat{V} | \Phi_{00}^{\varrho\sigma} \rangle \langle \Phi_{00}^{\varrho\sigma} | \hat{V} | \Phi_{0000}^{abcd} \rangle \langle \Phi_{0000}^{abcd} | \hat{V} | \Phi_{00}^{rs} \rangle \langle \Phi_{00}^{rs} | \hat{V} | \Phi \rangle}{(2\mu_0 - \mu_\varrho - \mu_\sigma)(4\mu_0 - \mu_a - \mu_b - \mu_c - \mu_d)(2\mu_0 - \mu_r - \mu_s)}, \tag{3.4}$$

from which the first and fourth factors in Eq. (3.4) we immediately recognise as

$$\frac{\langle \Phi | \hat{V} | \Phi_{00}^{rs} \rangle}{2\mu_0 - \mu_r - \mu_s} = t^{rs}. \quad (3.5)$$

With τ^{abcd} as well, the first term reduces to

$$\sum_{a \leq b \leq c \leq d} [\tau^{abcd}]^2. \quad (3.6)$$

Equation (3.1) may also be rewritten into the sum of a renormalisation term \mathcal{E}_R , representing the last three terms in Eq. (3.1), and the different contributions from excitations up to quadruple excitations in fourth order [16]. The single excitation term, \mathcal{E}_S , would then correspond to contributions from the first term in Eq. (3.1) containing $\langle \Phi_0^a | \hat{V} | \Phi_{00}^{rs} \rangle$, the double excitation term, \mathcal{E}_D , to contributions containing $\langle \Phi_{00}^{ab} | \hat{V} | \Phi_{00}^{rs} \rangle$, and similarly for the terms corresponding to triple and quadruple excitation, \mathcal{E}_T and \mathcal{E}_Q , respectively. The fourth-order correction then has the following form

$$\delta E_0^{(4)} = \mathcal{E}_R^{(4)} + \mathcal{E}_S^{(4)} + \mathcal{E}_D^{(4)} + \mathcal{E}_T^{(4)} + \mathcal{E}_Q^{(4)}. \quad (3.7)$$

This splitting is useful since it allows the different excitations to be considered separately, something that is also useful when implementing it in code. This was in fact utilised when the expressions were implemented in code. For the second and third factors in Eq. (3.4), we consider the multiple possibilities that arise from combinations of indices. We specifically choose to examine matrix elements involving transitions from double excitations to single excitations, for which the possible combinations will be described in more detail. All similarly derived expressions will only be presented in this section and not derived. More detailed steps are instead given in the Appendix. The first step is to write out the perturbation and replace it with the single- and double particle representations of the operators from Eqs. (2.13) and (2.15)

$$\begin{aligned} \langle \Phi_{0000}^{a000} | \hat{V} | \Phi_{00}^{rs} \rangle &= \langle \Phi_0^a | \hat{V} | \Phi_{00}^{rs} \rangle = \langle \Phi_0^a | \hat{V}_{\text{int}}^{\text{tot}} | \Phi_{00}^{rs} \rangle - \langle \Phi_0^a | \hat{U}_{\text{GP}} | \Phi_{00}^{rs} \rangle \\ &= \frac{1}{2} \sum_{j,k,l} \langle 0j | \hat{V}_{\text{int}} | kl \rangle \langle \Phi_0^a | \hat{a}_0^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k | \Phi_{00}^{rs} \rangle \\ &\quad \times (\delta_{j,a} \delta_{k,r} \delta_{l,s} + \delta_{j,0} \delta_{k,r} \delta_{l,0} + \delta_{j,0} \delta_{k,0} \delta_{l,s}) \\ &\quad - (N-1) \langle 00 || 0j \rangle \langle \Phi_0^a | \hat{a}_0^\dagger \hat{a}_j | \Phi_{00}^{rs} \rangle 2^{-\delta_{r,s}} (\delta_{j,r} \delta_{a,s} + \delta_{j,s} \delta_{a,r}). \end{aligned}$$

This sum will only give values when the variables take the values indicated by the Kronecker deltas. The Kronecker deltas are not needed since the other cases will cancel anyway. They are instead used to illustrate the different possibilities. The first of three possibilities we have for $\langle \Phi_0^a | \hat{a}_0^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k | \Phi_{00}^{rs} \rangle$ when going from a double excitation to a single excitation with the use of these four operators is to annihilate both of the excited particles, ϕ_r and ϕ_s , in the double-excitation state $|\Phi_{00}^{rs}\rangle$. We then need to create one particle in the single-particle ground state, ϕ_0 , and one in an excited state ϕ_a to reach $\langle \Phi_0^a |$. The other two possibilities are when we keep one of the excited particles, ϕ_r or

3. ANALYTICAL RESULTS

ϕ_s , and annihilate the other. We then also need to annihilate one of the particles in the ground state ϕ_0 . Finally, we need to create two particles in the ground state to be left with a single excited particle in either ϕ_r or ϕ_s , depending on which we annihilated. The possibilities for $\langle \Phi_0^a | \hat{a}_0^\dagger \hat{a}_j | \Phi_{00}^{rs} \rangle$ using the GP potential, can be identified in a similar way, though with only one creation operator and one annihilation operator. All of the possibilities then need to be written out explicitly and simplified

$$\begin{aligned} \langle \Phi_0^a | \hat{V} | \Phi_{00}^{rs} \rangle &= [\langle a0 \| rs \rangle + \langle a0 \| sr \rangle] \sqrt{N-1} (\sqrt{2})^{-\delta_{r,s}} \\ &\quad + (\langle 0r \| 00 \rangle^* \delta_{a,s} + \langle 0s \| 00 \rangle^* \delta_{a,r}) (\sqrt{2})^{-\delta_{r,s}} (N-2) \sqrt{N-1} \\ &\quad - (\langle 0r \| 00 \rangle^* \delta_{a,s} + \langle 0s \| 00 \rangle^* \delta_{a,r}) (\sqrt{2})^{-\delta_{r,s}} (N-1) \sqrt{N-1} \\ &= [\langle a0 \| rs \rangle + \langle a0 \| sr \rangle] \sqrt{N-1} (\sqrt{2})^{-\delta_{r,s}} \\ &\quad - (\langle 0r \| 00 \rangle^* \delta_{a,s} + \langle 0s \| 00 \rangle^* \delta_{a,r}) (\sqrt{2})^{-\delta_{r,s}} \sqrt{N-1}. \end{aligned} \quad (3.8)$$

Moving to the next case of double excitations, we get

$$\begin{aligned} \langle \Phi_{0000}^{ab00} | \hat{V} | \Phi_{00}^{rs} \rangle &= -\frac{1}{2} (N-1)(N-2) \langle 00 \| 00 \rangle + (N-3) [\langle 0r \| 0r \rangle + \langle 0s \| 0s \rangle] \\ &\quad + (N-3) [1 + (\sqrt{2}-1)(\delta_{a,r} + \delta_{r,s})] \langle 0a \| 0r \rangle \\ &\quad + \langle ab \| rs \rangle [2 + (\sqrt{2}-2)(\delta_{a,b} + \delta_{r,s}) + (3-2\sqrt{2})(\delta_{a,b}\delta_{r,s})]. \end{aligned} \quad (3.9)$$

