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A Study Of Cold Atoms In Optical Lattices Using The Bose-Hubbard Model With Local Three-Body Interactions

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Abstract*—A study of cold atoms in optical lattices has offered a powerful platform for exploring quantum many-body systems, particularly through the Bose-Hubbard Model (BHM). While the conventional BHM has been instrumental in describing the superfluid to Mott-insulator transition in systems with two-body interactions, it falls short in addressing the effects of local three-body interactions at zero temperature especially for polar molecules with long-range dipolar forces. This study aims to determine the thermodynamic properties of polar molecules in optical lattices using a modified Bose-Hubbard Model that includes local three-body interactions. The model Hamiltonian was constructed in the second quantization formalism and diagonalized using Fourier transformation. Thermodynamic quantities such as internal energy, specific heat capacity, and the Sommerfield were derived. Computational analysis and graphing were carried out using Mathcad software. The results reveal that the inclusion of three-body interactions significantly alters the energy spectrum and phase boundaries of the system. A quantum phase transition between the Mott-insulator and superfluid phases was identified, with a critical transition temperature estimated at 5.2 K. Notably, the specific heat peaked near the transition, indicating a second-order phase transition. The Sommerfeld coefficient also showed fermionic contributions near the Fermi surface, highlighting the interplay between bosons and fermions in the lattice. These findings offer new insights into strongly correlated bosonic systems and have promising applications in high-temperature superconductivity, magnetic heterostructures, quantum information processing, and the development of nano electronic devices such as field-effect transistors, switches, and memory units. This work contributes to a deeper understanding of thermodynamic behavior in quantum lattice systems and opens new avenues for theoretical and experimental investigations.

Keywords—Polar Molecules, Optical Lattices, Bose Hubbard Model, Superfluid-Mott Insulator Transition, Transition Temperature, Superfluidity.

Introduction

An optical lattice is a periodic potential which is formed by overlapping of two counter-propagating laser beams. Because of the interference of the counter-propagating laser beams an optical standing wave with wavelength $\frac{\lambda}{2}$ is created therefore, neutral atoms can be trapped via the Stark shift (Petrucciani, T. (2023). A two-dimensional periodic potential can be created by overlapping two optical standing waves in orthogonal direction while a three-dimensional lattice potential is formed by overlapping three orthogonal standing waves with different wavelengths where there is no cross interference between laser beams waves. They provide ideal loss-free potential in which Ultracold atoms may move and interact with one another (Grimme *et al*.,2000, Windpassinger *et al.*,2013*)* making it easy to observe and study them. The energy of an atom's internal states during interaction with an electromagnetic wave depends on the intensity of the light. Therefore, a spatially dependent intensity generates a spatially dependent potential energy. When such modulation is achieved through the interference of several laser beams, the resulting optical potential experienced by the atoms will feature distinct potential wells separated by a distance approximately equal to the laser wavelength. In experiments, the depths of these optical potential wells can reach the micro-Kelvin range. Despite this, atoms can be trapped in these potentials when cooled to low temperatures using laser and evaporative cooling techniques. Ultracold atoms interacting with a spatially modulated optical potential are quite similar to electrons in the ion-lattice potential of solid crystals (Sachdeva, R., 2013). However, optical lattices offer several advantages over solid-state systems. They can be made to be largely free from defects; such defects for example prevented the observation of Bloch oscillations in crystalline solids.

During the transition from insulating to metallic properties, the relationship between potential energy (P.E) and kinetic energy (K.E) plays a crucial role. Electrons become localized when P.E exceeds K.E, and they become delocalized, entering a superfluid state, when K.E surpasses P.E. Near zero temperature, the science governed by the Bose-Hubbard Hamiltonian can be

categorized into two distinct regimes (interaction dominated and kinetic energy dominated regimes). In the interaction-dominated regime, where the hopping parameter J is significantly smaller than the interaction energy U, the system is in the Mott insulator phase. Advances in quantum simulation techniques have made it possible to emulate complex many-body systems using ultracold atoms and molecules in optical lattices. These systems serve as quantum analog simulators, enabling the study of Hamiltonians that are otherwise analytically intractable or numerically intensive (Tarruell & Sanchez-Palencia, 2018). Thermodynamic properties such as internal energy, entropy, specific heat, and the partition function are crucial for understanding the equilibrium and non-equilibrium behavior of these quantum systems. Studies by Horace Kibe *et al*. (2017) and Ayodo (2008) emphasized the role of these properties in characterizing phase transitions and energy distributions in fermion-boson mixtures. Despite these advancements, there remains a lack of comprehensive studies focusing on the thermodynamic behavior of polar molecules under three-body interactions at zero temperature.

