# Effective four- and higher-body interactions of neutral bosons in optical lattices

W F Flynn, P R Johnson

*Department of Physics*

*4400 Massachusetts Ave., NW*

*American University*

*Washington, DC 20016-8058*

(Dated: May 4, 2010)

## Abstract

It has been shown that pair-wise interactions of atoms confined in the lowest vibrational states of optical lattices generate effective three-body interactions. Experiment into the collapse and revival dynamics of coherent states loaded into optical lattices has suggested the existence of measurable effective higher-body interactions. We present a process with which to quantify the strength of the effective three-, four- and higher-body interactions by use of the Bose-Hubbard model of interacting bosons. Using Wick's Theorem and third-order perturbation theory, we give an estimate of the effective four-body interaction energy as well as insight to calculating a third-order correction to the effective three-body interaction energy presented in current literature [1]. Understanding lattice interaction dynamics may allow for better models of higher temperature superconducting materials as well as lending more insight to understanding the dynamics of Bose-Einstein condensates loaded into optical traps.

## INTRODUCTION

In the past two decades, researchers have developed two ground-breaking phenomena. First is the ability to cool groups of atoms to fractions of a Kelvin. Today, this serves many purposes, most notably making for better atomic clocks. However, an effect called Bose-Einstein condensation has been only recently been realized. When bosons are cooled, the statistics that govern them, Bose statistics, make it most probable for all the particles to occupy the same quantum state, thus acting like a single entity with a single wave function. Although predicted decades ago, these macroscopic quantum objects, make it possible to study quantum phenomena on micron-scales.

Secondly, a process has been formulated with which scientists can use to create regular arrays of potential wells using standing waves of laser light. These three-dimensional crystals of light are called optical lattices and can be used to store and control an array of ultracold atoms suspended in vacuum. Called optical lattices, these experimental setups can be used to hold thousands of very cold atoms in regular arrays. The light forms 3-dimensional wells that trap the particles, just how atoms trap their electrons in solids. Similarly, just as electrons can tunnel from atom to atom in a solid, atoms in an optical lattice can tunnel from light well to light well. Yet unlike a solid, scientists can tune most parameters of the optical lattice, such as change well depth, well shape, atom separation, and much more. They even allow scientists to image the interior of the lattice, something that is impossible given a traditional solid.

Combined, these two technologies have allowed for the development of many interesting studies and subfields. One such field is the study of condensate scattering. Two groups of ultra cold atoms are loaded into different optical lattices and are suddenly released as the optical lattice is turned off. The atom groups form condensates and will form interference patterns as they the superimpose with some phase. As the phase changes, the interference changes between constructive and destructive, which forms a collapse and revival of interference patterns [3]. Much of the research of this article pertains to current research of collapse and revival dynamics of Bose-Einstein condensate scattering.

### Motivation

A larger motivation for this research is to study many-body problems in quantum mechanics. The most exotic and unexplained phenomena in quantum physics manifests as the number of interacting bodies grows large. These systems are often highly complicated and require increasingly sophisticated models to lend understanding into the physics behind them.

One such many-body problem is the study of high-temperature superconductors. Although the theory of ordinary superconductors is well-understood, the mechanism behind high-temperature superconductivity is still unknown after over 30 years of study. Superconductivity is widely studied because electrical current flows through the material with zero resistance – a process which gives off little heat and allows for the production of extremely strong magnetic fields. If understood, it is hoped that high-temperature superconductors will facilitate the manufacture of room temperature superconductors, which could revolutionize modern industry and make feasible many new technologies.

A leading model of high-temperature superconductivity supposes that electrons in the solid quantum tunnel from atom to atom, allowing electrons to move through a solid purely probabilistically and thus encountering zero resistance. However, due to their like charge, electrons will likely be repelled from tunneling into site already occupied by one or more electrons. Thus interactions, e.g. the Coloumb interaction, between electrons at a single site inhibits the material's ability to superconduct. It is theorized that the complex dynamics of high-temperature superconductors relies on this trade off between quantum tunneling and electron interactions, one granting and the other inhibiting the ability to superconduct.

### Objective

To investigate the dynamics of the trade off between electron interactions and quantum tunneling, one must study both closely. To do this one can consider modeling a high-temperature superconductor with an optical lattice loaded with ultracold atoms. Instead of electrons, or a species of neutral fermions, it is easier to first consider the lattice loaded with neutral bosons – atoms with integer spin. Thus, we consider a system where the evolution of a quantum state of the atoms in the lattice involves competition between tunneling processes (atoms quantum tunneling between adjacent lattice sites) and atom-atom interactions when multiple atoms occupy the same lattice site.

Traditionally, the interactions between atoms are treated pair-wise, even when more than two atoms occupy the same site. However, it was recently shown that pair-wise interactions of atoms confined in the lowest energy states of optical lattice wells generate effective three-body interactions, and this prediction was quickly verified by experiments looking at the collapse and revival dynamics of coherent states. Surprisingly, however, those experiments also showed clear evidence of four (and higher) body interactions [2]. It is assumed the same process that gave effective three-body interactions also gives effective four-body interactions. Calculating the energy of effective four- and higher-body interactions will directly contribute to the better understanding of lattice interactions of multiple neutral bosons in a single lattice site, which could be generalized to Fermi statistics in order to describe electron interactions in solids.

## MODEL

To begin describing this system, some assumptions must be made. To make matter simpler, the bosons loaded into the lattice are assumed to be spinless, structureless, massive particles. The energy of the bosons is assumed to so low that all are bosons are assumed to be in the ground state, the lowest vibrational energy state. Additionally, the lattice well depth is assumed to be so large that bosons cannot excite to traditional higher energy states, even by way of interaction with other particles.

The most fundamental aspect describing each atom is its wave function, $\varphi_\alpha(\vec{r})$, which is a function of function of $\vec{r} = \vec{r}(r, \theta, \phi)$. The explicit formulation is given below

$$\varphi(\vec{r}) = \sum_a \phi_a(\vec{r})\hat{a}_a. \tag{1}$$

One can approximate the superposition of many wave functions of bosons in the lattice as a coherent state, number state or Fock state. The state

$$|N_1 N_2 \ldots N_n \ldots\rangle$$

describes a state with $N_1$ atoms in the ground state, $N_2$ atoms in the first excited state, and so forth. To manipulate a given number state, one can operate on a state using a creation or annihilation operator. The creation operator, $\hat{a}_n^\dagger$, creates an additional atom in state $n$ while the annihilation operator $\hat{a}_n$ destroys an atom in state $n$. Given the number state $|N\rangle$, with just $N$ atoms in the ground state $\phi_0$,

$$\begin{aligned}
\hat{a}_1^\dagger |N\rangle &= \sqrt{N+1}\, |N+1\rangle & (2)\\
\hat{a}_1 |N\rangle &= \sqrt{N-1}\, |N-1\rangle & (3)\\
\hat{a}_1^\dagger \hat{a}_1 |N\rangle &= \sqrt{N(N-1)}\, |N\rangle & (4)
\end{aligned}$$

