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Thermodynamics Of Many Body Interactions In Optical Lattices

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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 transforms**. The thermodynamic properties of polar molecules confined in optical lattices were investigated using an extended Bose–Hubbard model incorporating local three-body interactions. Analysis focused on the temperature dependence of the grand canonical partition function, internal energy, and entropy. The partition function exhibited a strong exponential increase with temperature, becoming particularly pronounced above 20K, which reflects a rapid enhancement in accessible microstates and increased state degeneracy induced by three-body interactions. The internal energy showed a steep rise in the low-temperature regime (0–20 K), indicating dominant quantum fluctuations within the lattice. At higher temperatures, the internal energy gradually approached a saturation value of approximately 0.98J beyond 50K, suggesting thermodynamic stabilization of the system despite strong many-body correlations. Entropy increased monotonically with temperature, with a sharp rise observed below 30K, marking a transition from an ordered quantum state to a more disordered thermal regime. A maximum entropy was attained nearly at 115K, beyond which further temperature increase produced negligible changes, indicating thermal equilibrium. The consistent behavior of these thermodynamic quantities demonstrates that local three-body interactions substantially modify the energy landscape and statistical structure of bosonic systems in optical lattices, providing insight into equilibrium properties of strongly correlated quantum matter.**

Keywords—Entropy,Partition function, Polar Molecules, Optical Lattices, Bose Hubbard Model

Introduction

An optical lattice is a spatially periodic potential generated through the interference of two laser beams propagating in opposite directions. Their superposition produces a standing wave with a spatial period of λ/2, enabling the confinement of neutral atoms via the AC Stark effect (Petrucciani, 2023). By arranging standing waves along orthogonal axes, one can realize lattice geometries of different dimensionalities: two-dimensional lattices arise from two perpendicular standing waves, while three-dimensional lattice structures are obtained by superimposing three mutually orthogonal standing waves with distinct wavelengths to avoid cross-interference. These configurations create nearly ideal, dissipation-free trapping environments in which ultracold atoms can move and interact with minimal loss (Grimme et al., 2000; Windpassinger et al., 2013), facilitating precise experimental control and observation. The interaction between an atom and an electromagnetic field leads to a shift in the atom's internal energy levels that depends on the local light intensity. Consequently, spatial variations in intensity translate into position-dependent potential energies. When such variations are produced by the interference of multiple laser beams, the resulting optical potential consists of a periodic array of potential minima, typically separated by distances on the order of the laser wavelength. In laboratory settings, the depth of these potential wells can reach the microkelvin scale. Atoms cooled to ultralow temperatures through laser cooling and evaporative techniques can be effectively trapped within these lattices. The behavior of ultracold atoms in such periodically modulated optical potentials closely resembles that of electrons moving in the periodic potential of a crystalline solid (Sachdeva, 2013). Unlike solid-state systems, however, optical lattices are highly tunable and essentially defect-free, a feature that has enabled the observation of phenomena such as Bloch oscillations that are often obscured by imperfections in real crystals.The competition between potential energy and kinetic energy is

central to understanding the transition between insulating and conducting phases. When potential energy dominates, particles become localized, whereas dominance of kinetic energy leads to delocalization and superfluid behavior. At temperatures approaching absolute zero, systems described by the Bose–Hubbard Hamiltonian exhibit two principal regimes: an interaction-dominated regime and a kinetic-energy-dominated regime. In the former, where the tunneling amplitude JJJ is much smaller than the on-site interaction energy UUU, the system resides in the Mott insulating phase. Recent progress in quantum simulation has enabled the use of ultracold atoms and molecules in optical lattices as highly controllable platforms for mimicking complex many-body Hamiltonians that are otherwise difficult to solve analytically or numerically (Tarruell & Sanchez-Palencia,2018).Thermodynamic quantities—including internal energy, entropy, specific heat, and the partition function—play a fundamental role in characterizing both equilibrium and non-equilibrium properties of these quantum systems. Previous studies by Horace Kibe et al. (2017) and Ayodo (2008) highlighted the importance of these parameters in analyzing phase transitions and energy distributions in fermion–bosonmixtures.Nevertheless, comprehensive investigations into the thermodynamic behavior of polar molecules subject to three-body interactions at zero temperature remain limited, leaving an important gap in the current understanding of strongly correlated quantum systems.