The second to last case is that of triple excitations

$$\begin{aligned} \langle \Phi_{0000}^{abc0} | \hat{V} | \Phi_{00}^{rs} \rangle &= 2^{-\delta_{a,b}} [\langle ab \| 0r \rangle + \langle ab \| r0 \rangle] (\sqrt{2})^{\delta_{a,b}(1-\delta_{a,s})} (\sqrt{2})^{\delta_{a,s}(1-\delta_{a,b})} \\ &\quad \times (\sqrt{2})^{\delta_{b,s}(1-\delta_{a,b})} (\sqrt{6})^{\delta_{a,s}\delta_{a,b}} (\sqrt{2})^{\delta_{r,s}} \sqrt{N-2} \\ &\quad + 2^{-\delta_{a,b}} [\langle ab \| 0s \rangle + \langle ab \| s0 \rangle] (\sqrt{2})^{\delta_{a,b}(1-\delta_{a,r})} (\sqrt{2})^{\delta_{a,r}(1-\delta_{a,b})} \\ &\quad \times (\sqrt{2})^{\delta_{b,r}(1-\delta_{a,b})} (\sqrt{6})^{\delta_{a,r}\delta_{a,b}} (1-\delta_{r,s}) \sqrt{N-2} \\ &\quad - 2 \langle 0c \| 00 \rangle (\sqrt{2})^{\delta_{c,r}(1-\delta_{r,s})} (\sqrt{2})^{\delta_{c,s}(1-\delta_{r,s})} (\sqrt{3})^{\delta_{c,r}\delta_{r,s}} \sqrt{N-2}. \end{aligned} \quad (3.10)$$

Finally we consider the case of quadruple excitations

$$\begin{aligned} \langle \Phi_{0000}^{abcd} | \hat{V} | \Phi_{00}^{rs} \rangle &= 2^{-\delta_{a,b}} \langle ab \| 00 \rangle \sqrt{N-2} \sqrt{N-3} (\sqrt{2})^{\delta_{a,b}(1-\delta_{a,r})(1-\delta_{a,s})} \\ &\quad \times (\sqrt{2})^{(1-\delta_{a,b})(1-\delta_{a,s})\delta_{b,r}(1-\delta_{r,s})} (\sqrt{2})^{(1-\delta_{a,b})\delta_{a,s}(1-\delta_{b,r})(1-\delta_{r,s})} \\ &\quad \times (\sqrt{2})^{(1-\delta_{a,b})\delta_{a,r}(1-\delta_{b,s})(1-\delta_{r,s})} (\sqrt{2})^{(1-\delta_{a,b})(1-\delta_{a,r})\delta_{b,s}(1-\delta_{r,s})} \\ &\quad \times (\sqrt{3})^{(1-\delta_{a,b})\delta_{a,r}\delta_{r,s}} (\sqrt{3})^{(1-\delta_{a,b})\delta_{b,r}\delta_{r,s}} (\sqrt{6})^{\delta_{a,b}\delta_{a,r}(1-\delta_{r,s})} \\ &\quad \times (\sqrt{6})^{\delta_{a,b}\delta_{a,s}(1-\delta_{r,s})} 2^{\delta_{a,r}\delta_{b,s}(1-\delta_{a,b})} 2^{\delta_{a,s}\delta_{b,r}(1-\delta_{a,b})} (\sqrt{12})^{\delta_{a,b}\delta_{b,r}\delta_{r,s}}. \end{aligned} \quad (3.11)$$

With all matrix elements for RSPT derived, we move on to the second term in Eq. (3.1), which becomes

$$\delta E_0^{(2)} \sum_{r \leq s} \frac{|\langle \Phi | \hat{V} | \Phi_{00}^{rs} \rangle|^2}{(2\mu_0 - \mu_r - \mu_s)^2} = \delta E_0^{(2)} \sum_{r \leq s} \frac{|\langle \Phi | \hat{V}_{\text{int}}^{\text{tot}} - \hat{U}_{\text{GP}} | \Phi_{00}^{rs} \rangle|^2}{(2\mu_0 - \mu_r - \mu_s)^2}$$

$$= \delta E_0^{(2)} \sum_{r \leq s} [t^{rs}]^2. \quad (3.12)$$

The third term in Eq. (3.1) becomes

$$\begin{aligned} & 2\delta E_0^{(1)} \sum_{r \leq s} \sum_{\varrho \leq \sigma} \frac{\langle \Phi | \hat{V} | \Phi_{00}^{\varrho\sigma} \rangle \langle \Phi_{00}^{\varrho\sigma} | \hat{V} | \Phi_{00}^{rs} \rangle \langle \Phi_{00}^{rs} | \hat{V} | \Phi \rangle}{(2\mu_0 - \mu_\varrho - \mu_\sigma)(2\mu_0 - \mu_r - \mu_s)^2} \\ &= 2\delta E_0^{(1)} \sum_{r \leq s} \sum_{\varrho \leq \sigma} \frac{t^{\varrho\sigma} \langle \Phi_{00}^{\varrho\sigma} | \hat{V} | \Phi_{00}^{rs} \rangle t^{rs}}{(2\mu_0 - \mu_r - \mu_s)}. \end{aligned} \quad (3.13)$$

Finally, the fourth and last term in Eq. (3.1) becomes

$$\begin{aligned} & (\delta E_0^{(1)})^2 \sum_{r \leq s} \frac{|\langle \Phi | \hat{V} | \Phi_{00}^{rs} \rangle|^2}{(2\mu_0 - \mu_r - \mu_s)^3} = (\delta E_0^{(1)})^2 \sum_{r \leq s} \frac{|\langle \Phi | \hat{V}_{\text{int}}^{\text{tot}} - \hat{U}_{\text{GP}} | \Phi_{00}^{rs} \rangle|^2}{(2\mu_0 - \mu_r - \mu_s)^3} \\ &= (\delta E_0^{(1)})^2 \sum_{r \leq s} \frac{[t^{rs}]^2}{(2\mu_0 - \mu_r - \mu_s)}. \end{aligned} \quad (3.14)$$

In total, with the introduced factors, the fourth-order correction can be written as

$$\begin{aligned} \delta E_0^{(4)} &= \sum_{a \leq b \leq c \leq d} [\tau^{abcd}]^2 - \delta E_0^{(2)} \sum_{r \leq s} [t^{rs}]^2 - 2\delta E_0^{(1)} \sum_{r \leq s} \sum_{\varrho \leq \sigma} \frac{t^{\varrho\sigma} \langle \Phi_{00}^{\varrho\sigma} | \hat{V} | \Phi_{00}^{rs} \rangle t^{rs}}{(2\mu_0 - \mu_\varrho - \mu_\sigma)} \\ &+ (\delta E_0^{(1)})^2 \sum_{r \leq s} \frac{[t^{rs}]^2}{(2\mu_0 - \mu_r - \mu_s)}. \end{aligned} \quad (3.15)$$

We now give the first three orders of energy corrections using the same notation and the same factors

$$\delta E_0^{(1)} = -\frac{1}{2}N(N-1) \langle 00 || 00 \rangle, \quad (3.16)$$

$$\delta E_0^{(2)} = \sum_{r \leq s} (2\mu_0 - \mu_a - \mu_b) t^{rs}, \quad (3.17)$$

$$\delta E_0^{(3)} = \sum_{r \leq s, \varrho \leq \sigma} t^{rs} \langle \Phi_{00}^{rs} | \hat{V} | \Phi_{00}^{\varrho\sigma} \rangle t^{\varrho\sigma} + \frac{1}{2}N(N-1) \langle 00 || 00 \rangle \sum_{r \leq s} [t^{rs}]^2. \quad (3.18)$$

Finally, we note that when inserting contact interaction, the matrix elements are simply replaced with the integral of the form in Eq. (2.23) as

$$\langle ij | \hat{V} | kl \rangle \longrightarrow V_{ijkl}^{\text{cont}}. \quad (3.19)$$