To quantify the interaction energy between two atoms, the Bose-Hubbard Hamiltonian, $\hat{H}_2$, is used

$$\hat{H}_2 = \frac{U_2}{2} \int d^3r\, \varphi_a^\dagger(\vec{r})\varphi_b^\dagger(\vec{r})\varphi_c(\vec{r})\varphi_d(\vec{r}) = \frac{U_2}{2} \sum_{abcd} K_{abcd} \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_c \hat{a}_d. \tag{5}$$

Here, the function $K_{abcd}$ represents an integral of wave functions:

$$K_{abcd} = K_{0000}^{-1} \int d\vec{r}\, \phi_a \phi_b \phi_c \phi_d. \tag{6}$$

The operator $\hat{H}_2$ acting on $|N\rangle$ yields

$$\begin{aligned}
\hat{H}_2 |N\rangle &= \frac{U_2}{2} \sum_{abcd} K_{abcd} \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_c \hat{a}_d = \frac{U_2}{2} \sum_{ab} K_{ab00} \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_0 \hat{a}_0 \\
&= \frac{U_2}{2} \sum_{ab} K_{ab00} |\chi_{ab}\rangle
\end{aligned} \tag{7}$$

where $|\chi_{ab}\rangle$ is defined as

$$|\chi_{ab}\rangle = \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_0 \hat{a}_0 |N\rangle = N(N-1) \hat{a}_a^\dagger \hat{a}_b^\dagger |N-2\rangle\,. \tag{8}$$

Note that

$$\sum_{\alpha \neq 0} \frac{|\alpha\rangle \langle\alpha| \hat{H}_2 |N\rangle}{E_\alpha} = \frac{U_2}{2} \sum_{\alpha\neq 0} \sum_{ab} \frac{K_{abcd}}{E_\alpha} |\alpha\rangle \langle\alpha|\, \chi_{ab}\rangle = \frac{U_2}{2} \sum_{ab\neq 0} \frac{K_{ab00}}{E_{ab}} |\chi_{ab}\rangle \tag{9}$$

using the fact that, taking $|\alpha\rangle$ as a normalized Fock state, $|\alpha\rangle \langle\alpha|\, \chi_{ab}\rangle = |\chi_{ab}\rangle$, for the single state $|\alpha\rangle \propto |\chi_{ab}\rangle$, and $|\alpha\rangle \langle\alpha|\, \chi_{ab}\rangle = 0$ for the rest of the $|\alpha\rangle$. The notation $ab \neq 0$ means the sum over all $a, b$ except $a = b = 0$. Taking the adjoint gives

$$\sum_{\beta\neq 0} \frac{\langle N| \hat{H}_2 |\beta\rangle \langle\beta|}{E_\beta} = \frac{U_2}{2} \sum_{ab\neq 0} \frac{K_{00ab}}{E_{ab}} \langle\chi_{ab}|\,, \tag{10}$$

using the fact that $K_{ab00}^* = K_{00ab}$.

The Bose-Hubbard Hamiltonian only approximates the energy between interacting bosons for it only considers the energy of pairwise interactions. However, given any $N$ particles, there exists an intrinsic $N$-body interact which describes an interaction that cannot be explained by the superposition of pairwise interactions. One can imagine the $N$-body intrinsic interaction to occur when the wave functions of all $N$ particles overlap. Intrinsic interactions are the lowest-order approximation for interactions between $N$ particles. The use of Perturbation theory allows for more accurate, higher-order approximations of the interaction between $N$ bodies. To calculate the energy of an $N$-body interaction, these higher-order corrections for $N$ body interaction energy are simply added to the $N$-body intrinsic interaction energy, also know as the bare parameter interaction energy. Thus, the task becomes to calculate the interaction energy correction at higher-orders.

Additionally, higher-order perturbation allows nontrivial higher-body effective interactions to occur. Effective interaction are interactions that occur between "linked" pairwise interactions – pairwise interactions that are entangled via excitation of particles to forbidden excited states. The Heisenberg uncertainty principle can be written

$$\Delta E \delta t \geq \frac{\hbar}{2}, \tag{11}$$

stating that for small amounts of time, the energies of bosons in the lattice are uncertain. Therefore, despite not having enough energy to excite to higher vibrational states via collisions alone, bosons can excite to virtual excited states via collisions for these small amounts of time. However, for these atoms to de-excite, a collision must occur. If more than two bosons are present at a single lattice site, then it is possible for an atom to excite to and de-excite from a virtual state with interactions between two other, completely independent atoms. This is the basis for effective all interactions. It must be noted that in the long term, all particles must be in the ground state. This forces all effective interactions to end by recreating all atoms in the ground state. Higher-order effective interactions take place given sufficient atoms at a single lattice site and sufficiently high-order perturbation theory.

**PERTURBATION THEORY**

In order to quantify the four-body interaction energy, the analytic expression describing it must first be derived using perturbation theory. To begin, first and second-order perturbation is described. Let $E_m^{(n)}$ be the $n^{th}$-order correction to the $m$-body energy, so that

$$E_m = E_m^1 + E_m^2 + E_m^3 + \ldots = \frac{1}{m!} U_m N(N-1)\ldots(N-m+!), \tag{12}$$

where $U_m$ are the $m$-body "interaction" energies, and

$$U_m = Um^{(1)} + Um^{(2)} + Um^{(3)} + \ldots. \tag{13}$$

At a given order in perturbation theory, we can write

$$E^{(n)} = E_2^{(n)} + E_3^{(n)} + \ldots + E_{n+1}^{(n)}. \tag{14}$$

In general, $E_m^{(n)} = 0$ for $m > n+1$. In other words, at $n^{th}$-order, there will be only a maximum of $m = n+1$ body effective interactions.

### Feynman Diagrams

When discussing higher-order, multiparticle interactions, it is most efficient to use Feynman diagrams to describe specific interactions. This allows for distinctions to be made between interactions that share the same mathematical form. An example of a simple Feynman diagram is found below.

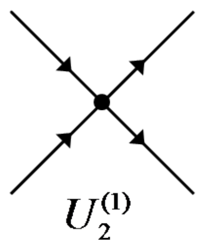


FIG. 1: Feynman Diagram representing an intrinsic two-body interaction.

The number of nodes in a given diagram represents the number of pairwise interactions in the effective interaction where $m = n$ pairwise interactions exist given $n^{th}$-order perturbation. Solid lines represent bosons in the ground state and dotted liens represent bosons in virtual states. Not all Feynman diagrams must be fully connected. Often given higher-order perturbation, many diagrams exist with a disconnected segment (see Figure 2).

In the following subsections, first-, second- and third- order perturbation theory is derivated, as are the applicable effective interaction energies for these orders.