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.

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

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.

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

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

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

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

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

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

$$= (\varepsilon_i - \mu)N \quad (1.7)$$

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

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

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

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

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

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

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

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

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,

$$E = -\mu N + \frac{W}{4}N(N-1) = \frac{W}{4}N^2 - \left(\frac{W}{4} + \mu\right)N \quad (2.0)$$

where N is the on-site particle number.

The value of N that minimizes the energy E

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

$$N = N_0 = \frac{1}{2} + 2\left(\frac{\mu}{W}\right) \quad (2.1)$$

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

$$N_0 = \frac{1}{2} + 2(1.5) = 4 \quad (2.2)$$

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:

$$E = -2tN - \mu N + \frac{W}{4}N(N-1) \quad (2.3)$$

Partition function

To determine the thermodynamic properties of bosons confined in the lattice, we begin by evaluating the grand canonical potential.

$$\Omega = -k_B T In Z \quad (2.4)$$

$$Z = e^{-\beta(H(q,p,N)-\mu N)} \quad (2.5)$$

$$\Omega = -k_B T In\left\{e^{-\beta(H(q,p,N)-\mu N)}\right\} \quad (2.6)$$

$$= -k_B T\{H(q,p,N) - \mu N\}$$

$$= -k_B T\left\{\frac{W}{4}N(N-1)\right\} \quad (2.7)$$

Substitute for $\frac{W}{4}N(N-1) = 1.75 \times 10^{-21} J$ and $K_B = 1.38 \times 10^{-23} J/K$ in $\Omega(T)$ we get, $\Omega(T) = -k_B T\left\{\frac{W}{4}N(N-1)\right\}$.

$$\Omega(T) = -1.38 \times 10^{-23} \times 1.75 \times 10^{-21}$$

$$= -2.415 \times 10^{-44} J$$

$$Z = e^{\frac{\Omega}{-KBT}} \quad (2.8)$$

Hence $Z = e^{\frac{-1.748 \times 10^{-21}}{T}}$ (2.9)

Internal energy

$$U - \mu N = -\frac{\partial}{\partial \beta}\ln Z(T,V,\mu) \quad (3.0)$$

$$= -\frac{\partial}{\partial \beta} In(e^{-\beta(H(q,p,N)-\mu N)}) + \mu N$$

$$= -2tN + \frac{W}{4}N(N-1) \quad (3.1)$$

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:

$$U(T) = E_o e^{-\frac{\Delta E}{K_B T}} \quad (3.2)$$

$$U(T) = \left\{\frac{W}{4}N(N-1)\right\} e^{-\frac{\Delta E}{K_B T}} \quad (3.3)$$

for $t = 0$

Entropy,

Entropy is the measure of disorder of particles in a system.

$$S = \int \frac{c_v}{T} dT \quad (3.4)$$

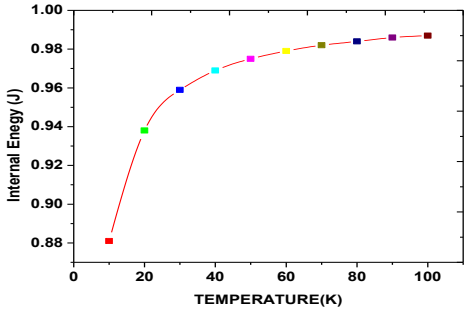
$$S = \left(K_B + \frac{E_o}{K_B T}\right) exp\left(-\frac{E_o}{100 k_B T}\right)$$