3.2. Fourth-Order Epstein-Nesbet

Here, we look at the same unperturbed wave function as in the previous section. Hence, the unperturbed Hamiltonian $\hat{H}_0^{\text{EN}} = \sum_i |\Phi_i\rangle \langle \Phi_i| \hat{H} |\Phi_i\rangle \langle \Phi_i|$ is expressed in eigenstates $|\Phi_i\rangle$ to \hat{H}_{CP} . Important for ENPT is thus the occurrence of matrix elements $\langle \Phi_i| \hat{H} |\Phi_i\rangle$ between identical states in the zeroth order energy correction as well as in the denominators. Only one of the matrix elements between identical states appear in RSPT with the double excitation. As such, the rest of these expressions need to be derived. More detailed steps are given in the Appendix. Between ground states we get

$$\langle \Phi | \hat{V} | \Phi \rangle = -\frac{1}{2} N(N-1) \langle 00 || 00 \rangle. \quad (3.20)$$

For single excitation states we instead get

$$\langle \Phi_0^a | \hat{V} | \Phi_0^a \rangle = -\frac{1}{2} N(N-1) \langle 00 || 00 \rangle + (N-1) \langle 0a || 0a \rangle. \quad (3.21)$$

Between double excitation states yields

$$\begin{aligned} \langle \Phi_{00}^{ab} | \hat{V} | \Phi_{00}^{ab} \rangle &= -\frac{1}{2} (N+1)(N-2) \langle 00 || 00 \rangle + (N-3) [\langle 0a || 0a \rangle + \langle 0b || 0b \rangle] \\ &\quad + 2 \langle ab || ab \rangle 2^{-\delta_{a,b}}. \end{aligned} \quad (3.22)$$

Second to last is the case of triple excitation states which gives

$$\begin{aligned} \langle \Phi_{000}^{abc} | \hat{V} | \Phi_{000}^{abc} \rangle &= -\frac{1}{2} (N+2)(N-3) \langle 00 || 00 \rangle \\ &\quad + [\langle 0a || 0a \rangle + \langle 0b || 0b \rangle + \langle 0c || 0c \rangle] (N-5) \\ &\quad + 2 [\langle ab || ab \rangle 2^{-\delta_{a,b}} + \langle ac || ac \rangle 2^{-\delta_{a,c}} + \langle bc || bc \rangle 2^{-\delta_{b,c}}], \end{aligned} \quad (3.23)$$

and lastly between quadruple excitation states, giving

$$\begin{aligned} \langle \Phi_{0000}^{abcd} | \hat{V} | \Phi_{0000}^{abcd} \rangle &= -\frac{1}{2} (N+3)(N-4) \langle 00 || 00 \rangle \\ &\quad + [\langle 0a || 0a \rangle + \langle 0b || 0b \rangle + \langle 0c || 0c \rangle + \langle 0d || 0d \rangle] (N-7) \\ &\quad + 2 [\langle ab || ab \rangle 2^{-\delta_{a,b}} + \langle ac || ac \rangle 2^{-\delta_{a,c}} + \langle ad || ad \rangle 2^{-\delta_{a,d}} \\ &\quad + \langle bc || bc \rangle 2^{-\delta_{b,c}} + \langle bd || bd \rangle 2^{-\delta_{b,d}} + \langle cd || cd \rangle 2^{-\delta_{c,d}}]. \end{aligned} \quad (3.24)$$

4. Numerical Results

4.1. Quantum Ring System with Contact Interaction

The system chosen for the application of RSPT and ENPT is a quantum ring using contact interaction with the particle number set to $N = 6$. The Hamiltonian of a ring system with the inclusion of the contact interaction term is [32]

$$\hat{H} = \sum_{i=1}^N -\frac{\hbar^2}{2\tilde{m}R^2} \frac{\partial^2}{\partial x_i^2} + \sum_{i<j}^N \frac{1}{R} g \delta(x_i - x_j), \quad (4.1)$$

where \hbar is the reduced Planck constant, \tilde{m} is the mass, R is the radius and g is the interaction strength. We use a periodic boundary condition, with $x \in (0, 2\pi]$. If we extract $\hbar^2/\tilde{m}R^2$, we get

$$\hat{H} = \frac{\hbar^2}{\tilde{m}R^2} \left(\sum_{i=1}^N -\frac{1}{2} \frac{\partial^2}{\partial x_i^2} + \sum_{i<j}^N \frac{g\tilde{m}R}{\hbar^2} \delta(x_i - x_j) \right). \quad (4.2)$$

Let us now consider the MF solution. The occupied MF orbital ϕ_0 obeys the GP equation

$$\frac{\hbar^2}{\tilde{m}R^2} \left(-\frac{1}{2} \frac{\partial^2}{\partial x^2} + \lambda |\phi_0|^2 \right) |\phi_0\rangle = \mu_0 |\phi_0\rangle, \quad (4.3)$$

where $\lambda \equiv g(N-1)\tilde{m}R/\hbar^2$. This orbital can be retrieved in the following basis

$$\chi_m(x) = \frac{1}{\sqrt{2\pi}} e^{imx}, \quad (4.4)$$

where $m = m_\ell \in \mathbb{Z}$, which reduces to only the quantum number for orbital angular momentum since we are only considering spin 0 bosons with $m_s = 0$ in this system. In fact, we note that one solution of Eq. (4.3) is when $m = 0$, giving the constant function $\phi_0 = 1/\sqrt{2\pi}$. In general, to find the occupied MF orbital we solve Eq. (4.3) self-consistently. Diagonalising the MF Hamiltonian expressed in the χ basis then gives us the ground state and all excited states, where the latter satisfy

$$\frac{\hbar^2}{\tilde{m}R^2} \left(-\frac{1}{2} \frac{\partial^2}{\partial x^2} + \lambda |\phi_0|^2 \right) |\phi_i\rangle = \mu_i |\phi_i\rangle, \quad (4.5)$$

with $i > 0$. The matrix elements $\langle \phi_i \phi_j | \hat{V}_{\text{int}} | \phi_k \phi_l \rangle$ can then be written as a linear combination of $\langle \chi_i \chi_j | \hat{V}_{\text{int}} | \chi_k \chi_l \rangle$. For contact interaction, $\langle \chi_i \chi_j | \hat{V}_{\text{int}} | \chi_k \chi_l \rangle$ is known analytically to be $g/2\pi$ for $-m^{(i)} - m^{(j)} + m^{(k)} + m^{(l)} = 0$ and 0 otherwise. This property simplifies calculations considerably. When orbital angular momentum is a good quantum number, any term from RSPT or ENPT in which a single particle was moved is expected to be zero, since it would violate conservation of momentum. For example the term $\langle \Phi_0^a | \hat{V} | \Phi_{00}^{rs} \rangle$,

4. NUMERICAL RESULTS

given in Eq. (3.8), will always be zero as a consequence of this. We can also see that the first-order contribution given in Eq. (2.49) will be zero for ENPT since the matrix elements are diagonal. Since zeroth order ENPT is the same as the sum of the first two orders of RSPT if we compare Eqs. (2.49) and (2.50) with Eq. (2.59), the total first order corrections for RSPT and ENPT are the same. When the energies are calculated self-consistently, the extracted factor is omitted, meaning that the calculated energies are given in units of $\hbar^2/\tilde{m}R$.

4.1.1. Sweep of g

As a first analysis of the chosen system, we set the basis size to be $|m| \leq 10$, $m \in \mathbb{Z}$ and do a sweep of g from $g = -\hbar^2/\tilde{m}R$ to $g = \hbar^2/\tilde{m}R$. We denote the different orders of RSPT and ENPT as RSPT $\#$ and ENPT $\#$, $\#$ representing the order of the perturbation. The calculated fourth-order energies using RSPT as well as ENPT are shown in panel (a) of Fig. 1, along with the numerically exact energies from CI in the same basis. In panel (b), the relative error for different orders of RSPT and ENPT as compared to CI from $|(E_{PT} - E_{CI})/E_{CI}|$ is plotted, PT being any of the two methods.