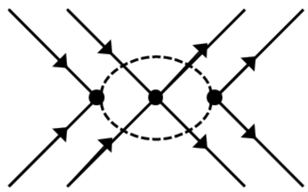

FIG. 2: A disconnected Feynman Diagram.

**Derivation of first-order interaction energy**

The first-order energy is

$$E^{(1)} = E_2^{(1)} = \left\langle N \left| \hat{H}_2 \right| N \right\rangle = \frac{1}{2} U_2 N(N-1), \tag{15}$$

with $N$ atoms in the ground state $\phi_0(\vec{r})$, and using $\left\langle N \left| \hat{a}_0^\dagger \hat{a}_0^\dagger \hat{a}_0 \hat{a}_0 \right| N \right\rangle = N(N-1)$. Therefore $U_2^{(1)} = U_2$, the bare parameter interaction energy.

**Derivation of second-order interaction energies**

If we set the ground state energy to zero, i.e. $E_0 = 0$, the second-order energy is given by

$$\begin{aligned} E^{(2)} &= -\sum_{\alpha \neq 0} \frac{\left\langle N \left| \hat{H}_2 \right| \alpha \right\rangle \left\langle \alpha \left| \hat{H}_2 \right| N \right\rangle}{E_\alpha} \\ &= -\left(\frac{U_2}{2}\right)^2 \sum_{ab} \sum cd \neq 0 \frac{K_{00ab} K_{cd00}}{E_{cd}} \left\langle \chi_{ab} \mid \chi_{cd} \right\rangle \end{aligned} \tag{16}$$

Note that the sum $\sum_{ab}$ is unrestricted. Using the definition

$$\begin{aligned} \left\langle \chi_{ab} \mid \chi_{cd} \right\rangle &= \left\langle N \left| \hat{a}_0^\dagger \hat{a}_0^\dagger \hat{a}_0 \hat{a}_0 \hat{a}_0^\dagger \hat{a}_0^\dagger \hat{a}_0 \hat{a}_0 \right| N \right\rangle \\ &= N(N-1) \left\langle N-2 \left| \hat{a}_0 \hat{a}_0 \hat{a}_c^\dagger \hat{a}_d^\dagger \right| N-2 \right\rangle, \end{aligned} \tag{17}$$

we have

$$E^{(2)} = -\left(\frac{U_2}{2}\right)^2 N(N-1) \sum_{ab} \sum_{cd \neq 0} \frac{K_{00ab} K_{cd00}}{E_{cd}} \left\langle \hat{a}_a \hat{a}_b \hat{a}_c^\dagger \hat{a}_d^\dagger \right\rangle. \tag{18}$$

where $\langle \ldots \rangle$ is shorthand for $\langle N-2 | \ldots | N-2 \rangle$.

In order to evaluate $\left\langle \hat{a}_a \hat{a}_b \hat{a}_c^\dagger \hat{a}_d^\dagger \right\rangle$, we can employ Wick's theorem to turn this into a counting exercise; we use contractions between operators to achieve a sum of normal ordered operators and commutation relations. Often these normal ordered terms give rise to numerical substitutions which drastically simplify the result. Thus, we evaluate $\left\langle \hat{a}_a \hat{a}_b \hat{a}_c^\dagger \hat{a}_d^\dagger \right\rangle$ using Wick's theorem, which gives

$$\begin{aligned}\left\langle \hat{a}_a \hat{a}_b \hat{a}_c^\dagger \hat{a}_d^\dagger \right\rangle = &\left\langle : \hat{a}_a \hat{a}_b \hat{a}_c^\dagger \hat{a}_d^\dagger : \right\rangle + \left\langle : \wick{\c1{\hat{a}}_a \hat{a}_b \c1{\hat{a}}_c^\dagger} \hat{a}_d^\dagger : \right\rangle + \left\langle : \wick{\c1{\hat{a}}_a \hat{a}_b \hat{a}_c^\dagger \c1{\hat{a}}_d^\dagger} : \right\rangle + \left\langle : \hat{a}_a \wick{\c1{\hat{a}}_b \c1{\hat{a}}_c^\dagger} \hat{a}_d^\dagger : \right\rangle \\ &+ \left\langle : \hat{a}_a \wick{\c1{\hat{a}}_b \hat{a}_c^\dagger \c1{\hat{a}}_d^\dagger} : \right\rangle + \left\langle : \wick{\c1{\hat{a}}_a \c2{\hat{a}}_b \c1{\hat{a}}_c^\dagger \c2{\hat{a}}_d^\dagger} : \right\rangle + \left\langle : \wick{\c1{\hat{a}}_a \c2{\hat{a}}_b \c2{\hat{a}}_c^\dagger \c1{\hat{a}}_d^\dagger} : \right\rangle .\end{aligned} \tag{19}$$

The double colons :: denote the normal ordering, which is when all annihilation operators are to the right of all creation operators in a product of creation and annihilation operators. The contractions give the Kronecker $\delta$ terms, e.g.,

$$\wick{\c1{\hat{a}}_b \c1{\hat{a}}_c^\dagger} = \delta_{ac}, \tag{20}$$

and all normal-ordered, uncontracted operators have indices set to zero since the initial and final state have all atoms in the $a = 0$ state. The term $\left\langle \hat{a}_0^\dagger \hat{a}_0^\dagger \hat{a}_0 \hat{a}_0 \right\rangle$ doest not appear, however, because of the restriction $c = d \neq 0$. The four single contractions $\left\langle : \wick{\c1{\hat{a}}_a \hat{a}_b \c1{\hat{a}}_c^\dagger} \hat{a}_d^\dagger : \right\rangle$ are all identical under the symmetries $a \longleftrightarrow b$ and $c \longleftrightarrow d$, and similarly the two double contractions are likewise identical.

Therefore,

$$\left\langle \hat{a}_a \hat{a}_b \hat{a}_c^\dagger \hat{a}_d^\dagger \right\rangle = 4 \left\langle \hat{a}_0^\dagger \hat{a}_0 \right\rangle \delta_{ac} + 2\delta_{ac}\delta_{bd}. \tag{21}$$

Using $\left\langle \hat{a}_0^\dagger \hat{a}_0 \right\rangle = \left\langle N-2 \left| \hat{a}_0^\dagger \hat{a}_0 \right| N-2 \right\rangle = N-2$, the second-order energy becomes

$$E^{(2)} = -\frac{1}{2!} U_2^2 N(N-1) \sum_{cd \neq 0} \frac{K_{00cd} K_{cd00}}{E_{cd}} - \frac{1}{3!} 6 U_2^2 N(N-1)(N-2) \sum_{a \neq 0} \frac{K_{000a} K_{a000}}{E_a} \tag{22}$$

and

$$U_2^{(2)} = -U_2^2 \sum_{cd \neq 0} \frac{K_{00cd} K_{cd00}}{E_{cd}} \tag{23}$$

$$U_3^{(2)} = -6 U_2^2 \sum_{a \neq 0} \frac{K_{000a} K_{a000}}{E_a} \tag{24}$$

### Derivation of third-order interaction energies

The formula for the third-order energy is

$$E^{(3)} = \sum_{\alpha \neq 0} \sum_{\beta \neq 0} \frac{\left\langle N \left| \hat{H}_2 \right| \alpha \right\rangle \left\langle \alpha \left| \hat{H}_2 \right| \beta \right\rangle \left\langle \beta \left| \hat{H}_2 \right| N \right\rangle}{E_\alpha E_\beta} - \left\langle N \left| \hat{H}_2 \right| N \right\rangle \sum_{\alpha \neq 0} \frac{\left\langle N \left| \hat{H}_2 \right| \alpha \right\rangle \left\langle \alpha \left| \hat{H}_2 \right| N \right\rangle}{E_\alpha^2}. \tag{25}$$

The right hand side (RHS) of the above expression has the effect of subtracting away from disconnected diagrams.