Methodology

The standard Bose-Hubbard Model (BHM) for 1s electrons in a tight binding lattice which allows electrons to hop between nearest neighbors is given by.

$$H = -t\Sigma_{(ij)\sigma}\, C^{+}{}_{i}C_{j} + hc + \Sigma_{i}(\varepsilon_{i} - \mu)C^{+}{}_{i}C_{j} + \Sigma_{ijk}\frac{W_{ijk}}{6}n_{i}n_{j}n_{k} \quad (1.0)$$

Where ‹*i, j*› counts nearest neighbor pairs once. In the following discussion the on-site energy ε_i will be assumed to be the same on all sites. μ is the chemical potential included to fix the particle number as in Grand Canonical Ensemble.

This Hamilton in (1) can be diagonalized by Fourier transformation from position space to momentum space by using creation and annihilation operators.

The Fourier transforms for creation and annihilation operators.

$$\partial^{+}_{k\sigma} = \frac{1}{\sqrt{m}}\sum_j e^{ikr_j}c^{+}_{j\sigma} \quad (1.1)$$

$$\partial_{k\sigma} = \frac{1}{\sqrt{m}}\sum_j e^{-ikr_j}c_{j\sigma} \quad (1.2)$$

Where *m* is the number of lattice sites and for simplicity, we shall consider it equal to one.

The inverse operators will then be.

$$c^{+}_{j\sigma} = \frac{1}{\sqrt{m}}\sum_j e^{-ikr_j}a^{+}_{k\sigma} \quad (1.3)$$

$$c_{j\sigma} = \frac{1}{\sqrt{m}}\sum_j e^{ikr_j}\, a_{k\sigma} \quad (1.4)$$

All bosons are maximally delocalized with probability $\frac{1}{m}$ to be found on an arbitrary lattice site. The wave function of every boson is spread over the whole lattice which indicates the superfluid state where all bosons can move freely over the whole lattice.

The Hamiltonian in (1) can be decomposed into three parts thus.

H=Hopping term (H_1) +Kinetic energy term(H_2) +three body interaction term (H_3)

$$H_1 = -t\sum_{\langle i,j\rangle\sigma} c^{+}_{i}c_j + hc \quad (1.5)$$

$$H_1 = -t\sum_{\langle i,j\rangle\sigma}\sum_{kk'i}(e^{-ikr_j}\partial^{+}_{k_\sigma}e^{ik'r_j}a_{k'\sigma} + e^{-ik'r_j}\partial^{+}_{k'_\sigma}e^{ikr_i}a_{k\sigma})$$

$$= \frac{-t}{m}\sum_{k\delta}(e^{-ik\delta} + e^{ik\delta})\partial^{+}_{k\sigma}a_{k\sigma}\delta_{kk'}$$

The summation over the lattice site gives a factor related to the lattice structure typically represented as ∂ in momentum space

$$= -2t\partial^{+}_{k\sigma}a_{k\sigma} = -2tN \quad (1.6)$$

Where the $\partial^{+}_{k\sigma}a_{k\sigma} = N$(lattice sites)

$$H_2 = \sum_i(\varepsilon_i - \mu)\, c^{+}_{i}c_i$$

$$= (\varepsilon_i - \mu)\sum_i\sum_k e^{ikr_i - ikr_i}\partial^{+}_{k\sigma}a_{k\sigma} = (\varepsilon_i - \mu)N \quad (1.7)$$

$$H_3 = \sum_{i\neq j\neq k}\left(\frac{W_{i,j,k}}{6}\right)n_i n_j n_{k\mathrm{j}}$$

where;

n_i is the number operator at site i.

$W_{i,j,k}$is the interaction strength between three different sites.

