The Bose-Hubbard Hamiltonian

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I. INTRODUCTION

One of the exciting prospects of the physics of dilute bose gasses is the realization of optical lattices. The combination of many body physics together with a high degree of tunability makes these systems promising test beds for theoretical techniques and novel devices. In particular given their high degree of quantum coherence they represent the (long term) possibility of a universal quantum simulator or even computer[7,4]. As a general discussion is beyond both the scope of this paper and the author's understanding, this paper will focus on perhaps the simplest non-trivial example namely the bose-hubbard system. One sense in which it is non-trivial is that its zero-temperature quantum phase transition has no direct d+1 dimensional classical phase transition.[1] But really an experimental observation of a phase transition, driving by quantum fluctuations rather than thermal ones is quite remarkable. In fact we will essentially narrow our focus further to the zero temperature limit. This paper will first 'get a feeling' for the system discussing it in an intuitive way. Next, to ground the discussion a bit I will review an 'early' realization of such a system, namely the experiment of Greiner et. al. (2002)[2]. We will next move on to the theoretical treatment; first deriving the expected phase diagram from mean field theory, then having a look at some of the scaling properties. Finally we will note some of the exciting future prospects for this field.

II. MEET THE BOSE-HUBBARD SYSTEM

The Bose Hubbard system is best thought of as a bunch of atoms with no internal structure in an external 'egg-carton' potential. The atoms can move by hopping between nearest neighbor sites. The also interact by an on-site mechanism that penalizes double or more