The left hand side (LHS) can be written as

$$E_{LHS}^{(3)} = \left( \sum_{\alpha \neq 0} \frac{\left\langle N \left| \hat{H}_2 \right| \alpha \right\rangle \langle \alpha |}{E_\alpha} \right) \hat{H}_2 \left( \sum_{\alpha \neq 0} \frac{| \beta \rangle \left\langle \beta \left| \hat{H}_2 \right| N \right\rangle}{E_\beta} \right) \tag{26}$$

Using our previous results and definition, and relabeling indices when helpful for clarity, gives

$$\begin{aligned} E_{LHS}^{(3)} &= \left( \frac{1}{2} U_2 \sum_{ab \neq 0} K_{00ab} \frac{\langle \chi_{ab} |}{E_{ab}} \right) \frac{1}{2} U_2 \sum_{cdef} K_{cdef} \hat{a}_c^\dagger \hat{a}_d^\dagger \hat{a}_e \hat{a}_f \left( \frac{1}{2} U_2 \sum_{gh \neq 0} K_{gh00} \frac{| \chi_{gh} \rangle}{E_{gh}} \right) \\ &= \left( \frac{U_2}{2} \right)^3 \sum_{ab \neq 0} \sum_{cdef} \sum_{gh} \frac{K_{00ab} K_{cdef} K_{gh00}}{E_{ab} E_{gh}} \langle \chi_{ab} | \, \hat{a}_c^\dagger \hat{a}_d^\dagger \hat{a}_e \hat{a}_f \, | \chi_{gh} \rangle \end{aligned} \tag{27}$$

Since

$$\langle \chi_{ab} | \, \hat{a}_c^\dagger \hat{a}_d^\dagger \hat{a}_e \hat{a}_f \, | \chi_{gh} \rangle = \langle N | \, \hat{a}_0^\dagger \hat{a}_0^\dagger \hat{a}_a \hat{a}_b \hat{a}_c^\dagger \hat{a}_d^\dagger \hat{a}_e \hat{a}_f \hat{a}_g^\dagger \hat{a}_h^\dagger \hat{a}_0 \hat{a}_0 \, | N \rangle = N(N-1) \left\langle \hat{a}_a \hat{a}_b \hat{a}_c^\dagger \hat{a}_d^\dagger \hat{a}_e \hat{a}_f \hat{a}_g^\dagger \hat{a}_h^\dagger \right\rangle , \tag{28}$$

and the shorthand $\langle \ldots \rangle = \langle N-2 | \ldots | N-2 \rangle$, we have that

$$E_{LHS}^{(3)} = \left( \frac{U_2}{2} \right)^3 N(N-1) \sum_{ab \neq 0} \sum_{cdef} \sum_{gf \neq 0} \frac{K_{00ab} K_{cdef} K_{gh00}}{E_{ab} E_{gh}} \left\langle \hat{a}_a \hat{a}_b \hat{a}_c^\dagger \hat{a}_d^\dagger \hat{a}_e \hat{a}_f \hat{a}_g^\dagger \hat{a}_h^\dagger \right\rangle \tag{29}$$

Using the first- and second-order results, we have the RHS

$$E_{RHS}^{(3)} = - \left( \frac{U_2}{2} \right)^3 N^2 (N-1)^2 \sum_{ab} \sum_{cd \neq 0} \frac{K_{00ab} K_{cd00}}{E_{cd}^2} \left\langle \hat{a}_a \hat{a}_b \hat{a}_c^\dagger \hat{a}_d^\dagger \right\rangle \tag{30}$$

*RHS terms*

We previously found that

$$\left\langle \hat{a}_a \hat{a}_b \hat{a}_c^\dagger \hat{a}_d^\dagger \right\rangle = 4(N-2)\delta_{ac} + 2\delta_{ac}\delta_{bd}, \tag{31}$$

using $\left\langle hata_0^\dagger \hat{a}_0 \right\rangle = N-2$, which gives

$$E_{RHS}^{(3)} = -\frac{U_2^3}{2} N^2 (N-1)^2 (N-2) \sum_{a \neq 0} \frac{K_{000a} K_{a000}}{E_a^2} - \frac{U_2^3}{4} N^2 (N-1)^2 \sum_{ab \neq 0} \frac{K_{00ab} K_{ab00}}{E_{ab}^2}. \tag{32}$$

To express this as separate $N$-body terms, we note that

$$N^2(N-1)^2(N-2) = N(N-1)(N-2)(N-3)(N-4) + 6N(N-1)(N-2)(N-3) + 6N(N-1)(N-2) \tag{33}$$

and

$$N^2(N-1)^2 = N(N-1)(N-2)(N-3) + 4N(N-1)(N-2) + 2N(N-1). \tag{34}$$

Therefore, the contribution to the five-body interaction energy is (after factoring out $N(N-1)(N-2)(N-3)(N-4)/5!$)

$$U^{(3)}_{RHS,5} = -60U_2^3 \sum_{a\neq 0} \frac{K_{000a}K_{a000}}{E_a^2}. \tag{35}$$

The contribution to the four-body interaction energy, after factoring out $N(N-1)(N-2)(N-3)/4!$, is

$$U^{(3)}_{RHS,4} = -72U_2^3 \sum_{a\neq 0} \frac{K_{000a}K_{a000}}{E_a^2} - 6U_2^3 \sum_{ab\neq 0} \frac{K_{00ab}K_{ab00}}{E_{ab}^2}. \tag{36}$$

The contribution to the three-body interaction energy, after factoring out $N(N-1)(N-2)/3!$, is

$$U^{(3)}_{RHS,3} = -18U_2^3 \sum_{a\neq 0} \frac{K_{000a}K_{a000}}{E_a^2} - 6U_2^3 \sum_{ab\neq 0} \frac{K_{00ab}K_{ab00}}{E_{ab}^2}. \tag{37}$$

