Superfluid-Insulator Transition in a Lattice Boson Gas

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Atoms in a Bose-Einstein Condensate can, under the influence of a periodic potential, make a quantum phase transition from the more usual superfluid (SF) phase to an insulating phase known as a Mott Insulator (MI). This transition is characterized by the destruction of long range phase coherence and number squeezing arising, so that each lattice site has a well defined number of atoms. The MI phase is being investigated to better understand the behavior of ultra-cold atoms, and to implement fine control over atomic systems for possible uses including quantum computers.

I. INTRODUCTION

The Bose-Einstein Condensate(BEC) phase of cold bosonic atoms in an atomic trap is characterized by a condensation of nearly all atoms into the lowest momentum state. This state is described by a order parameter which acts like a macroscopic wavefunction describing the collective quantum mechanical behavior of the atoms in the trap. Externally imposing a periodic potential onto the BEC requires switching from a continuum description to a lattice boson gas description. The behavior of bosons in this potential are described by two parameters[1], the tunnel coupling between adjacent lattice sites and the short range repulsive interaction between bosons on the same lattice site, For small potential strengths, the tunneling term dominates the energy and the gas remains in a superfluid(SF) state similar to the original BEC. However, for a critical strength of the potential, the system undergoes a quantum phase transition to a phase where atoms are localized to a single lattice site. This phase, the Mott Insulator (MI) phase is characterized by number squeezing and an energy gap in the excitation spectrum. The energy gap arises because the lowest lying excitation of the MI phase requires the creation of a particle-hole pair. For small tunnel couplings, this is equal to the on-site repulsion of two atoms sharing a lattice site.

The transition between these two phases of the boson gas take place at absolute zero and is driven by quantum mechanical fluctuations and the competition between two energy terms in the Hamiltonian – the on-site repulsion versus the kinetic energy. In contrast, classical phase transitions such as melting or the onset of ferromagnetism are characteristically driven by thermal fluctuations and a trade off between energy and entropy in the free energy. However, at absolute zero, all thermal fluctuations are frozen out and the entropy is zero, so classical phase transitions are impossible. Quantum fluctuations, however, are always present and enable phase transitions even at absolute zero. Indeed, even at very low but non-zero temperatures quantum fluctuations can dwarf thermal fluctuations.

The transition to the MI phase is not only an interesting example of a quantum phase transition in a strongly interacting system, but shows promise as a means of finely controlling atom-atom interactions for use in quantum computation[2]. An atoms behavior in the trapping potential can be made to depend on the magnetic sublevels of the atom. By defining these sublevels as a qubit, the one- and two-qubit logic operations required for universal quantum computation may be realized.

II. THEORY

It is well known that static electromagnetic fields cannot create a trapping potential. However, an oscillating field can create an effective trapping potential that confines the atoms to, for instance, the nodes or anti-nodes of the electric field. This principle is used with low frequency fields to trap atoms or ions for many low temperature experiments. If instead optical frequency fields are used this technique can create a lattice of micron sized potential wells[1], each capable of hosting a small number of atoms. The simplest case is a pair of counter propagating laser beams to form a 1D standing wave, but higher dimensional lattices may be formed by adding additional beams. In 2D and 3D, each of the crystallographic lattices may be formed by using an appropriate configuration of lasers.

Unsurprisingly, the wave vectors of the generating lasers correspond directly to the reciprocal lattice vectors of the resulting lattice. In particular, a 2D lattice generated by three coplanar waves with wave vectors $\boldsymbol{k_1}$, $\boldsymbol{k_2}$, and $\boldsymbol{k_3}$ has the reciprocal lattice vectors $(\boldsymbol{k_2} - \boldsymbol{k_1})$ and $(\boldsymbol{k_3} - \boldsymbol{k_1})$. Similarly for 3D, four waves are required and the reciprocal lattice vectors are $(\boldsymbol{k_2} - \boldsymbol{k_1})$, $(\boldsymbol{k_3} - \boldsymbol{k_1})$, and $(\boldsymbol{k_4} - \boldsymbol{k_1})$. This condition can easily be deduced by requiring that Bragg scattering conserve energy[3]. Bragg scattering occurs when $\boldsymbol{\Delta k} = \boldsymbol{K}$, a reciprocal lattice vector. However, to conserve energy and momentum, $\boldsymbol{\Delta k}$ must be balanced by absorption and emission of photons from the pump beams. This leads to the conclusion that the reciprocal lattice is generated by the differences in the wave vectors. In addition this determines restriction on other lasers used as part of the trap, for instance to assist in cooling. Once the first 4 beams determine the reciprocal lattice vectors, additional waves must satisfy $\boldsymbol{k_i} = \sum_{j=2}^{4} a_j \cdot (\boldsymbol{k_1} - \boldsymbol{k_j})$ if they are not to disrupt the lattice structure.