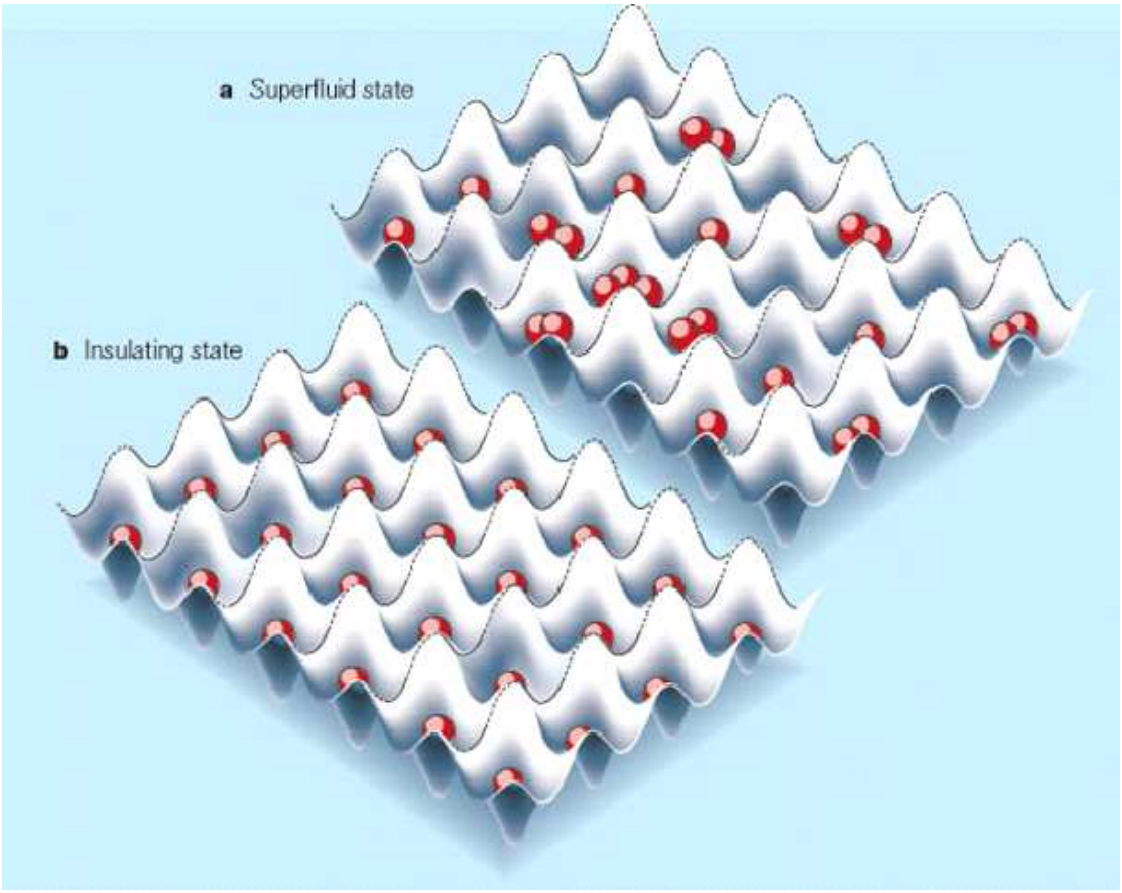

FIG. 1: A cartoon view of the Bose-Hubbard Hamiltonian[3]

occupancy. The exact form of the Hamiltonian can be 'derived' or perhaps more accurately 'motivated' starting with the Hamiltonian of a weakly interacting bose gas described by an effective s-wave interaction, and assuming that all particles are in the lowest band . We then can expand the boson operators in terms of Wannier functions in a usual tight binding approximation.[4] This allows us to express the Hamiltonian in terms of b_i and $b_i^\dagger$, creation and annialation opperators at the different sites, where we denote the site index by i. The final result is as follows.

$$H = -J \sum_{\langle i,j \rangle} b_j^\dagger b_i + \mu \sum_i n_i + \frac{U}{2} \sum_i n_i(n_i - 1) \tag{2.1}$$

where n_i is $b_i^\dagger b_i$ and the operators satisfy boson commutator relation $[b_i, b_j^\dagger] = \delta_{i,j}$ et cetera. The coefficients J and U can be defined in terms of overlap terms of Wannier functions but at this level it is more intuitive to view equation 2.1 as the starting point since each term can be understood physically.

The first term is a hopping term that annihilates a particle only to create it at a neighboring site. The next term is an external potential, which in general can depend on the site (for instance it could provide a random potential for a disordered system) and in particular, as important experimentally, must have a global harmonic shape to keep the atoms from leaking out. This term being conjugate to the total number, we can see that by changing μ by a fixed global amount this term can be used to go between the canonical and grand-canonical formulations; as such μ is referred to as the chemical potential. Lastly, the interaction term. There are other forms but I choose this one since written in this form it is manifestly clear that when the occupation is 0 or 1 this term will be zero and only for $n \geq 2$ will this term contribute a positive energy.

Now we are ready to understand figure 1. For the moment we will ignore the chemical potential term. Further, lets imagine that the number of atoms equals the number of lattice sites. Lets first consider what the system might look like if $J \gg U$. In this case the hopping kinetic term will dominate favoring a delocalized state. Since we can neglect interactions we expect all the atoms to be in the lowest single particle state. Thus at zero temperature we expect the ground state to be a coherent state with all N atoms occupying the $q = 0$ state, which is referred to as the 'super fluid' state. Written in terms of the creation operators,

$$|\Psi_{SF}\rangle \propto (\sum_i b_i^\dagger)^N |0\rangle \tag{2.2}$$

where we have for simplicity dropped the normalization factor. This description is instructive because it allows you to visualize algebraically what this state looks like if we expanded it in the basis with a fixed particle number at each site. What we just imagine doing is multiplying out the $(\sum b^\dagger)^N$ term as one big multinomial. In each term an atom will 'land' at a site with a probability independent of every other atom, thus in the large N limit the number of atoms at each lattice site will be a Poisson distribution; in particular there is a finite probability that there are zero one two or more atoms at a given lattice site. This is represented by picture 'a' of figure 1.

This then leads to the important observation that the expectation value of the interaction term would be non-zero. And that in particular that as U and J change to the opposite limit $U \gg J$ the ground state must change to the so called 'mott insulator' state with exactly one atom occupying every site,

$$|\Psi_{MI}\rangle \propto (\prod_i b_i^\dagger)|0\rangle \tag{2.3}$$

which is represented in figure 1 as picture 'b.'