The contribution to the two-body interaction energy, after factoring out $N(N-1)/2!$, is

$$U^{(3)}_{RHS,2} = -U_2^3 \sum_{ab\neq 0} \frac{K_{00ab}K_{ab00}}{E_{ab}^2}. \tag{38}$$

*Five-body interaction energy*

Apply Wick's Theorem to $\left\langle \hat{a}_a\hat{a}_b\hat{a}_c^\dagger\hat{a}_d^\dagger\hat{a}_e\hat{a}_f\hat{a}_g^\dagger\hat{a}_h^\dagger \right\rangle$, we obtain two, three, four and five-body terms. The six-body term corresponding to $\left\langle : \hat{a}_a\hat{a}_b\hat{a}_c^\dagger\hat{a}_d^\dagger\hat{a}_e\hat{a}_f\hat{a}_g^\dagger\hat{a}_h^\dagger : \right\rangle$ with no contractions vanishes because of the restriction of $a = b \neq 0$ and $g = h \neq 0$. Five-body terms are generated by a single contraction. However, the restrictions $a = b \neq 0$ and $g = h \neq 0$ imply that either $a$ or $b$ must be contracted with either $g$ or $h$. Therefore, the five-body term is given by

$$\left\langle : \hat{a}_a \hat{a}_b \hat{a}_c^\dagger \hat{a}_d^\dagger \hat{a}_e \hat{a}_f \hat{a}_g^\dagger \, \hat{a}_h^\dagger : \right\rangle = \left\langle 4\hat{a}_0^3 \right\rangle \delta_{ag} = 4(N-2)(N-3)(N-4)\delta_{ag}, \tag{39}$$

with $b = c = d = e = f = h = 0$, and the factor of 4 from the four equivalent contractions. This gives

$$E^{(3)}_{LHS,5} = 4\left(\frac{U_2}{2}\right)^3 N(N-1)(N-2)(N-3)(N-4)\sum_{a\neq 0}\frac{K_{000a}K_{a000}}{E_a^2} \tag{40}$$

using $K_{0000} = 1$. Factoring out $N(N-1)(N-2)(N-3)(N-4)/5!$, we obtain

$$U^{(3)}_{LHS,5} = 60U_2^3 \sum_{a\neq 0}\frac{K_{000a}K_{a000}}{E_a^2}. \tag{41}$$

Adding the LHS and the RHS contributions gives

$$U^{(3)}_{LHS,5} + U^{(3)}_{RHS,5} = 60U_2^3 \sum_{a\neq 0}\frac{K_{000a}K_{a000}}{E_a^2} - 60U_2^3 \sum_{a\neq 0}\frac{K_{000a}K_{a000}}{E_a^2} = 0 \tag{42}$$

*Four-body interaction energy*

Four-body terms are generated by double contractions of $\left\langle \hat{a}_a \hat{a}_b \hat{a}_c^\dagger \hat{a}_d^\dagger \hat{a}_e \hat{a}_f \hat{a}_g^\dagger \hat{a}_h^\dagger \right\rangle$. Because of the restriction $a = b \neq 0$ and $g = h \neq 0$, either $a$ or $b$ and also either $g$ or $h$ must be contracted. This gives the following terms:

$$\begin{aligned} \left\langle \hat{a}_a \hat{a}_b \hat{a}_c^\dagger \hat{a}_d^\dagger \hat{a}_e \hat{a}_f \hat{a}_g^\dagger \hat{a}_h^\dagger \right\rangle &= 8\left\langle : \hat{a}_a \, \hat{a}_b \hat{a}_c^\dagger \hat{a}_d^\dagger \hat{a}_e \hat{a}_f \hat{a}_g^\dagger \, \hat{a}_h^\dagger : \right\rangle + 8\left\langle : \hat{a}_a \hat{a}_b \hat{a}_c^\dagger \hat{a}_d^\dagger \hat{a}_e \hat{a}_f \hat{a}_g^\dagger \, \hat{a}_h^\dagger : \right\rangle \\ &+ 2\left\langle : \hat{a}_a \, \hat{a}_b \hat{a}_c^\dagger \hat{a}_d^\dagger \hat{a}_e \hat{a}_f \hat{a}_g^\dagger \, \hat{a}_h^\dagger : \right\rangle + 16\left\langle : \hat{a}_a \, \hat{a}_b \hat{a}_c^\dagger \, \hat{a}_d^\dagger \hat{a}_e \, \hat{a}_f \hat{a}_g^\dagger \, \hat{a}_h^\dagger : \right\rangle \\ &= (8\delta_{ac}\delta_{bg} + 8\delta_{ac}\delta_{eh} + 2\delta_{ah}\delta_{bg} + 16\delta_{bc}\delta_{fg}(N-2)(N-3), \end{aligned} \tag{43}$$

where the factors 8,8,2, and 16 are the number of equivalent contractions and $\left\langle \hat{a}_0^{\dagger 2}\hat{a}_0^2 \right\rangle = (N-2)(N-3)$. Inserting Kronecker deltas for the contractions, setting all other indicies to zero, and dividing by $N(N-1)(N-2)(N-3)/4!$ gives

$$\begin{aligned} U^{(3)}_{LHS,4} &= 24U_2^3 \sum_{a,b\neq 0}\frac{K_{00ab}K_{a000}K_{b000}}{E_{ab}E_b} + 24U_2^3 \sum_{a,b\neq 0}\frac{K_{000a}K_{000b}K_{ab00}}{E_a E_{ab}} \\ &+ 6U_2^3 \sum_{ab\neq 0}\frac{K_{00ab}K_{0000}K_{ab00}}{E_{ab}^2} + 48U_2^3 \sum_{a,b\neq 0}\frac{K_{000a}K_{a00b}K_{b000}}{E_a E_b}. \end{aligned} \tag{44}$$

The first two terms are equal. Meanwhile,

$$U_{RHS,4}^{(3)} = -72 U_2^{(3)} \sum_{a\neq 0} \frac{K_{000a} K_{0000} K_{a000}}{E_a^2} - 6 U_2^3 \sum_{ab\neq 0} \frac{K_{00ab} K_{0000} K_{ab00}}{E_{ab}^2}. \tag{45}$$

Adding the LHS and RHS gives

$$U_4^{(3)} = 48 U_2^3 \sum_{a,b\neq 0} \frac{K_{00ab} K_{a000} K_{b000}}{E_{ab} E_b} + 48 U_2^3 \sum_{a,b\neq 0} \frac{K_{000a} K_{a00b} K_{b000}}{E_a E_b} - 72 U_2^3 \sum_{a\neq 0} \frac{K_{000a} K_{0000} K_{a000}}{E_a^2}. \tag{46}$$