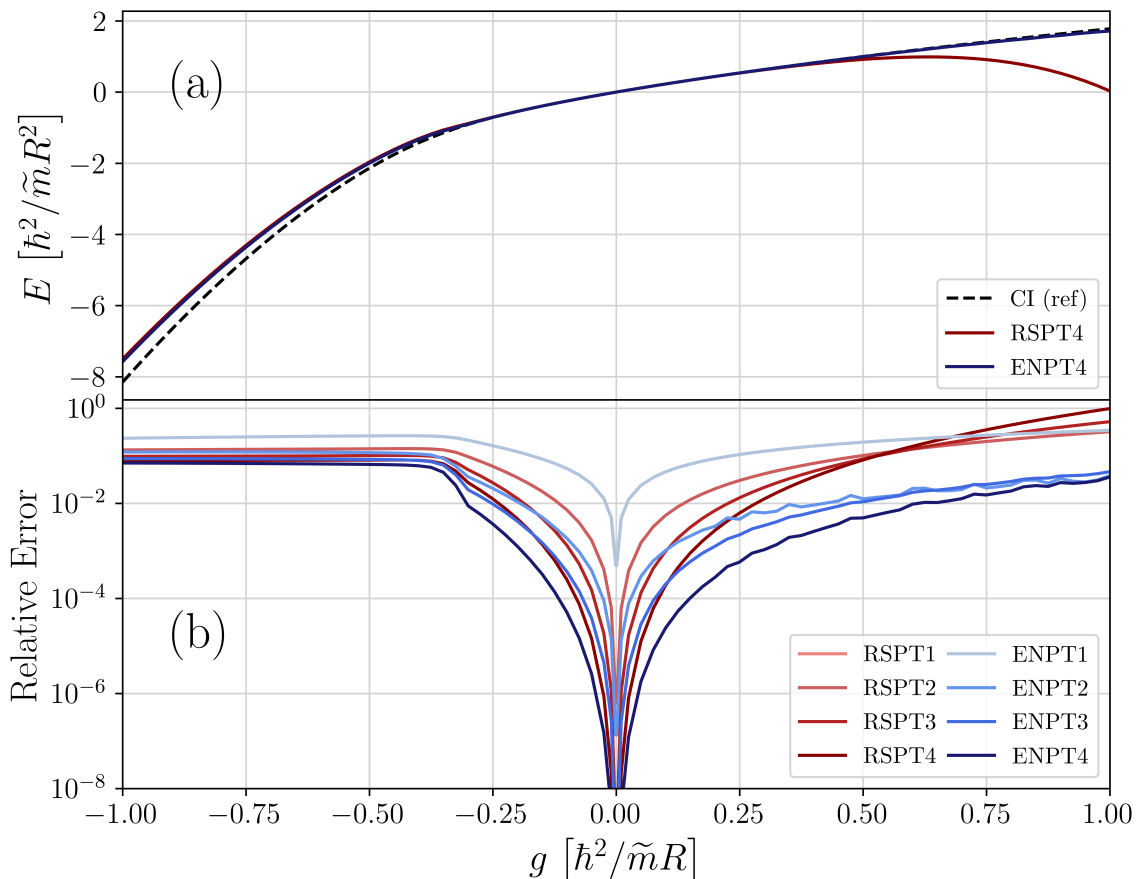


Figure 1: Panel (a) shows the calculated energies as a function of g of RSPT4 and ENPT4, using CI as a reference. (b) shows the relative error as a function of g of RSPT1, RSPT2, RSPT3 and RSPT4 as well as ENPT1, ENPT2, ENPT3 and ENPT4 as compared to the exact result of CI with a logarithmic scale for the relative error.

From the result in panel (a) of Fig. 1, we see that ENPT performs better than RSPT for all values of g , but especially for $g > 0.5\hbar^2/\tilde{m}R$. RSPT1 and ENPT1 overlap since the corrections are the same. That ENPT4 so closely follows CI is promising for further development of the method. The methods generally perform better with increasing order. The large deviation of RSPT4 for $g > 0.5\hbar^2/\tilde{m}R$ is not promising for its potential uses in this range, especially as it performs worse than lower orders of RSPT as can be seen in panel (b). This indicates that RSPT does not converge since the correction grows larger with increasing g , and that there is likely no use in going to higher orders in this range. Each order of ENPT seems to be smaller, suggesting that it converges. When we are going up to $g = \pm\hbar^2/\tilde{m}R$, we are in fact considering very high interaction strengths since the GP equation, given in Eq. (4.3), contains not just g , but λ . λ gives the relation of the interaction energy to the kinetic energy. In our case, using $N = 6$, this means that $\lambda = 2.5$ for $g = 0.5\hbar^2/\tilde{m}R$ and $\lambda = 5$ for $g = \hbar^2/\tilde{m}R$. The value $\lambda = 2.5$ is already quite large and the fact that the two models, but especially ENPT closer to $\lambda = 5$, show such good agreement with CI is promising. An overall similar behaviour is expected for other types of interactions besides contact interaction.

We also note from Fig. 1 that the ENPT corrections oscillate slightly for $g > 0$. This can be traced back to the degeneracy in the excited one-body orbitals ϕ when $\phi_0 = 1/\sqrt{2\pi}$. When there are degenerate states, the chosen basis is arbitrary in the manifold, unless explicitly specified. The expression in the denominators of the ENPT corrections, given in Eq. (2.60), have a basis dependence. Thus, when a random basis in the manifold is chosen by the program, the solution will differ slightly. In the expressions for RSPT, only chemical potentials appear, which do not depend on the chosen basis.

4.1.3. Comparison of Single Up to Quadruple Excitations

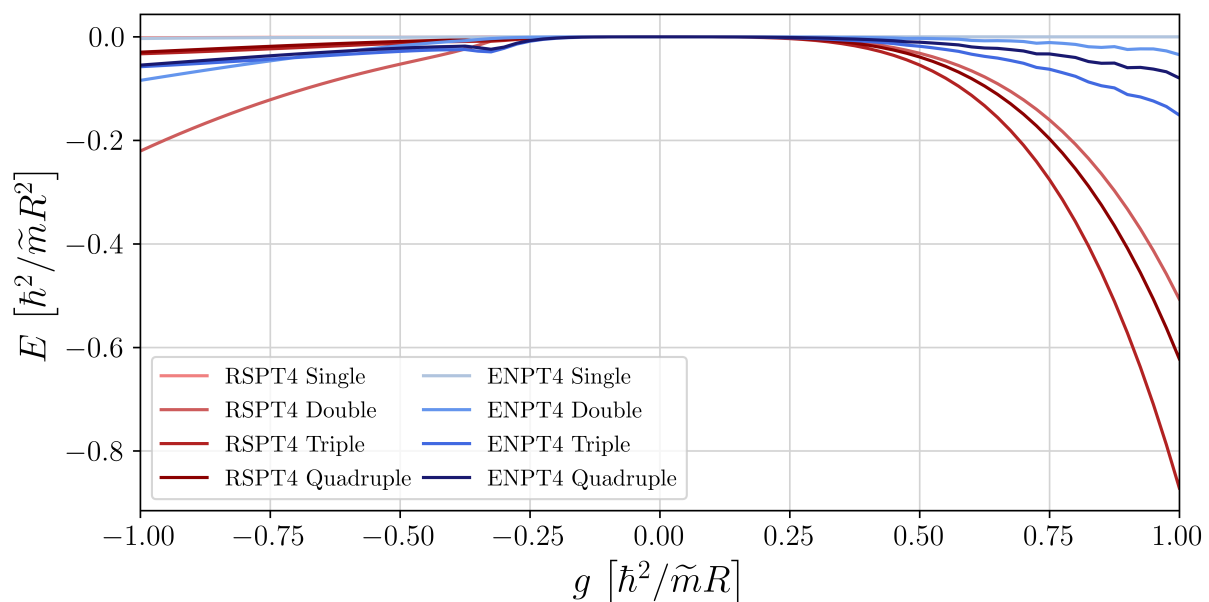


Figure 2: The plot shows the energy contributions in fourth order from single, double, triple and quadruple excitations for both RSPT and ENPT as a function of g .