III. THE OPTICAL LATTICE EXPERIMENT

While the field has grown enormously since its inception a mere half decade ago I will primarily discuss the first experiment of Greiner, Bloch et. al.[2] The system is essentially 10^6 Rb87 (which are bosons) atoms that are trapped in a harmonic magnetic trap and cooled via optical doppler, subdoppler and evaporative cooling techniques to milli Kelvin temperatures. The atoms are then loaded into an optical lattice made up of counter propagating lasers that are chosen to have a frequency that is detuned from a transition of the atoms (which are all in the same internal state). This off-resonance condition causes the atoms to not be significantly heated yet be attracted to the high intensity regions of the induced electric field. This creates an effective periodic potential with a periodicity half the wavelength of the laser light. In their setup they used three pairs of counter-propagating beams to make the potential three dimensional.

The interesting knob that they could still tune was the intensity of the laser light. By increasing the intensity the Wannier functions became more localized decreasing the magnitude of the hopping parameter J. Thus they could tune the system between the superfluid and mott insulator regimes discussed above. So how did they tell if a phase transition was

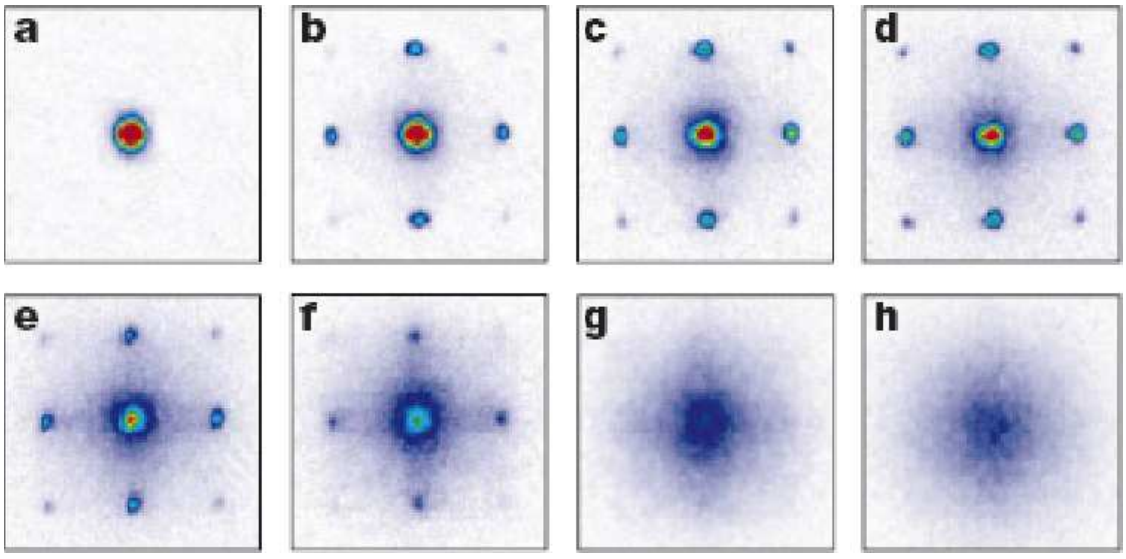

FIG. 2: A series of expansion images. Increasing U/J as a $\rightarrow$ h. [2]

occurring? Well, they had a look! i.e. they expanded the system and took an absorbtion image. What would we expect in the different phases? In the superfluid phase each atom is globally coherent so its probability of ending up at a particular location is a coherent superposition of traveling from each lattice site and in particular has a sharply peaked distribution with bragg peaks corresponding to the lattice spacing. (At very low barrier to hopping the atoms are more or less uniform which corresponds to picture 'a'). However in the Mott insulator the probability of an atom being at a particular location is an incoherent sum and the resulting image is much more diffuse.

Aside from the (in my opinion) very aesthetically pleasing element of this result, In some respects the results aren't all that spectacular; in particular its not clear that there is any 'transition' at all i.e. it certainly isn't abrupt – it is hard to imagine getting scaling exponents for instance. Though a few points should be made. First, since there is a overall harmonic potential, certainly the chemical potential ins't constant across the sample so in particular it is not clear that the system doesn't break up into domains which might dull the effects of any transition that is occurring, neither have we discussed yet exactly what transition we would expect to see. In fact at constant particle number density we would only expect a transition at exactly integer filling. However, though the quantitative significance of the experiment may be limited – as a 'proof of principle' it is clear the experiment is invaluable.