*Three-body interaction energy*

Three-body terms are generated by triple contractions of $\left\langle \hat{a}_a \hat{a}_b \hat{a}_c^\dagger \hat{a}_d^\dagger \hat{a}_e \hat{a}_f \hat{a}_g^\dagger \hat{a}_h^\dagger \right\rangle$. This gives the following terms:

$$\begin{aligned} \left\langle \hat{a}_a \hat{a}_b \hat{a}_c^\dagger \hat{a}_d^\dagger \hat{a}_e \hat{a}_f \hat{a}_g^\dagger \hat{a}_h^\dagger \right\rangle &= 8 \left\langle : \hat{a}_a\, \hat{a}_b \hat{a}_c^\dagger\, \hat{a}_d^\dagger\, \hat{a}_e\, \hat{a}_f \hat{a}_g^\dagger\, \hat{a}_h^\dagger : \right\rangle + 8 \left\langle : \hat{a}_a \hat{a}_b \hat{a}_c^\dagger\, \hat{a}_d^\dagger\, \hat{a}_e\, \hat{a}_f \hat{a}_g^\dagger\, \hat{a}_h^\dagger : \right\rangle \\ &+ 16 \left\langle : \hat{a}_a\, \hat{a}_b \hat{a}_c^\dagger\, \hat{a}_d^\dagger \hat{a}_e\, \hat{a}_f \hat{a}_g^\dagger\, \hat{a}_h^\dagger : \right\rangle . \end{aligned} \tag{47}$$

Using $\left\langle \hat{a}_0^\dagger \hat{a}_0 \right\rangle = N-2$, and dividing by $N(N-1)(N-2)/3!$ gives

$$\begin{aligned} U_{LHS,3}^{(3)} &= 6 U_2^3 \sum_{ab\neq 0} \sum_{c\neq 0} \frac{K_{00ab} K_{ba0c} K_{c000}}{E_{ab} E_c} + 6 U_2^3 \sum_{a\neq 0} \sum_{bc\neq 0} \frac{K_{00a0} K_{a0bc} K_{bc00}}{E_a E_{bc}} \\ &+ 12 U_2^3 \sum_{ab\neq 0} \sum_{c\neq 0} \frac{K_{00ab} K_{b00c} K_{ca00}}{E_{ab} E_{ca}} \end{aligned} \tag{48}$$

Using $\left\langle \hat{a}_0^\dagger \hat{a}_0 \right\rangle = N-2$, and dividing by $N(N-1)(N-2)/3!$ gives

$$U_{RHS,3}^{(3)} = -18 U_2^3 \sum_{a\neq 0} \frac{K_{000a} K_{0000} K_{a000}}{E_a^2} - 6 U_2^3 \sum_{ab\neq 0} \frac{K_{00ab} K_{0000} K_{ab00}}{E_{ab}^2} \tag{49}$$

These are produced by triple contractions of $\left\langle \hat{a}_a \hat{a}_b \hat{a}_c^\dagger \hat{a}_d^\dagger \hat{a}_e \hat{a}_f \hat{a}_g^\dagger \hat{a}_h^\dagger \right\rangle$ and these contractions give rise rise to three types of terms:

$$\begin{aligned} \left\langle \hat{a}_a \hat{a}_b \hat{a}_c^\dagger \hat{a}_d^\dagger \hat{a}_e \hat{a}_f \hat{a}_g^\dagger \hat{a}_h^\dagger \right\rangle &\to \frac{1}{2} \times 4 \times \left\langle : \hat{a}_f \hat{a}_h^\dagger : \right\rangle \left( \hat{a}_a \dot{\hat{a}}_c^\dagger \right) \left( \hat{a}_b \dot{\hat{a}}_d^\dagger \right) \left( \hat{a}_e \dot{\hat{a}}_g^\dagger \right) \\ &+ \frac{1}{2} \times 4 \times \left\langle : \hat{a}_b \hat{a}_d^\dagger : \right\rangle \left( \hat{a}_e \dot{\hat{a}}_g^\dagger \right) \left( \hat{a}_f \dot{\hat{a}}_h^\dagger \right) \left( \hat{a}_a \dot{\hat{a}}_c^\dagger \right) \\ &+ \frac{1}{2} \times 4 \times \left\langle : \hat{a}_d^\dagger \hat{a}_f : \right\rangle \left( \hat{a}_a \dot{\hat{a}}_c^\dagger \right) \left( \hat{a}_e \dot{\hat{a}}_g^\dagger \right) \left( \hat{a}_b \dot{\hat{a}}_h^\dagger \right) \\ &\to 2 \left\langle \hat{a}_h^\dagger \hat{a}_f \right\rangle \delta_{ac} \delta_{bd} \delta_{eg} + 2 \left\langle \hat{a}_d^\dagger \hat{a}_b \right\rangle \delta_{ef} \delta_{fg} \delta_{ac} + 2 \left\langle \hat{a}_d^\dagger \hat{a}_f \right\rangle \delta_{ac} \delta_{eg} \delta_{bh}. \end{aligned} \tag{50}$$

They are all proportional to $(U_2/2)^3 N(N-1)\left\langle \hat{a}_0^\dagger \hat{a}_0 \right\rangle = (U_2/2)^3 N(N-1)(N-2)$, and so we can write

$$E_3^{(3)} = \frac{1}{6}\delta U_3^{(3)} N(N-1)(N-2), \tag{51}$$

with

$$\delta U_3^{(3)} = \delta U_{3,1}^{(3)} + \delta U_{3,2}^{(3)} + \delta U_{3,3}^{(3)}, \tag{52}$$

and

$$\delta U_{3,1}^{(3)} = \frac{3U_2^3}{4} \times 2 \sum_{ab\neq 0} \sum_{c\neq 0} \frac{K_{00ab} K_{abc0} K_{c000}}{E_{ab} E_c} \tag{53}$$

$$\delta U_{3,2}^{(3)} = \frac{3U_2^3}{4} \times 2 \sum_{a\neq 0} \sum_{bc\neq 0} \frac{K_{000a} K_{a0bc} K_{bc00}}{E_a E_{bc}} \tag{54}$$

$$\delta U_{3,3}^{(3)} = \frac{3U_2^3}{4} \times 8 \sum_{ab\neq 0} \sum_{cb\neq 0} \frac{K_{00ab} K_{a0c0} K_{bc00}}{E_{ab} E_{bc}} \tag{55}$$

*Two-body energy*

These are produced by quadruple contractions of $\left\langle \hat{a}_a \hat{a}_b \hat{a}_c^\dagger \hat{a}_d^\dagger \hat{a}_e \hat{a}_f \hat{a}_g^\dagger \hat{a}_h^\dagger \right\rangle$. There are four equivalent terms to yield

$$\left\langle \hat{a}_a \hat{a}_b \hat{a}_c^\dagger \hat{a}_d^\dagger \hat{a}_e \hat{a}_f \hat{a}_g^\dagger \hat{a}_h^\dagger \right\rangle \to 4\delta_{ac}\delta_{bd}\delta_{eg}\delta_{fh} \tag{56}$$

giving

$$E_2^{(3)} = 4 \times \left(\frac{U_2}{2}\right)^3 N(N-1) \sum_{ab\neq 0} \sum_{ef\neq 0} \frac{K_{00ab} K_{abcf} K_{ef00}}{E_{ab} E_{ef}}. \tag{57}$$