4. NUMERICAL RESULTS

Next we would like to compare the fourth-order contributions in energy from single, double, triple and quadruple excitations with RSPT and ENPT for different interaction strengths g . This is shown in Fig. 2 above. We notice that the contributions for RSPT are larger in magnitude than for ENPT and contribute more to the total energy estimate shown in panel (a) of Fig 1. For $g > 0$, the contributions from triple excitations are the largest of the four contributions for both RSPT and ENPT. This suggests that we cannot so easily remove it, though Pople et al. excluded it for some systems in the case of fermions in one of their papers [16] as mentioned in Sec. 1.

4.1.2. Comparison of Basis Sizes

The two methods were studied for their dependence on the one-body basis size. The bases used were $|m| \leq 5$, $|m| \leq 10$, $|m| \leq 15$ and $|m| \leq 20$, giving sizes of 11, 21, 31 and 41 respectively. RSPT4, ENPT4 as well as first order from PT, PT1, since this is the same for both RSPT and ENPT as noted earlier, are calculated in terms of relative error as compared to CI and plotted against the different basis sizes using two values for g , $-0.5 \hbar^2/\tilde{m}R$ and $0.5 \hbar^2/\tilde{m}R$. This is shown in Fig 3.

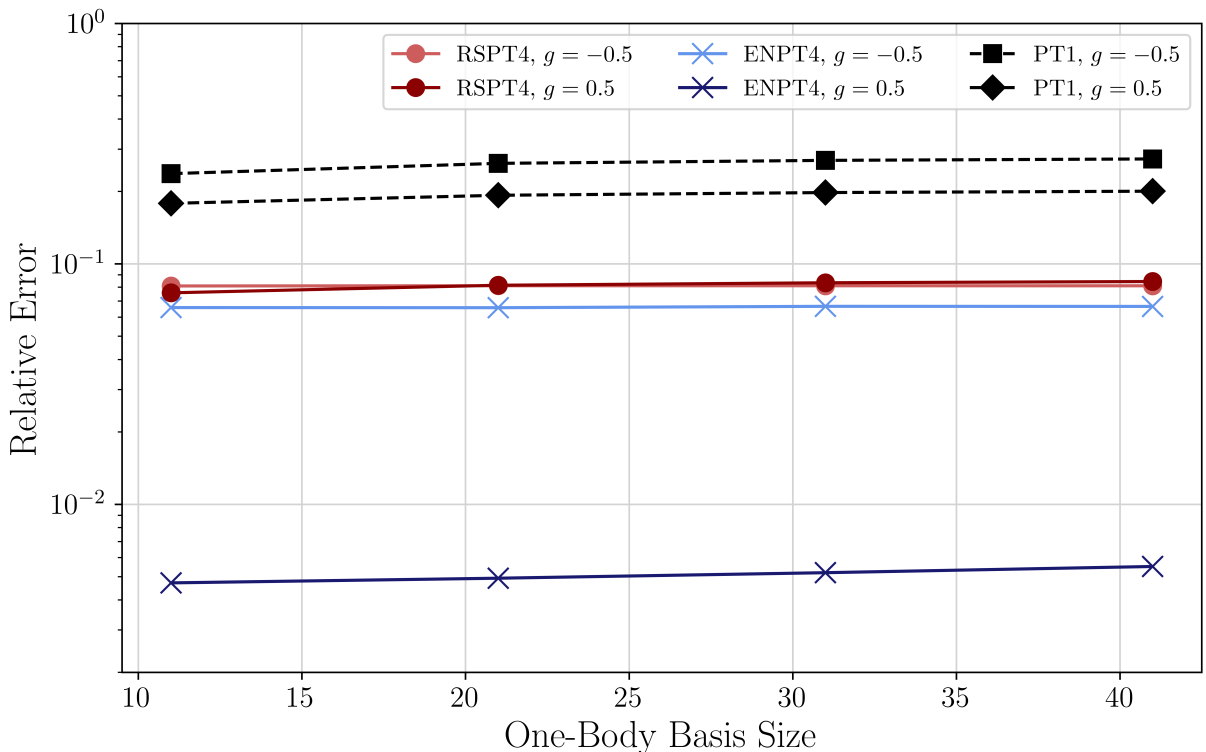


Figure 3: In the plot, the relative error of RSPT4, ENPT4 and PT1 as compared to CI are plotted against different basis sizes, for $g \pm 0.5$ in units of $\hbar^2/\tilde{m}R$.

RSPT4 and ENPT4 both display little dependence on the one-body basis size, meaning that the result in Fig. 1 would not change significantly if the basis size would have been increased.

5. Summary

The main result in this work is the derivation of expressions for the terms in fourth-order energy correction from two different perturbation methods, RSPT and ENPT, using the GP equation for a single-component BEC. To reduce the computational workload, we wrote these corrections in a manner suitable for implementation in numerical software. This was done both through the introduction of factors that could be calculated and then stored in the form of matrices early on, to then be able to retrieve the already calculated values from it. Another thing that was utilised was that the fourth-order expression can be split into five terms, of which four contain unique forms of matrix elements corresponding to contributions from single up to quadruple excitations. The general form of the GP equation was used for the derivations to facilitate different choices of particle interaction more easily.

The other result of this work is the computational implementation of the fourth-order correction and subsequent application to a one-dimensional quantum ring system with contact interaction for a particle count of $N = 6$. The one-component perturbative methods of RSPT and ENPT that were implemented computationally were then benchmarked against the numerically exact method of CI and both gave good agreement. Fourth order was also found to be an improvement over third order. For negative interaction strengths, the two methods performed very similar to each other, but with ENPT coming out ahead. For high interaction strengths, ENPT performed significantly better than RSPT and close to the result from CI. The results were also plotted as a function of the one-body basis size in terms of the relative error as compared to CI. This showed stable dependencies on the basis size for both methods that are almost constant.

6. Outlook

With the fourth-order expressions derived and analysis having been performed on a quantum ring system, the question of what research this might lead to in the future arises. The answer to this is that there are a great number of avenues that might be explored, some of which will be discussed below.

Having implemented the fourth-order correction for a one-component bosonic system, it is also possible to include other species of atoms with different intra- and inter-species interaction strengths. This allows for more possibilities, but builds upon the expressions that have already been derived. Also, this work only considered the simplest case of one dimension. Extensions of the work to two or three dimensions is another possible avenue to explore.

Fifth order and beyond seems perhaps to be the most natural extension of this work and fifth order would not be a big endeavour to derive. The only new thing that enters in the expression is the factor $\langle \Phi_{0000}^{abcd} | \hat{V}_{\text{GP}} | \Phi_{0000}^{\alpha\beta\chi\delta} \rangle$, which was partially derived between same states when deriving the denominators in ENPT. Sixth order would take a lot more effort due to the possibility to have six excited particles. This would introduce a lot of cases to be considered. The drawback of going to fifth order is the very large extra computational load. To get a better understanding of the physics, PT on the states could also be considered. This would require the derivation of the expressions for the wave functions in different orders.