IV. THE BOSE-HUBBARD THEORY

The hubbard hamiltonian has a long history of use primarily to study the superconductor-insulator transition in fermi systems. However in 1989 M.P.A. Fisher et. al.[5] extensively analyzed the Bose version of the theory. In particular since space does not allow a more extensive discussion I will focus on two important elements. The use of mean field theory to derive the general structure of the phase diagram. And the import of renormalization of the time dimension for a $T = 0$ quantum phase transition, which will lead to for example generalized Josephson scaling relations. Again since these are rather technical issues and space is limited I will discuss these points rather heuristically; (this will hopefully have the added benefit of disguising some of my ignorance as well.)

Let us begin by discussing the mean field theory (MFT). As usual we make the infinite

range hopping assumption. I.e. our Hamiltonian becomes

$$H = -\sum_{i,j} J_{i,j} b_j^\dagger b_i + \mu \sum_i n_i + \frac{U}{2} \sum_i n_i(n_i - 1) \tag{4.1}$$

We can exactly digitalize the interaction term which we will denote H_0 denote the hopping term as H_1 and ignore for now the chemical potential. We can now express the partition function in the standard interaction picture. $Z \propto \langle Texp[-\int_0^\beta d\tau H_1]\rangle$ where the average is taken over the ensemble given by diagonalizing H_0 and T is the time order operator. Now we can introduce a complex field $\psi_i(\tau)$ conjugate to b_i and perform a Hubbard-Stratonovich transformation we end up with a functional integral over ψ of an effective action of the form

$$S = \sum_{i,j} \int d\tau J_{i,j}^{-1} \psi_i^* \psi_j - \sum_i ln\langle Texp[\int d\tau \psi_i b_i^\dagger + h.c.]\rangle \tag{4.2}$$

Note that if we included the chemical potential this term is also local. Further note the sum over space as well as (integral) over time. In the limit temperature goes to zero, time goes to infinity. This point is key for the discussion of quantum phase transitions below. The average is now on site and can be computed as a cumulant expansion in powers of ϕ. This action for ψ can then be approximated and molded in in the usual landau form

$$S = \beta N \frac{1}{2} r|\psi|^2 + u|\psi|^4 + ... \tag{4.3}$$

where r has the form

$$r = \chi(1 - zJ\chi) \tag{4.4}$$

$$\chi = \frac{n+1}{Un - \mu} + \frac{n}{\mu - U(n-1)} \tag{4.5}$$

where n is a step function in μ/U. For each integer value of n you can solve $r = 0$ i.e. the phase transition line, generating the phase diagram in figure 3. Of course as with all MFT, it does not adequately account for fluctuations (here in the superfluid order perameter). In particular MFT is thought to be a particularly bad approximation at the tip of the 'mott lobes.' The numerical simulation seems to bare this out as seen in figure 4.

Let us now move on to a property unique to $T = 0$ quantum phase transitions: The importance of the time dimention. As with all things in stat. mech. the partition function is central. In classical mechanics momentum and position commute and we can perform gaussian integration to eliminate the momentum dependance from the partition function. We are then left with an integral over space. If we express this in functional integration