## DERIVATION OF FOUR-BODY INTERACTION ENERGY

In order to find an analytic form describing the 4-body effective interaction energy, we must simplify the terms given in Equation 46 in the previous section. There we are given

$$U_4^{(3)} = 48U_2^3 \sum_{a,b\neq 0} \frac{K_{00ab} K_{a000} K_{b000}}{E_{ab} E_b} + 48U_2^3 \sum_{a,b\neq 0} \frac{K_{000a} K_{a00b} K_{b000}}{E_a E_b} - 72U_2^3 \sum_{a\neq 0} \frac{K_{000a} K_{0000} K_{a000}}{E_a^2}. \tag{58}$$

It is apparent that before these sums be evaluated, the quantity $K_{abcd}$ should be calculated. To achieve this, recall

$$K_{nm} = \int d^3x \varphi_{n00}(\vec{r})\, \varphi_{m00}(\vec{r})\, \varphi_{000}(\vec{r})\, \varphi_{000}(\vec{r}) \tag{59}$$

where

$$\varphi_{nlm}\left(\vec{r}\right) = N_{nl} r^l e^{-r^2/2} L_n^{l+1/2}\left(r^2\right) Y_{lm}\left(\theta, \phi\right). \tag{60}$$

Here, $L_n^\alpha(X)$ is the generalized Laguerre polynomial of degree $n$ and $Y_{lm}(\theta, \phi)$ represent the spherical harmonics. The constants $N_{nl}$ are given by

$$N_{nl} = \sqrt{\frac{2^{2n+2l+2} n!(n+l)!}{(2n+2l+1)!}} \tag{61}$$

Notice that $Y_0^0(\theta, \phi) = \frac{1}{2\sqrt{\pi}}$, $L_0^\alpha(r^2) = 1$ and $N_{00} = 2$. This reveals that $\varphi(\vec{r}) = \pi^{-3/4} e^{-x^2/2}$. Given these facts, we convert $K_{mn}$ to spherical coordinates and simplify

$$K_{nm} = \int d\phi d\theta dr \frac{4}{16\pi^3} N_{n0} N_{m0} r^2 \sin\theta e^{-2r^2} L_n^{1/2}\left(r^2\right) L_m^{1/2}\left(r^2\right) \tag{62}$$

We can integrate to with respect to $\theta$ and $\phi$:

$$\begin{aligned} K_{nm} &= \frac{N_{n0} N_{m0}}{4\pi^3} \int_0^{2\pi} d\phi \int_0^\pi d\theta \sin\theta \int_0^\infty dr\ r^2 e^{-2r^2} L_n^{1/2}\left(r^2\right) L_m^{1/2}\left(r^2\right) \\ &= \frac{N_{n0} N_{m0}}{\pi^2} \int_0^\infty dr r^2 e^{-2r^2} L_n^{1/2}\left(r^2\right) L_m^{1/2}\left(r^2\right) \end{aligned} \tag{63}$$

To integrate the Laguerre polynomials, we will use their complex formulation, where $L_n^\alpha(z) = \frac{1}{2\pi i} \oint_\gamma dt \frac{1}{(1-t)^{\alpha+1} t^{n+1}} e^{-zt/(1-t)}$, where $\gamma$ is some contour in the complex plane. Thus

$$\begin{aligned} K_{nm} &= \frac{N_{n0} N_{m0}}{\pi^2} \int_0^\infty dr\ r^2 e^{-2r^2} \left( \frac{1}{2\pi i} \oint_{\gamma_1} dt \frac{1}{(1-t)^{3/2} t^{n+1}} e^{-r^2 t/(1-t)} \right) \\ &\times \left( \frac{1}{2\pi i} \oint_{\gamma_2} dT \frac{1}{(1-T)^{3/2} T^{m+1}} e^{-r^2 T/(1-T)} \right) \\ &= \frac{N_{n0} N_{m0}}{\pi^2} \left( \frac{1}{2\pi i} \right)^2 \oint_{\gamma_1} dt \oint_{\gamma_2} dT \frac{1}{(1-t)^{3/2}(1-T)^{3/2}} \frac{1}{t^{n+1} T^{m+1}} \\ &\times \int_0^\infty dr\ r^2 e^{-2r^2} e^{-r^2 t/(1-t)} e^{-r^2 T/(1-T)} \end{aligned} \tag{64}$$

Take $\gamma_1 : |t| < 1$ and $\gamma_2 : |T| < |t| < 1$. Then, we have

$$\int_0^\infty dr\ r^2 e^{-2r^2} e^{-r^2 t/(1-t)} e^{-r^2 T/(1-T)} = \frac{\pi^{1/2}}{4} \frac{(t-1)^3/2(T-1)^{3/2}}{(2-t-T)^3/2}. \tag{65}$$

Using this, we have

$$\begin{aligned} K_{nm} &= \frac{N_{n0} N_{m0}}{\pi^{3/2}} \left( \frac{1}{2\pi i} \right)^2 \oint_{\gamma_1} dt \oint_{\gamma_2} dT \frac{1}{(1-t)^{3/2}(1-T)^{3/2}} \frac{1}{t^{n+1} T^{m+1}} \\ &\times \frac{\pi^{1/2}}{4} \frac{(t-1)^3/2(T-1)^{3/2}}{(2-t-T)^3/2}. \end{aligned} \tag{66}$$

To compute the contour integrals, the Cauchy Residue Theorem is used. Recall, given a function $f$ with discontinuity $z_0$,

$$f^{(n)}(z_0) = \frac{n!}{2\pi i}\oint_\gamma \frac{f(z)dz}{(z-z_0)^{n+1}} \tag{67}$$

where $f^{(n)}$ denotes the $n$-th derivative of $f$. Our paths $\gamma_1$ and $\gamma_2$ only contain a single discontinuity each, at $t = T = 0$. Therefore,

$$\frac{1}{2\pi i}\oint_{gamma_2} \frac{(2-t-T)^{-3/2}}{(T-0)^{m+1}} = \frac{1}{m!}\left.(2-t-T)^{-3/2}\right|_{T=0} = \frac{2}{(2-t)^{3/2+m}}\frac{\Gamma(m+3/2)}{\sqrt{(\pi)}m!} \tag{68}$$

Moving on to the second contour integral, we have

$$\frac{1}{2\pi i}\oint_{gamma_1} \frac{(2-t)^{-3/2-m}}{(t-0)^{n+1}} = \frac{1}{n!}\left.(2-t)^{-3/2-m}\right|_{t=0} = \frac{1}{2^{3/2+m+n}}\frac{\Gamma(m+n+3/2)}{n!\,\Gamma(m+3/2)} \tag{69}$$