The main use of MBPT is to systems with higher particle numbers. For low particle numbers, CI gives numerically exact solutions, and is thus the preferred option. CI cannot be used beyond a few particles however, since the computation time grows to be too large. MBPT is thus one possible option to describe systems containing more particles than it is feasible for CI to deal with. In this regime, comparisons to CI for benchmarking the accuracy is then not possible, and thus other methods will have to be applied, such as comparing third and fourth order for signs of convergence.

Beyond contact interaction, which was the interaction type considered in this thesis, other types of interaction could also be analysed. One example is the long-range dipolar interaction. Since the derived expressions in MBPT with GP was done with an interaction term that is general, the work is more easily extended to these other types of interaction. The choice of external potential greatly influences the behaviour of the system. A common choice of external potential is the harmonic oscillator (HO). An analytical solution also exists when using HO basis functions

The standard GP equation is chosen to optimise the ground state and not the virtual orbitals. Optimising these as well could result in better results, see for example [33] and

references therein. In using the general form of the GP equation, the GP potential within it is often used in a manner that ignores an exchange of particles. This exchange was included in this work, but the effect of including it or not is something that could be investigated.

Increasing the basis size very rapidly increases the time required to run the code. To set it in perspective, the basis size of 21 took in the order of a few minutes to run, whilst the basis size of 41 took many hours on a standard workstation running MATLAB. To make it more feasible to analyse larger bases, measures have to be taken. One solution with great potential is the implementation of arrays and factors that effectively store values to be reused such as in the work of Pople et al. [16]. Calculations would then not have to be repeated, which is one of the main contributors to the long run times. Such factors were used in this work with t^{rs} and τ^{abcd} , but even more sophisticated factors and arrays would be required for similar systems as well as more complex ones. One may also look at writing the program in such a way that many instances can run parallel to each other. This would reduce the effect of everything having to run sequentially.

Comparisons with other more sophisticated methods could also be tested. It could then help in implementing methods such as QCISD or Coupled Cluster [21]. Beyond potentially aiding in development of other methods, this would serve as a step towards modelling a higher number of particles in the intermediate particle-number regime and beyond, which is relatively unexplored territory as of yet. One could also modify the GP equation to include the LHY correction through extended GP. The work could then be used to analyse a self-bound correlated Bose-Einstein condensate that is stabilised by quantum fluctuations through this LHY correction. Such correlated Bose gases of larger particle numbers is unable to be treated with the method of CI due to the heavy computational load that is needed and could instead be analysed with MBPT using extended GP.

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As a final note, I would like to acknowledge Jim Klintrup and Simon Tropp for their work creating the cover page and their willingness to share it with me.

Appendix:

More Detailed Derivations

Here, more detailed steps are given for most of the derivations of the expressions appearing in fourth-order RSPT and ENPT.

RSPT

From a double excitation state to any other, we get

$$\begin{aligned}
\langle \Phi_{0000}^{ab00} | \hat{V} | \Phi_{00}^{rs} \rangle &= \langle \Phi_{00}^{ab} | \hat{V} | \Phi_{00}^{rs} \rangle = \langle \Phi_{00}^{ab} | \hat{V}_{\text{int}}^{\text{tot}} | \Phi_{00}^{rs} \rangle - \langle \Phi_{00}^{ab} | \hat{U}_{\text{GP}} | \Phi_{00}^{rs} \rangle \\
&= \frac{1}{2} \sum_{i,j,k,l} \langle ij | \hat{V}_{\text{int}} | kl \rangle \langle \Phi_{00}^{ab} | \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k | \Phi_{00}^{rs} \rangle \\
&\quad - \sum_{i,k} (N-1) \langle 0i || 0k \rangle \langle \Phi_{00}^{ab} | \hat{a}_i^\dagger \hat{a}_k | \Phi_{00}^{rs} \rangle \\
&= -\frac{1}{2} (N+1)(N-2) \langle 00 || 00 \rangle \\
&\quad + (N-3) [\langle 0r || 0r \rangle + \langle 0s || 0s \rangle] \\
&\quad + (N-3) [1 + (\sqrt{2}-1)(\delta_{a,r} + \delta_{r,s})] \langle 0a || 0r \rangle \\
&\quad + \langle ab || rs \rangle [2 + (\sqrt{2}-2)(\delta_{a,b} + \delta_{r,s}) + (3-2\sqrt{2})(\delta_{a,b}\delta_{r,s})], \quad (\text{A.1})
\end{aligned}$$

and from double to triple

$$\begin{aligned}
\langle \Phi_{0000}^{abc0} | \hat{V} | \Phi_{00}^{rs} \rangle &= \langle \Phi_{000}^{abc} | \hat{V} | \Phi_{00}^{rs} \rangle = \langle \Phi_{000}^{abc} | \hat{V}_{\text{int}}^{\text{tot}} | \Phi_{00}^{rs} \rangle - \langle \Phi_{000}^{abc} | \hat{U}_{\text{GP}} | \Phi_{00}^{rs} \rangle \\
&= \frac{1}{2} \sum_{i,j,l} \langle ij | \hat{V}_{\text{int}} | 0l \rangle \langle \Phi_{000}^{abc} | \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_0 | \Phi_{00}^{rs} \rangle \\
&\quad - \sum_i (N-1) \langle 0i || 00 \rangle \langle \Phi_{000}^{irs} | \hat{a}_i^\dagger \hat{a}_0 | \Phi_{00}^{rs} \rangle \\
&= \langle 0c || 00 \rangle (\sqrt{2})^{\delta_{c,r}(1-\delta_{r,s})} (\sqrt{2})^{\delta_{c,s}(1-\delta_{r,s})} (\sqrt{3})^{\delta_{c,r}\delta_{r,s}} (N-3) \sqrt{N-2} \\
&\quad + 2^{-\delta_{a,b}} [\langle ab || 0r \rangle + \langle ab || r0 \rangle] (\sqrt{2})^{\delta_{a,b}(1-\delta_{a,s})} (\sqrt{2})^{\delta_{a,s}(1-\delta_{a,b})} \\
&\quad \times (\sqrt{2})^{\delta_{b,s}(1-\delta_{a,b})} (\sqrt{6})^{\delta_{a,s}\delta_{a,b}} (\sqrt{2})^{\delta_{r,s}} \sqrt{N-2} \\
&\quad + 2^{-\delta_{a,b}} [\langle ab || 0s \rangle + \langle ab || s0 \rangle] (\sqrt{2})^{\delta_{a,b}(1-\delta_{a,r})} (\sqrt{2})^{\delta_{a,r}(1-\delta_{a,b})} \\
&\quad \times (\sqrt{2})^{\delta_{b,r}(1-\delta_{a,b})} (\sqrt{6})^{\delta_{a,r}\delta_{a,b}} (1-\delta_{r,s}) \sqrt{N-2} \\
&\quad - \langle 0c || 00 \rangle (\sqrt{2})^{\delta_{c,r}(1-\delta_{r,s})} (\sqrt{2})^{\delta_{c,s}(1-\delta_{r,s})} (\sqrt{3})^{\delta_{c,r}\delta_{r,s}} (N-1) \\
&\quad \times \sqrt{N-2} \\
&= 2^{-\delta_{a,b}} [\langle ab || 0r \rangle + \langle ab || r0 \rangle] (\sqrt{2})^{\delta_{a,b}(1-\delta_{a,s})} (\sqrt{2})^{\delta_{a,s}(1-\delta_{a,b})} \\
&\quad \times (\sqrt{2})^{\delta_{b,s}(1-\delta_{a,b})} (\sqrt{6})^{\delta_{a,s}\delta_{a,b}} (\sqrt{2})^{\delta_{r,s}} \sqrt{N-2}
\end{aligned}$$