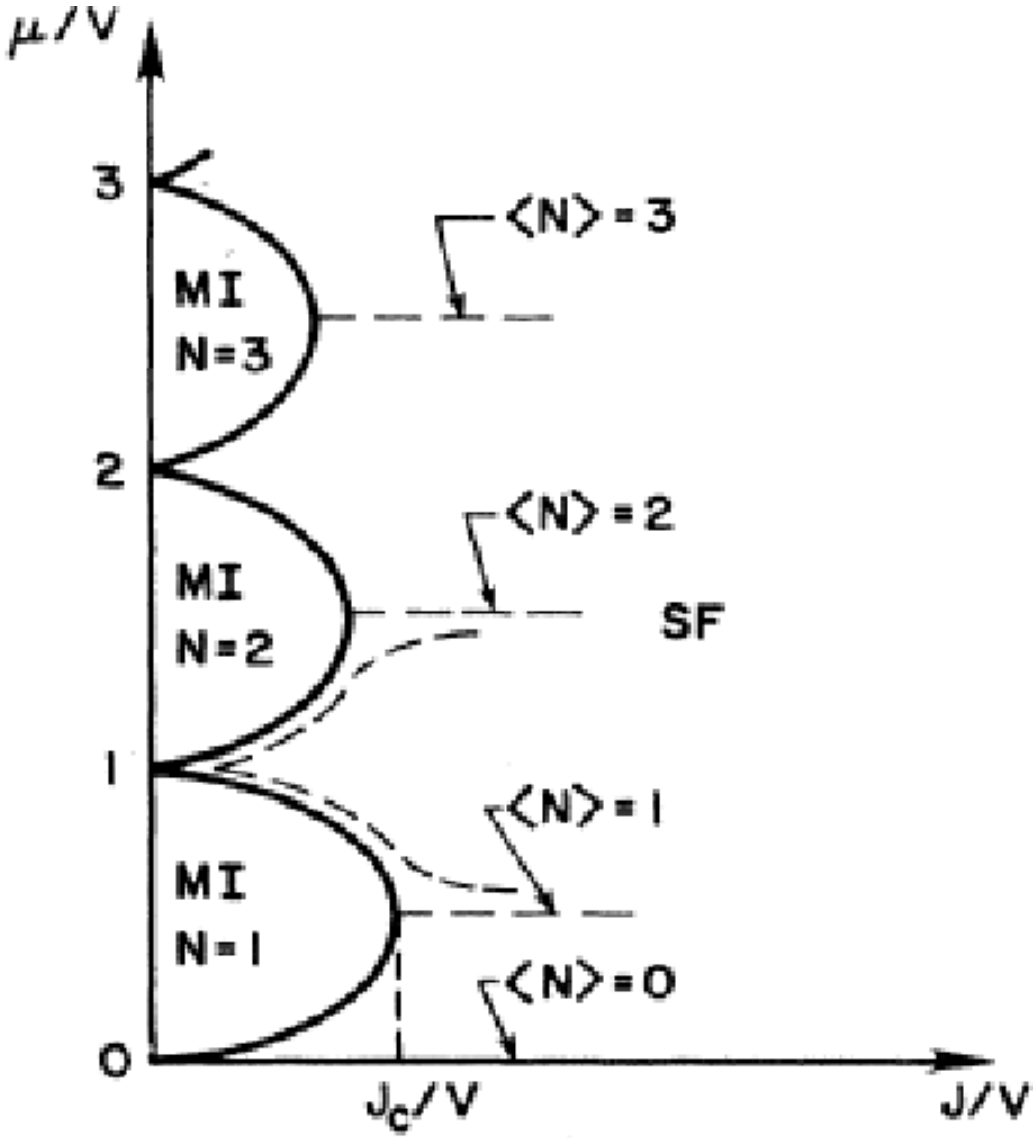

FIG. 3: Phase diagram from [5]. For direct reference to discussion V should be replaced by U . J_c corresponds to $\frac{U}{6z}$ where z is the lattice connectivity