$\frac{1}{6}$ corrects for overcounting permutations of i, j, k

$$= \frac{W}{6m^2}\left\{\sum_{k_1k_2k_3k_4}\left(e^{-i(k_1-k_2)r_i - i(k_3-k_4)r_i}a^{+}_{k+\sigma}a_{k\sigma}\partial^{+}_{k'-\sigma}a_{k'\sigma}\right)\right.$$

$$+ \sum_{k_1k_2k_3k_4}\left(e^{-j(k_1-k_2)r_j - j(k_3-k_4)r_j}a^{+}_{k+\sigma}a_{k\sigma}\partial^{+}_{k'-\sigma}a_{k'\sigma}\right)$$

$$+ \left.\sum_{k_1k_2k_3k_4}\left(e^{-k(k_1-k_2)r_k - k(k_3-k_4)r_k}a^{+}_{k+\sigma}a_{k\sigma}\partial^{+}_{k'-\sigma}a_{k'\sigma}\right)\right.$$

where we let $k_1 = k+\sigma, k_2 = k, k_3 = k^{'} - \sigma \text{ and } k_4 = k'$

$$= \frac{W}{6m^2}\left(\begin{array}{c}\sum_{kk'}a^{+}_{k+\sigma}a_{k\sigma}\partial^{+}_{k'-\sigma}a_{k'\sigma} + \sum_{kk'}a^{+}_{k+\sigma}a_{k\sigma}\partial^{+}_{k'-\sigma}a_{k'\sigma} + \\ \sum_{kk'}a^{+}_{k+\sigma}a_{k\sigma}\partial^{+}_{k'-\sigma}a_{k'\sigma}\end{array}\right)$$

$$= \frac{6}{6m^2}\left(\sum_i n_i(n_i-1) + \sum_i n_j\left(n_j-1\right) + \sum_i n_k(n_k-1)\right)$$

$$= \frac{W}{4}N(N-1) \quad (1.8)$$

Finally, the full Hamiltonian includes a kinetic energy term (from hopping) −2tN, a chemical potential term −μN and the three-body interaction term $\frac{W}{4}N(N-1)$.

$$H = -2tN - \mu N + \frac{W}{4}N(N-1) \quad (1.9)$$

This is the modified Hamiltonian which has the three-body interaction part.

When the interaction dominates the Hamiltonian ($t = 0$)then the on-site particle number states are the Eigenstates of the Hamiltonian, and the energy E is given by,

$$E = -\mu N + \frac{W}{4}N(N-1) = \frac{W}{4}N^2 - \left(\frac{W}{4} + \mu\right)N \quad (1.9)$$

where N is the on-site particle number.

The value of N that minimizes the energy E

$$\frac{\partial E}{\partial N} = \frac{WN}{2} - \left(\frac{W}{4} + \mu\right) = 0$$

$$N = N_0 = \frac{1}{2} + 2\left(\frac{\mu}{W}\right) \quad (2.0)$$

where N_0 is the value of N for E to be minimum. This value of N will be rounded off to the nearest whole number, say N_0 for the energy E to be minimum say E_0 and Eqn. (1.9) shows that the value of N_0 will depend on the chosen values of $\frac{\mu}{w}$. Similar values are given by (Bruder et al., 2005) such that $\frac{\mu}{w}$= 1.5, $\frac{\mu}{w}$=0.75, $\frac{\mu}{w}$=0.5 and $\frac{\mu}{w}$=0.25

$$N_0 = \frac{1}{2} + 2(1.5) = 4 \quad (2.1)$$

For N_0>2, however, the bosonic Hubbard model has no Pauli exclusion and allows each site to have higher occupation.

Now at very low temperatures when the bosons are trapped in an optical lattice, the number of trapped atoms is fixed, then μ can be taken to be zero (μ=0), and Equation (1.9) can be used to write the energy E as:

$$E = -2tN - \mu N + \frac{W}{4}N(N-1) \quad (2.2)$$

Grand Canonical Partition Function

$$\rho(q,p,N) = \frac{1}{h^{3N}N!}\frac{1}{Z(T,V,\mu)}\, e^{-}\beta(H(q,p,N) - \mu N) \quad (2.3)$$

While the partition function for this ensemble is given by;

$$Z(T,V,\mu) = \sum_{N=0}^{\infty}\int \frac{d^{3N}\, qd^{3N}p}{h^{3N}N!} e^{-}\beta(H(q,p,N) - \mu N) \quad (2.4)$$

$$\sum_{N=0}^{\infty}\int d^{3N}qd^{3N}p\rho(q,p,N) = 1 \quad (2.5)$$

Using the normalization factor $h^{3N}N!$

$$Z = e^{-\beta(H(q,p,N)-\mu N)} \quad (2.6)$$

Thermodynamic properties

Internal energy

$$U - \mu N = -\frac{\partial}{\partial\beta}\ln Z(T,V,\mu)$$
$$= -\frac{\partial}{\partial\beta} In(e^{-\beta(H(q,p,N)-\mu N)}) + \mu N$$
$$= -2tN + \frac{W}{4}N(N-1) \quad (2.7)$$

We express the energy of the system at any temperature as a function of temperature by multiplying the ground state energy by the thermal activation factor given by: $e^{-\frac{\Delta E}{K_B T}}$ where k_B is the Boltzmann's constant and ΔE is the energy gap.