APPENDIX:
MORE DETAILED DERIVATIONS

$$\begin{aligned}
& + 2^{-\delta_{a,b}} [\langle ab \parallel 0s \rangle + \langle ab \parallel s0 \rangle] (\sqrt{2})^{\delta_{a,b}(1-\delta_{a,r})} (\sqrt{2})^{\delta_{a,r}(1-\delta_{a,b})} \\
& \times (\sqrt{2})^{\delta_{b,r}(1-\delta_{a,b})} (\sqrt{6})^{\delta_{a,r}\delta_{a,b}} (1 - \delta_{r,s}) \sqrt{N-2} \\
& - 2 \langle 0c \parallel 00 \rangle (\sqrt{2})^{\delta_{c,r}(1-\delta_{r,s})} (\sqrt{2})^{\delta_{c,s}(1-\delta_{r,s})} (\sqrt{3})^{\delta_{c,r}\delta_{r,s}} \sqrt{N-2}. \quad (\text{A.2})
\end{aligned}$$

Lastly, from double to quadruple excitation states we get

$$\begin{aligned}
\langle \Phi_{0000}^{abcd} | \hat{V} | \Phi_{00}^{rs} \rangle & = \langle \Phi_{0000}^{abcd} | \hat{V}_{\text{int}}^{\text{tot}} | \Phi_{00}^{rs} \rangle - \langle \Phi_{0000}^{abcd} | \hat{U}_{\text{GP}} | \Phi_{00}^{rs} \rangle = \langle \Phi_{0000}^{abcd} | \hat{V}_{\text{int}}^{\text{tot}} | \Phi_{00}^{rs} \rangle \\
& = \frac{1}{2} \sum_{i,j} \langle ij | \hat{V}_{\text{int}} | 00 \rangle \langle \Phi_{0000}^{abrs} | \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_0 \hat{a}_0 | \Phi_{00}^{rs} \rangle \\
& = 2^{-\delta_{a,b}} \langle ab \parallel 00 \rangle \sqrt{N-2} \sqrt{N-3} (\sqrt{2})^{\delta_{a,b}(1-\delta_{a,r})(1-\delta_{a,s})} \\
& \quad \times (\sqrt{2})^{(1-\delta_{a,b})(1-\delta_{a,s})\delta_{b,r}(1-\delta_{r,s})} (\sqrt{2})^{(1-\delta_{a,b})\delta_{a,s}(1-\delta_{b,r})(1-\delta_{r,s})} \\
& \quad \times (\sqrt{2})^{(1-\delta_{a,b})\delta_{a,r}(1-\delta_{b,s})(1-\delta_{r,s})} (\sqrt{2})^{(1-\delta_{a,b})(1-\delta_{a,r})\delta_{b,s}(1-\delta_{r,s})} \\
& \quad \times (\sqrt{3})^{(1-\delta_{a,b})\delta_{a,r}\delta_{r,s}} (\sqrt{3})^{(1-\delta_{a,b})\delta_{b,r}\delta_{r,s}} (\sqrt{6})^{\delta_{a,b}\delta_{a,r}(1-\delta_{r,s})} \\
& \quad \times (\sqrt{6})^{\delta_{a,b}\delta_{a,s}(1-\delta_{r,s})} 2^{\delta_{a,r}\delta_{b,s}(1-\delta_{a,b})} 2^{\delta_{a,s}\delta_{b,r}(1-\delta_{a,b})} (\sqrt{12})^{\delta_{a,b}\delta_{b,r}\delta_{r,s}} \quad (\text{A.3})
\end{aligned}$$

ENPT

For the ground state we have

$$\begin{aligned}
\langle \Phi | \hat{V} | \Phi \rangle & = \langle \Phi | \hat{V}_{\text{int}}^{\text{tot}} | \Phi \rangle - \langle \Phi | \hat{U}_{\text{GP}} | \Phi \rangle \\
& = \frac{1}{2} \langle 00 \parallel 00 \rangle \langle \Phi | \hat{a}_0^\dagger \hat{a}_0^\dagger \hat{a}_0 \hat{a}_0 | \Phi \rangle - (N-1) \langle 00 \parallel 00 \rangle \langle \Phi | \hat{a}_0^\dagger \hat{a}_0 | \Phi \rangle \\
& = \frac{1}{2} \langle 00 \parallel 00 \rangle N(N-1) - \langle 00 \parallel 00 \rangle N(N-1) = -\frac{1}{2} N(N-1) \langle 00 \parallel 00 \rangle, \quad (\text{A.4})
\end{aligned}$$

between the same single excitation states

$$\begin{aligned}
\langle \Phi_0^a | \hat{V} | \Phi_0^a \rangle & = \langle \Phi_0^a | \hat{V}_{\text{int}}^{\text{tot}} | \Phi_0^a \rangle - \langle \Phi_0^a | \hat{U}_{\text{GP}} | \Phi_0^a \rangle \\
& = \sum_i \left[\frac{1}{2} \langle 0i | \hat{V}_{\text{int}} | 0i \rangle \langle \Phi_0^a | \hat{a}_i^\dagger \hat{a}_0^\dagger \hat{a}_i \hat{a}_0 | \Phi_0^a \rangle - (N-1) \langle 0i \parallel 0i \rangle \langle \Phi_0^a | \hat{a}_i^\dagger \hat{a}_i | \Phi_0^a \rangle \right] \\
& = \frac{1}{2} \langle 00 \parallel 00 \rangle (N-1)(N-2) + 2 \langle 0a \parallel 0a \rangle (N-1) \\
& \quad - \langle 00 \parallel 00 \rangle (N-1)^2 - (N-1) \langle 0a \parallel 0a \rangle \\
& = \langle 00 \parallel 00 \rangle (N-1) \left(\frac{1}{2} (N-2) - (N-1) \right) \\
& \quad + (N-1) \langle 0a \parallel 0a \rangle \\
& = -\frac{1}{2} N(N-1) \langle 00 \parallel 00 \rangle + (N-1) \langle 0a \parallel 0a \rangle, \quad (\text{A.5})
\end{aligned}$$

and between double

$$\langle \Phi_{00}^{ab} | \hat{V} | \Phi_{00}^{ab} \rangle = \langle \Phi_{00}^{ab} | \hat{V}_{\text{int}}^{\text{tot}} | \Phi_{00}^{ab} \rangle - \langle \Phi_{00}^{ab} | \hat{U}_{\text{GP}} | \Phi_{00}^{ab} \rangle$$

$$\begin{aligned}
&= \frac{1}{2} \sum_{i,j} \langle ij | \hat{V}_{\text{int}} | ij \rangle \langle \Phi_{00}^{ab} | \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_i \hat{a}_j | \Phi_{00}^{ab} \rangle \\
&\quad - \sum_i (N-1) \langle 0i | 0i \rangle \langle \Phi_{00}^{ab} | \hat{a}_i^\dagger \hat{a}_i | \Phi_{00}^{ab} \rangle \\
&= \frac{1}{2} \langle 00 | 00 \rangle (N-2)(N-3) \\
&\quad + 2^{-\delta_{a,b}} [2 \langle 0a | 0a \rangle (N-2) 2^{\delta_{a,b}} + 2 \langle 0b | 0b \rangle (N-2) 2^{\delta_{a,b}}] \\
&\quad + 2 \langle ab | ab \rangle 4^{-\delta_{a,b}} 2^{\delta_{a,b}} \\
&\quad - (N-1) \langle 00 | 00 \rangle (N-2) \\
&\quad + 2^{-\delta_{a,b}} [- (N-1) \langle 0a | 0a \rangle 2^{\delta_{a,b}} - (N-1) \langle 0b | 0b \rangle 2^{\delta_{a,b}}] \\
&= \langle 00 | 00 \rangle (N-2) \left(\frac{1}{2} (N-3) - (N-1) \right) \\
&\quad + [2(N-2) - (N-1)] (\langle 0a | 0a \rangle + \langle 0b | 0b \rangle) \\
&\quad + 2 \langle ab | ab \rangle 2^{-\delta_{a,b}} \\
&= -\frac{1}{2} (N+1)(N-2) \langle 00 | 00 \rangle + (N-3) [\langle 0a | 0a \rangle + \langle 0b | 0b \rangle] \\
&\quad + 2 \langle ab | ab \rangle 2^{-\delta_{a,b}}, \tag{A.6}
\end{aligned}$$