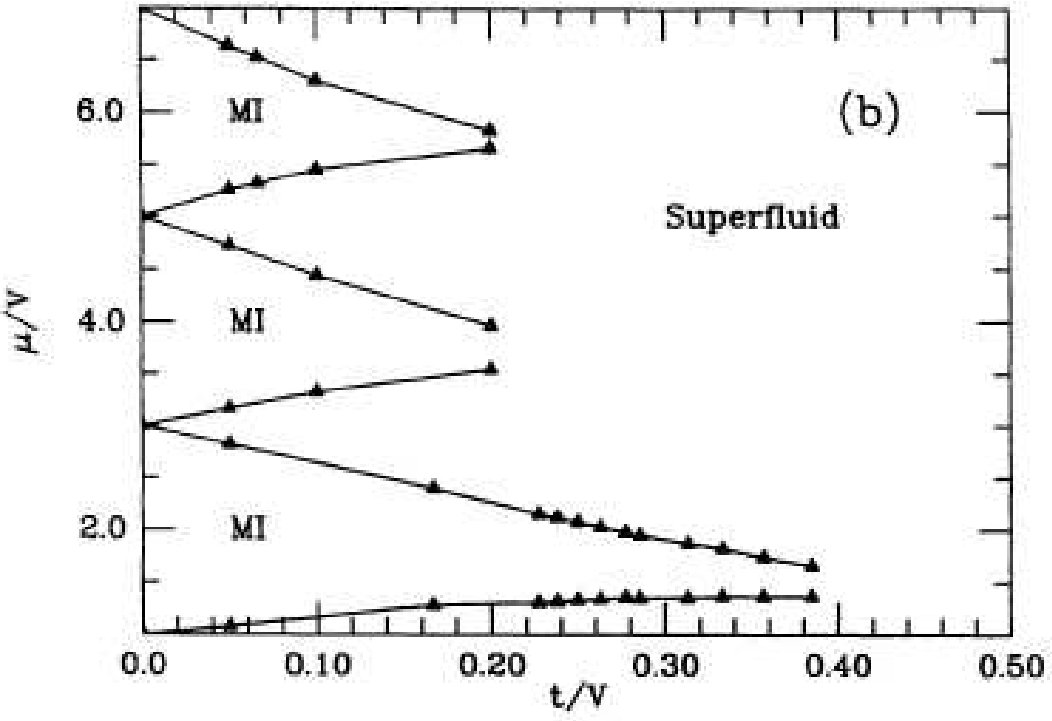

FIG. 4: numerical simulation of bose hubbard hamiltonian [6]

the terms in an effective action approach such as in Landau theory will be expressed as an integral of a lagrangian density of space only. In quantum field theory for instance we will also have to perform the calculation $Z = Tre^{-S}$. However the trace is over hilbert space not *dpdq*. There isn't a simple analogue integrating over momentum coordinates. Let us think in terms of a quantum field theory. If we think of the β as the imaginary time axis our effective action will not only integrate our lagrangian density over space but also the time dimension as well as we saw in equation 4.2. Thus when we perform the a renormalization of the length scales we will also have to renormalize in the time dimension.

To see what this means for scaling we will following the discussion of Fisher. First we need to remember that μ is effectivly an external field. Let δ be the reduced μ at a critical phase transition. As a usual assumption of our scaling the correlation length will diverge with δ as $\xi \ |\delta|^{-\nu}$. However we will also need to rescale our 'imaginary time' axis in our functional integral. In many respects we are able to bring over most of our tools from classical phase transitions with the only proviso that our d space dimensional quantum theory would have to be be described by a d+1 space dimensional classical theory. By analogy with the space dimentions there will be a characteristic energy scale Ω ($\hbar = 1$) that defines a characteristic time scale that will be diverging also. Thus we assume $\Omega^{-1} \ |\delta|^{-z\nu}$ which defines z. (note this is not the lattice connectivity above). Following usual scaling arguments we find for instance that the singular part of the free energy scales $\nu(d + z)$ and not just d!

Much more could be said of the Fisher paper as it is a quite rich discussion including estimations of critical dimensions and RG calculations. In particular they also discuss the effects of disorder. However given the limited space we will end discussion of it here. In closing let me just remark that while the details of the theory may not be exactly applicable to Optical lattices, the theoretical framework is convincing enough that a 'topological deformation' of the theory should be applicable. In particular it provides a paradigm and language to discuss and analyze the experimental results. For example is it the last word on nature of the phase transition at the multicritical point at the tip of the mott lobe? I would bet against it, however I am fairly sure it will be foundation of what come next.

V. CONCLUSIONS

In many respects this area of research is in its infancy. For instance there are many exciting direction that experiments are taking. The intensity of the laser field is hardly the only tuneable parameter. In particular using a light amplitude modulator can create interesting potential energy landscapes. Fermions could replace bosons. Feshbach resonances can in principle be used to tune the interaction between atoms. More that one hyperfine species could be used. The potential on the theoretical side is equally deep. In particular a fascinating issue is quantum simulation or even computation which raise the potential of exploring systems and concepts in a complexity class different than the classical one, touching on fundamental questions about what is knowable given a specified resource – even in principle. These highly tunable yet intrinsically complex system promise to be at the forefront as physics tries to understand the ultimate limits (or lack thereof) of the reductionist paradigm. How's that for a conclusion!

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