The energy of the quasi particles for superconductivity is a very small quantity and is generally 1% of the minimum energy of the system (Ayodo, 2008).

Therefore, at any temperature T, the energy of the system is given by:

$$U(T) = E_o e^{-\frac{\Delta E}{K_B T}} \quad (2.8)$$

$$U(T) = \left\{\frac{W}{4}N(N-1)\right\} e^{-\frac{\Delta E}{K_B T}} \quad (2.9)$$

for $t = 0$

Specific heat capacity

$$C_V = \left\{-2tN + \frac{W}{4}N(N-1)\right\}\frac{\Delta E}{K_B T^2} e^{-\frac{\Delta E}{K_B T}} \quad (3.0)$$

Estimation of the coupling constant numerical value W

According to Buchler H.P *et al* (2007), (for three-body interactions with cold polar molecules)

$$W = \left(\frac{R_o}{a}\right)^3 E_{kin} = \left(\frac{R_o}{a}\right)^3 \left(\frac{\hbar^2}{ma^2}\right) \quad (3.1)$$

Where R_o –parameter space to the region $|r_i - r_j|$
a-lattice spacing
m- atomic mass

$$W = 3.5 \times 10^{-21} J$$

$$C_V = 1.75 \times 10^{-21}\left(\frac{\Delta E}{K_B T^2} e^{-\frac{\Delta E}{K_B T}}\right) \quad (3.2)$$

and $\Delta E = 0.01E_o = 1.75 \times 10^{-23} J.$ (3.3)

Phase Transition

Given $\left(\frac{\partial C_V}{\partial T}\right)_{T=T_C} = 0$. (3.4)

$$T_C = \frac{\Delta E}{2K_B} \quad (3.5)$$

Sommerfeld coefficient (γ)

$$\gamma = \frac{c_v}{T}$$

$$\gamma = \frac{2.23\times10^{-21}}{T^3} e^{-\frac{1.27}{T}} \quad (3.6)$$

Grand canonical potential

To obtain the thermodynamic properties of the bosons trapped in the lattice we determine the grand canonical potential

$$\Omega = -k_B T In Z = -k_B T\left\{\frac{W}{4}N(N-1)\right\} \quad (3.7)$$

RESULTS AND DISCUSSION

Internal Energy Versus Temperature

For any given thermodynamic system, the higher the temperature, the higher the internal energy should be. The increase in internal energy tends to be exponential in the temperature range 0 K to 20 K but tends to flatten at a value approximately 0.98J as the temperature approaches 80 K. The value of the internal energy smoothly increases as the temperature is increased, and then starts to plateau after T≅50 K. This means that a fermion-dominated system behaves like electron gas. The three-body system is a micro interaction of a boson (pair) and a fermion. Higher energy values correspond to states where the fermions dominate the system with higher angular momentum values. A weak coupling is still exhibited in this phase and the bosons are still in phase. These results are in good agreement with the ones observed by Ayodo *et al.*, (2008). The internal energy of the system increases with temperature. At low temperature $\sim 0 - 20\,K$ there is a rapid increase in internal energy indicating the system is dominated by quantum fluctuations. The sharp rise in internal energy at $T = 10 - 20K$ suggests a crossover from superfluid to Mott insulator regime where thermal fluctuations set in as observed by Büchler *et al*. (2007) and Silva-Valencia & Souza (2011).