The confined boson gas was originally explored theoretically by Fisher *et al.*[4] for the case of superfluid ^{4}He in an disordered external potential. The phase diagram for this system includes not only the SF and MI phases but another phase called the Bose Glass(BG) phase. The BG phase has localized atomic wavefunctions and no long range coherence, so it is an insulator, but does not have an energy gap. The case without disorder is simpler, as well as realizable in dilute gas systems. In the case where the strength of the potential is great enough that atoms may only move from site to site by tunneling, the behavior of atoms in a periodic potential is governed by the second quantization Hamiltonian[5]:

$$H = -J \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \frac{1}{2} \sum_i \hat{n}_i(\hat{n}_i - 1) \qquad (1)$$

Here, J is the tunneling matrix element, $\langle i, j \rangle$ is the sum over adjacent lattice sites, and U is the strength of the short range repulsion felt by atoms in the same potential well. Repulsive interactions between atoms in neighboring lattice sites, tunneling to next-nearest neighbors, and spatial inhomogeneities in the trapping potential have all been neglected. The ground state can be found in mean field theory by minimizing the ground state energy with a fixed density number of total atoms.

For small U/J the tunneling term dominates the behavior, corresponding to delocalized atoms minimizing kinetic energy. The mean field ground state has all of the atoms in identical extended Bloch states, and is thus described by a macroscopic order parameter. By the uncertainty principle, the well defined phase between each potential well must be traded against uncertainty in the occupation numbers, so the superfluid state has large fluctuations about the mean number of particles in each well. However, as the U/J crosses a critical value, the system makes a transition into the MI phase. In this phase, the energy is dominated by the on-site interactions and the ground state is a collection of Fock states where the number of particles per site is well determined and uniform. Correspondingly, by the uncertainty principle the lack of fluctuations in the particle number must correspond to a complete lack of phase coherence. The long range phase coherence of the superfluid phase is in a sense converted into the number ordering of the insulator phase. The critical value for the transition depends on the dimension of the lattice, the coordination number of the lattice, and the average particle density. For a 3D lattice with 1 atom per site and coordination number z, the critical value is predicted to be $U/J = 5.8z$.

The transition to the MI phase is also characterized by the appearance of an energy gap. While in the SF phase there existed low lying excitations of the kinetic energy, the lowest excitation of the MI phase requires creating a particle-hole pair. For $U \gg J$ the energy of this excitation is simply U. Detection of this energy gap is one possible way to detect the MI phase [5].

III. EXPERIMENTAL REALIZATION

MI states can be realized by first trapping a dilute atomic gas in a low frequency magnetic trap and using standard laser cooling techniques to cool them below the BEC transition temperature. Once the gas condenses into a BEC, additional lasers are used to generate the chosen optical lattice. While many experimental configurations are possible, it is advantageous for robustness to use $d+1$ beams to create a d-dimensional lattice. Such lattices are insensitive to fluctuations in the relative phases of the beams. Such fluctuations merely cause the lattice to slightly shift intact.

The hallmark of coherence is interference, and this provides a mechanism to distinguish the SF from the MI phases of the boson gas. If the trapping potential is turned off and the gas allowed to freely expand and fall onto a detector, the individual lattice sites will act as an array of mutually coherent point sources, resulting in an observable interference pattern on the detector. This is entirely equivalent to the diffraction pattern generated by illuminating a grating with a coherent light source. The MI phase, however, has no phase coherence, and under free expansion generates a uniform distribution, in the same manner as an array of incoherent light sources would produce. It is observed that for strong applied fields the detected pattern is uniform, while for weak fields there is an interference pattern. The MI transition is also reversible. If the potential is increased past the critical field, then decreased below it again, the system rapidly recovers it phase coherence. All of these effects have been experimentally observed by Greiner *et al.* [5]. In addition, the onset of the incoherent background in the interference pattern corresponded to the value of U/J numerically predicted by mean field theory as the transition threshold.