Combining these two results, we have have

$$K_{nm} = \frac{N_{n0}N_{m0}}{m!\,n!\,\pi^2}\frac{\Gamma(m+n+3/2)}{2^{5/2+m+n}} \tag{70}$$

However, there exist some relationships between gamma functions and factorials, which can be used to manipulate the formula for $K_{nm}$ into a form more easily comparable to related results in the literature.

$$\begin{aligned}
K_{nm} &= \frac{N_{n0}N_{m0}}{m!\,n!\,\pi^2}\frac{\Gamma(m+n+3/2)}{2^{3/2+m+n}} \\
&= \sqrt{\frac{2^{2n+2}(n!)^2}{(2n+1)!}}\sqrt{\frac{2^{2m+2}(m!)^2}{(2m+1)!}}\frac{\sqrt{2}}{2^{m+n+2}2\pi^2 m!\,n!}\Gamma(m+n+3/2) \\
&= \frac{2^{n+1}n!}{\sqrt{(2n+1)!}}\frac{2^{m+1}m!}{\sqrt{(2m+1)!}}\frac{\sqrt{2}}{2^{m+n+2}2\pi^2 m!\,n!}\frac{(2n+2m+1)!!\sqrt{\pi}}{2^{n+m+1}} \\
&= \frac{1}{(2\pi)^{3/2}}\frac{(2n+2m+1)!!}{2^n 2^m\sqrt{(2n+1)!(2m+1)!}}
\end{aligned} \tag{71}$$

## ESTIMATE OF EFFECTIVE FOUR-BODY INTERACTION ENERGY

Using the results from Equations 46 and 71, it is now possible to evaluate $U_4^{(3)}$. We have that

$$U_4^{(3)} = 48U_2^3\sum_{a,b\neq 0}\frac{K_{00ab}K_{a000}K_{b000}}{E_{ab}E_b} + 48U_2^3\sum_{a,b\neq 0}\frac{K_{000a}K_{a00b}K_{b000}}{E_aE_b} - 72U_2^3\sum_{a\neq 0}\frac{K_{000a}K_{0000}K_{a000}}{E_a^2}. \tag{72}$$

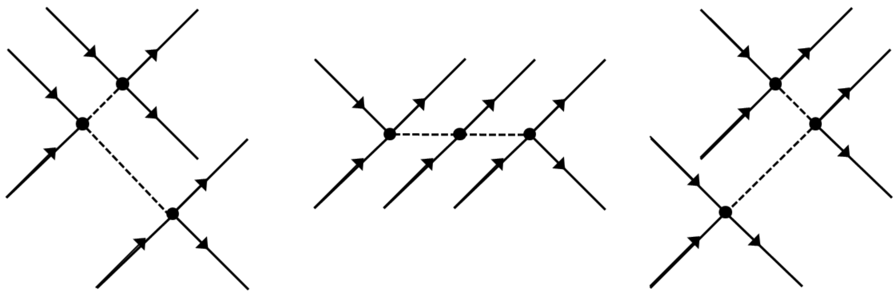

FIG. 3: Four-body Feynman Diagrams.

where the $K_{abcd}$ are given above in Eq 71. The first two terms can be described in terms of the following Feynman diagrams. Using Wolfram Mathematica, preliminary estimates for two of the sums have been calculated.

$$\sum_{a,b\neq 0} \frac{K_{00ab}K_{a000}K_{b000}}{E_{ab}E_b} \approx 0.144138 \tag{73}$$

$$\sum_{a,b\neq 0} \frac{K_{000a}K_{a00b}K_{b000}}{E_a E_b} \approx 0.0968428 \tag{74}$$

$$\tag{75}$$

Using these results, an estimate for $U_4^{(3)}$ has been determined:

$$U_4^{(3)} = 48U_2^3(0.144138) + 48U_2^3(0.0968428) - 72U_2^3 \sum_{a\neq 0} \frac{K_{000a}K_{0000}K_{a000}}{E_a^2} = 11.5671U_2^3 - 72U_2^3 \sum_{a\neq 0} \frac{K_{000a}K_{000}}{E_a^2} \tag{76}$$

## INSIGHT INTO THREE-BODY CORRECTION AT THIRD-ORDER

It has been realized that the third-order perturbations allow interactions like that show in Figure 4 to exist.

Up to this point, because each virtual states must excite from and de-excite to the ground state, all wave function had zero angular momentum, i.e., $l = m = 0$, due to conservation of angular momentum. But this third-order, effective three-body interaction allows for all excited states to have some angular momentum associated with it. At the first pairwise interaction, one excited state may take the form $\hat{a}_{nlm}$ but the other other excited state exiting that interaction must then take the form $\hat{a}_{nl-m}$ due to conservation of angular momentum. At the intermediate interaction, the exiting excited state must have the same

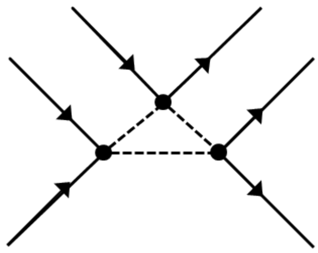

FIG. 4: Three-body correction Feynman Diagram.

angular momentum as the incoming excited state. This ensures that angular momentum is conserved. A similar procedure can be followed to calculate this energy correction; like the four-body correction, it involves evaluating the terms $K_{abcd}$. However, these terms are complicated by the addition of $l$ and $m$:

$$K_{n\nu} = \int d\phi d\theta dr \frac{N_{nl} N_{\nu l}}{\pi} r^{2l} \sin\theta e^{-2r^2} L_n^{l+1/2}\left(r^2\right) L_\nu^{l+1/2}\left(r^2\right) Y_{lm}\left(\theta,\phi\right) Y_{l-m}\left(\theta,\phi\right) \tag{77}$$

## CONCLUSION

The work presented in this article displays a framework with which to calculate the four-body and higher-body effective interactions as to more accurately represent the interaction energy of interacting neutral bosons in optical lattices. The methods employed were used due to the ability to be generalized to calculate higher-body effects. The current results can be used to better describe the collapse and revival mechanics of scattering of Bose-Einstein condensates.

This work, however, represents a preliminary venture into a project where there is much more to be researched. More rigorous estimates of the four-body correction must be calculated and compared to work presented by Bloch [2], as well as the third-order three-body correction evaluated. One could then attempt to calculate the five- and six-body corrections using fourth- and fifth-order perturbation theory. These results should similarly be compared to experimental results. Lastly, the Bose-Hubbard Hamiltonian may be replaced by one that accounts for tunneling – only then can a robust model of high temperature superconductors be achieved.

[1] Johnson P R, et al, 2009 New J. Phys. 11 093022

[2] Bloch I 2008 Nature 453 1016

[3] Bloch I, Dalibard J and Zwerger W 2008 Rev. Mod. Phys. 80 885