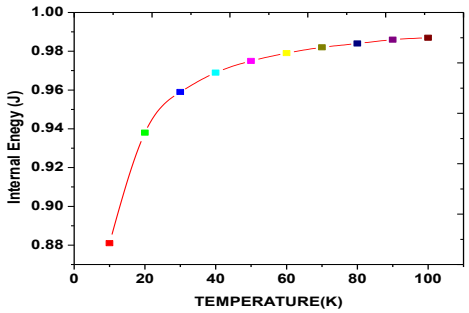

Figure 1.0: Internal energy versus Temperature

Specific Heat Capacity

The shape of the specific heat curve exhibits fluctuations. Specific heat values are too low in the temperature range from 40 K to 90 K. One feature that was found to be more interesting is that the highest peak of the curve occurred at $5.2K$. This happens to be very near the λ-transition temperature for liquid ^{4}He, which is 2.2 K. Below this temperature liquid ^{4}He becomes a superfluid. However, experimental observations by Chan *et al.* (1996) showed shifts in the transition temperature at which peaks in the value of the specific heat occurred. This can be accounted for since, experimentally, a highly porous material called aerogel was used to control the flow of liquid ^{3}He into liquid ^{4}He and changes in the thermodynamic quantities of the mixture were observed for different liquid ^{3}He concentrations. However, our theoretical model assumes a bulk mixture, meaning without aerogel, of the two liquids. Furthermore, our calculations do not include the flow properties of the two liquids. The normal-superfluid phase transition in pure liquid ^{4}He is a second order phase transition, whereas the phase change in the mixture of liquid ^{3}He into liquid ^{4}He is characterized with a lot of fluctuations with no discontinuity. In our three-body model, bosons and fermions are supposed to be interacting via a pair interaction, and the whole assembly is supposed to be in thermal equilibrium. The specific heat C_V has maximum and minimum, and the maximum value of C_V is around 5.2 K. This depicts that the system is unstable at the peak and a second order phase transition (normal metal to superconducting state) occurs due to absence of latent heat. In general, the total specific heat of any system is the sum of several different excitations. Specific heat needs to be explored in order to unravel the magnitude of different contributions to the total specific heat. The shape of the C_V curve is different from the shape of the curve for internal energy *E*. It should be acceptable that the specific heat C_V for a fermion dominated system will be different from a boson dominated system. It is the Pauli Exclusion Principle that restricts the flow of fermions from one level to another as the temperature changes from $-10K\ to\ 0K$. Thus, the system may refuse to absorb heat resulting in a negative specific heat. The actual transition temperature of the mixture is at 5.2 K, below which the whole mixture goes into the superfluid state. At a temperature above the Tc the energy of the system is so high that the energy gap does not exist anymore due to the increased agitation of the particles. The bosonic pair breaks up and the mixed ensemble gives out the energy exhibiting a lot of fluctuations. The superfluid state will no longer exist. The theoretical specific heat capacity and transition temperature were found to be $7.48 \times 10^{-21} J/Kg$ and $T_C = 5.2K$ respectively. The heat capacity is exponentially small at low temperatures. The results compare with that of Horace E Kibe *et al.*, (2017) on their study on Thermodynamics of S-Wave Pairing in Uranium and Cerium Based Heavy Fermion Compounds at low temperatures.

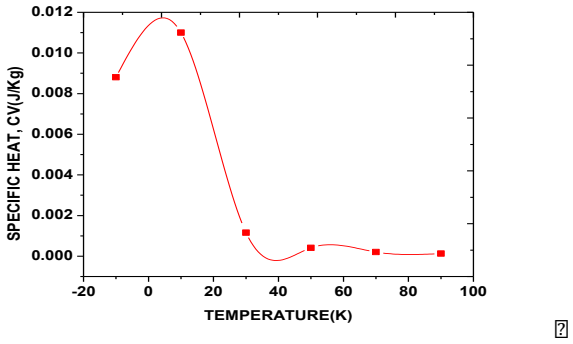

Figure 1.1: Specific heat capacity versus temperature

Sommerfeld coefficient

The Sommerfeld coefficient, representing the electronic specific heat, peaks at 11.1K with a value of 0.001121J/Kg.K. This result suggests enhanced fermionic contributions near the Fermi surface due to hybridization or coexistence of fermions with bosons in the optical lattice. The increase in the Sommerfeld coefficient with temperature indicates increased density of states near the Fermi level, aligning with theoretical predictions for mixed boson-fermion systems Kibe *et al.*, (2017). This is also in agreement with Peotta and Törmä (2015)**,** who demonstrated superfluidity in flat-band systems where fermionic states contribute to bosonic behavior.

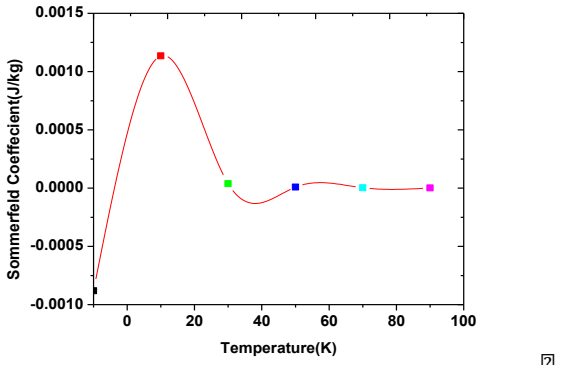

Figure 1.3: Sommerfield coefficient versus temperature

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