$$S(T) = 0.08628 + \frac{127}{T} e^{\frac{-127}{T}} \quad (3.5)$$

RESULTS AND DISCUSSION

Internal Energy Versus Temperature

The curve of internal energy versus temperature was obtained from plotting equation 3.3 and its observed that for any given thermodynamic system, the higher the temperature, the higher should be the internal energy. 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 plateaus 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. This results are in good agreement with the ones observed by Lusamamba., (2015) and Ayodo., (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 sets in as observed by Büchler (2007) and Silva-Valencia & Souza (2011).This study's key contribution lies in demonstrating that three-body coupling directly alters the energy landscape of optical lattices, creating new stability conditions for quantum phases. The results extend the theoretical understanding of superfluid energy dynamics, offering a bridge between atomic-scale Bose–Einstein condensates and macroscopic superconducting systems where energy stabilization governs phase coherence.

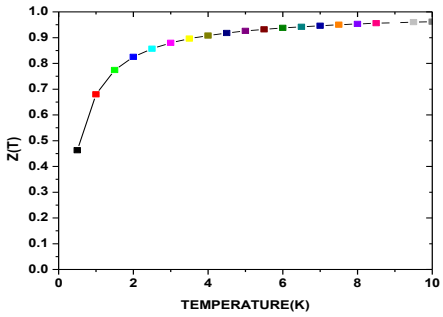


Partition function

The curve of partition function versus temperature was plotted from equation 2.9. From the curve, there is an exponential rise in the value of the partition function Z. The reason for this kind of behavior is that at very low temperatures there are very few energy states that can be occupied by the particles in the assembly. However, at higher temperatures, the number of energy levels available for particle occupation could be large, and these could be called the excited states of the assembly of particles. There is an optimum state occupied such that further increase in temperature does not alter the number occupied by the excited states. This arises given the ensemble has a fixed number of bodies. This behavior aligns with statistical mechanics principles, where the partition function serves as a generating function for thermodynamic quantities. The observed trend supports the theoretical framework in which the three body interaction terms enhances state degeneracy, affecting the thermal distribution Fisher (1989).

The behavior of the partition function reinforces the model's strength in predicting phase transitions and thermodynamic stability. It establishes a direct link between lattice-level particle interactions and macroscopic observables such as entropy and heat capacity. Scientifically, this underscores the contribution of this study to understanding statistical thermodynamics of superfluid systems**,** particularly the entropy-driven ordering transitions relevant in superconducting frameworks.

Partition function versus Temperature



Entropy

The curve of entropy versus temperature was obtained by plotting equation 3.5. The values of entropy increase with temperature just like the internal energy. At temperatures below 30K, entropy increases rapidly signifying a transition from an ordered superfluid phase to a more disordered normal phase. The curve reaches a maximum around 115K Indicating a thermal equilibrium state where further increase in temperature do not significantly increase disorder. The behavior is consistent with earlier findings by Kibe *et al.* (2017) and serves as a thermodynamic indicator of the phase transition observed in this system. Therefore, the lower the interaction of the particles the lower the value of entropy and *vice versa*. At higher temperatures molecules have higher vibrational energies, creating more disorder and hence more entropy. Furthermore, the curve of entropy exhibits a steady increase with temperature, indicating a progressive occupation of available microstates. The relationship between specific heat and entropy highlights the system's increasing disorder and energy accessibility, which aligns with theoretical expectations for correlated electron systems. This behavior mirrors findings in bismuth-based cuprate models, where similar entropy trends were reported as temperature rose, confirming that electron interactions significantly influence thermal properties (Odhiambo & Makokha, 2018).

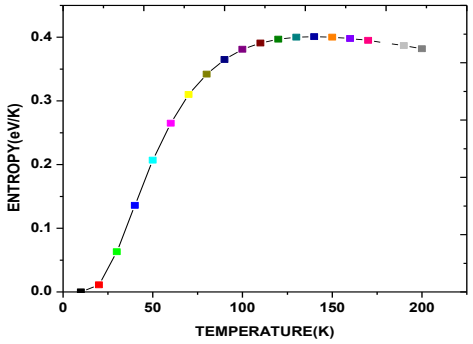


Figure 5.5 Entropy against Temperature

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