For a triple excitation state we get

$$\begin{aligned}
\langle \Phi_{000}^{abc} | \hat{V} | \Phi_{000}^{abc} \rangle &= \langle \Phi_{000}^{abc} | \hat{V}_{\text{int}}^{\text{tot}} | \Phi_{000}^{abc} \rangle - \langle \Phi_{000}^{abc} | \hat{U}_{\text{GP}} | \Phi_{000}^{abc} \rangle \\
&= \frac{1}{2} \sum_{i,j} \langle ij | \hat{V}_{\text{int}} | ij \rangle \langle \Phi_{000}^{abc} | \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_i \hat{a}_j | \Phi_{000}^{abc} \rangle \\
&\quad - \sum_i (N-1) \langle 0i | 0i \rangle \langle \Phi_{000}^{abc} | \hat{a}_i^\dagger \hat{a}_i | \Phi_{000}^{abc} \rangle \\
&= \frac{1}{2} \langle 00 | 00 \rangle (N-3)(N-4) \\
&\quad + 2 \langle 0a | 0a \rangle (N-3) + 2 \langle 0b | 0b \rangle (N-3) + 2 \langle 0c | 0c \rangle (N-3) \\
&\quad + 2^{\delta_{a,b} \delta_{a,c}} [4^{-\delta_{a,b}} 2 \langle ab | ab \rangle 2^{\delta_{a,b}(1-\delta_{a,c})} \\
&\quad + 4^{-\delta_{a,c}} 2 \langle ac | ac \rangle 2^{\delta_{a,c}(1-\delta_{a,b})} + 4^{-\delta_{b,c}} 2 \langle bc | bc \rangle 2^{\delta_{b,c}(1-\delta_{a,b})}] \\
&\quad - (N-1) \langle 00 | 00 \rangle (N-3) - (N-1) \langle 0a | 0a \rangle \\
&\quad - (N-1) \langle 0b | 0b \rangle - (N-1) \langle 0c | 0c \rangle \\
&= \langle 00 | 00 \rangle (N-3) \left(\frac{1}{2} (N-4) - (N-1) \right) \\
&\quad + (2(N-3) - (N-1)) [\langle 0a | 0a \rangle + \langle 0b | 0b \rangle + \langle 0c | 0c \rangle] \\
&\quad + 2 [\langle ab | ab \rangle 2^{-\delta_{a,b}} + \langle ac | ac \rangle 2^{-\delta_{a,c}} + \langle bc | bc \rangle 2^{-\delta_{b,c}}] \\
&= -\frac{1}{2} (N+2)(N-3) \langle 00 | 00 \rangle \\
&\quad + [\langle 0a | 0a \rangle + \langle 0b | 0b \rangle + \langle 0c | 0c \rangle] (N-5) \\
&\quad + 2 [\langle ab | ab \rangle 2^{-\delta_{a,b}} + \langle ac | ac \rangle 2^{-\delta_{a,c}} + \langle bc | bc \rangle 2^{-\delta_{b,c}}], \tag{A.7}
\end{aligned}$$

APPENDIX:
MORE DETAILED DERIVATIONS

and finally between the same quadruple excitation states we have

$$\begin{aligned}
\langle \Phi_{0000}^{abcd} | \hat{V} | \Phi_{0000}^{abcd} \rangle &= \langle \Phi_{0000}^{abcd} | \hat{V}_{\text{int}}^{\text{tot}} | \Phi_{0000}^{abcd} \rangle - \langle \Phi_{0000}^{abcd} | \hat{U}_{\text{GP}} | \Phi_{0000}^{abcd} \rangle \\
&= \frac{1}{2} \sum_{i,j} \langle ij | \hat{V}_{\text{int}} | ij \rangle \langle \Phi_{0000}^{abcd} | \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_i \hat{a}_j | \Phi_{0000}^{abcd} \rangle \\
&\quad - \sum_i (N-1) \langle 0i || 0i \rangle \langle \Phi_{0000}^{abcd} | \hat{a}_i^\dagger \hat{a}_i | \Phi_{0000}^{abcd} \rangle \\
&= \frac{1}{2} \langle 00 || 00 \rangle (N-4)(N-5) \\
&\quad + 2 \langle 0a || 0a \rangle (N-4) + 2 \langle 0b || 0b \rangle (N-4) \\
&\quad + 2 \langle 0c || 0c \rangle (N-4) + 2 \langle 0d || 0d \rangle (N-4) \\
&\quad + 2 [\langle ab || ab \rangle 2^{-\delta_{a,b}} + \langle ac || ac \rangle 2^{-\delta_{a,c}} + \langle ad || ad \rangle 2^{-\delta_{a,d}} \\
&\quad + \langle bc || bc \rangle 2^{-\delta_{b,c}} + \langle bd || bd \rangle 2^{-\delta_{b,d}} + \langle cd || cd \rangle 2^{-\delta_{c,d}}] \\
&\quad - (N-1) \langle 00 || 00 \rangle (N-4) \\
&\quad - (N-1) \langle 0a || 0a \rangle - (N-1) \langle 0b || 0b \rangle \\
&\quad - (N-1) \langle 0c || 0c \rangle - (N-1) \langle 0d || 0d \rangle \\
&= (N-4) \langle 00 || 00 \rangle \left(\frac{1}{2} (N-5) - (N-1) \right) \\
&\quad + (2(N-4) - (N-1)) [\langle 0a || 0a \rangle + \langle 0b || 0b \rangle + \langle 0c || 0c \rangle \\
&\quad + \langle 0d || 0d \rangle] \\
&\quad + 2 [\langle ab || ab \rangle 2^{-\delta_{a,b}} + \langle ac || ac \rangle 2^{-\delta_{a,c}} + \langle ad || ad \rangle 2^{-\delta_{a,d}} \\
&\quad + \langle bc || bc \rangle 2^{-\delta_{b,c}} + \langle bd || bd \rangle 2^{-\delta_{b,d}} + \langle cd || cd \rangle 2^{-\delta_{c,d}}] \\
&= -\frac{1}{2} (N+3)(N-4) \langle 00 || 00 \rangle \\
&\quad + [\langle 0a || 0a \rangle + \langle 0b || 0b \rangle + \langle 0c || 0c \rangle + \langle 0d || 0d \rangle] (N-7) \\
&\quad + 2 [\langle ab || ab \rangle 2^{-\delta_{a,b}} + \langle ac || ac \rangle 2^{-\delta_{a,c}} + \langle ad || ad \rangle 2^{-\delta_{a,d}} \\
&\quad + \langle bc || bc \rangle 2^{-\delta_{b,c}} + \langle bd || bd \rangle 2^{-\delta_{b,d}} + \langle cd || cd \rangle 2^{-\delta_{c,d}}]. \tag{A.8}
\end{aligned}$$

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