IV. QUANTUM GATES

Quantum computation holds the elusive promise of performing many computations asymptotically more efficiently than computers based on classical physics are able to. Unfortunately, physical implementation of quantum computers are limited by the hard to reconcile goals of having strong coupling between the qubits in order to quickly perform logic operations, while maintaining weak coupling any external system that would tend to disrupt quantum superpositions. Neutral atoms in an optical trap are an interesting choice because they couple relatively weakly to electromagnetic noise from outside sources compared with ion based systems, but at close range can have strong dipole interactions possibly allowing fast quantum gates. Quantum computation requires a universal set of gates[6]. Roughly speaking, a universal set of logical gates is the combination of arbitrary single-qubit rotations plus an entangling two-qubit gate. When qubits are built using two levels of an atom or ion, the single-qubit operations are usually Rabi oscillations from an applied field, either directly on resonance or using a Raman transition. The entangling gate is more complicated. Two common examples are the controlled not (CNOT) and a two-qubit phase gate. CNOT is the quantum equivalent of a logical XOR defined:

$$\begin{aligned}
|0\rangle_1|0\rangle_2 &\rightarrow |0\rangle_1|0\rangle_2 \\
|0\rangle_1|1\rangle_2 &\rightarrow |0\rangle_1|1\rangle_2 \\
|1\rangle_1|0\rangle_2 &\rightarrow |1\rangle_1|1\rangle_2 \\
|1\rangle_1|1\rangle_2 &\rightarrow |1\rangle_1|0\rangle_2
\end{aligned} \tag{2}$$

while a phase gate negates one of the four two-qubit basis elements, for instance:

$$\begin{aligned}
|0\rangle_1|0\rangle_2 &\rightarrow |0\rangle_1|0\rangle_2 \\
|0\rangle_1|1\rangle_2 &\rightarrow |0\rangle_1|1\rangle_2 \\
|1\rangle_1|0\rangle_2 &\rightarrow -|1\rangle_1|0\rangle_2 \\
|1\rangle_1|1\rangle_2 &\rightarrow |1\rangle_1|1\rangle_2
\end{aligned} \tag{3}$$

Neutral atoms in an optical lattice can implement this phase gate by inducing collisions between atoms in two hyperfine levels in a controlled fashion[2].

The effect of the trapping potential on atoms is directly tied to polarization. By making an appropriate choice of atomic levels and lasers, it is possible to arrange for one hyperfine level to only be trapped by right circular polarized light and another only by left circular polarized light. A 1D lattice formed by two beams with linear polarization is an equal superposition of left and right circular components. Thus, they actually form two independent lattices, one for zero bits, and one for one bits. The two lattices can be translated with respect to one another by changing the polarization angle between the two beams.

Thus, consider a two adjacent sites in a configuration where the lattices for each polarization line up. Then, rotate the polarization of one beam to move the σ^+ lattice to the right by about one lattice spacing then back. Only if the right atom is in the - state and the left atom is in the + state will the two have interacted. If the states involved in the collision are such that there is no induced transition, the only effect of the interaction is an additional dynamical phase $e^{iEt/\hbar}$ where E is the interaction energy associated with bringing the two atoms close to each other. Since any other state of the two atoms will not result in a collision, adjusting the interaction time so the integrated phase is π results in performing a phase gate on the atoms in the two lattice wells.

V. DISCUSSION AND CONCLUSIONS

Creation of a Mott insulator phase by applying a periodic potential has been observed, as well as the ability to transfer back and forth between the insulating and superfluid phases. By using hyperfine levels of the ground state of an alkali atom is is possible to implement a two-qubit phase quantum gate. That, coupled with one-qubit rotations is sufficient to implement a universal quantum computer. This system has some advantages, such as using neutral atoms with couple to the environment much less than ions, and the possibility of doing gate operations on an entire set of qubits at once. However while it is in principle straightforward to implement a rotation on a single atom using laser pulses to induce Rabi oscillations, since the appropriate laser wavelengths are on the same order as the lattice periodicity, it is in practice difficult to address a single atom within the lattice without also rotating adjacent atoms. In addition, as described, it is impossible to selectively perform the phase gate on a single pair of atoms. However, every other proposed framework for quantum computation also has serious unresolved issues, so exploring neutral atom systems may be fruitful.

Regardless of whether the MI phase is of use in quantum computing or other atomic scale engineering tasks, this is a marvelous way to examine the behavior of a quantum phase transition in an extremely clean and controlled fashion. Of particular significance is that since atoms confined by the lattice potential may be confined to a volume much smaller than the average density in the free BEC, the atom-atom interactions could not be treated as small perturbations, but were in fact responsible for the entire effect. This allows studying of strongly interacting bosons in a much more controllable environment that previous systems such as superfluid ^{4}He or cooper pairs in a superconductor. In particular, the ability to vary arbitrarily between the weakly and strongly interacting limits is remarkable.

It would be interesting to see an experimental validation of Fisher *et al.*'s prediction of a gapless Bose Glass phase. This might be achieved by introducing some quasi-random noise into the trapping potential and looking for intermediate field strengths where there is substantial incoherent background in the interference pattern indicating the loss of phase coherence, but with no observable excitation gap.

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