Contributed Papers

Metal Insulator Transition in Strongly Correlated Electron Systems

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Strongly interacting quantum systems exhibit some of the most interesting phenomena in condensed matter physics. Until very recently the study of these systems has been confined to either numerical simulations of rather small systems (which still have an enormous number of quantum states) or approximate analytical methods which are uncontrolled. Most of the effort concentrated on the fermionic systems. In the last few years the bosonic systems have attracted a lot of interest.[1,2,3,4,5] Examples of the bosonic strongly correlated systems include short coherence length superconductors, Josephson junction arrays, the dynamics of flux lines in high temperature superconductors and the quantum hall effect.[6] The essential physics of all of these problems is the competition between the hopping matrix elements and the short range strong repulsion. The minimum model which contains the basic physics of the problem is the so called Bose Hubbard model:

$$H = -t\sum_{ij} b_i^\dagger b_j - \mu\sum_i \hat{n}_i + \frac{1}{2}U\sum_i \hat{n}_i(\hat{n}_i - 1) \quad , \quad \hat{n}_i = b_i^\dagger b_i \tag{1}$$

where b_i is the boson annihilation operator at site i, t is the hopping matrix element between the site i and j, U is the strength of the on-site repulsion, and μ is the chemical potential. The approximate form of the zero temperature ($T = 0$) phase diagram can be understood by starting from the strong- coupling or "atomic" limit.[1,7,8] In this limit, the kinetic energy vanishes ($t = 0$) and every site is occupied by a fixed number of bosons, n_0. The ground-state boson occupancy (n_0) is then chosen in such a way as to minimize the on-site energy. For a finite deviation from integer filling, a finite amount of energy (gap) is required to move a particle through the lattice. The bosons are localized, producing a Mott insulator. This energy gap decreases with increasing strength of the hopping matrix elements until it vanishes and the bosons condense into the superfluid phase. As the strength of the hopping matrix elements increases, the range of the chemical potential μ about which the system is incompressible decreases. The Mott-insulator phase will completely disappear at a critical value of the hopping matrix elements.

The Hamiltonian, Eq. (1), has been studied numerically with the Quantum Monte Carlo Method, e.g.,[2,4,5] and analytically by mean field approximations,[9] renormalisation group[3,7] and other techniques.[5] Here we present an analytical approach[10] which allows us to calculate the Mott-insulator - superfluid phase boundary at zero temperature with an accuracy comparable to the best available numerical results. We proceed as follows. We determine the energy the of the Mott insulator in many body perturbation theory in powers of the kinetic energy. We compare the energy of the Mott - insulator with the energy of a so called "defect state" in which one additional boson (or one additional hole) is in an extended state. The energy of the defect state is also determined with many body perturbation theory. The Mott - insulator superfluid transition occurs when the energy of the "defect state" and the Mott - insulator state are equal. To zeroth order in t/U the Mott insulating state is given by. To zeroth order in t/U the Mott insulating state is given by

$$|\Psi_{\rm Mott}(n_0)\rangle^{(0)} = \prod_{i=1}^{N} \frac{1}{\sqrt{n_0!}} \left(b_i^\dagger\right)^{n_0} |0\rangle \tag{2}$$

where n_0 is the number of bosons on each site, N is the number of sites in the lattice and $|0\rangle$ is the vacuum state. The defect phase is characterized by one additional particle (hole) which moves coherently throughout the lattice. The ansatz for the "defect state" to zeroth order in t/U is determined by degenerate perturbation theory:

$$\begin{aligned} |\Psi_{\rm Def}(n_0)\rangle^{(0)}_{\rm particle} &= \frac{1}{\sqrt{n_0+1}} \sum_i f_i b_i^\dagger |\Psi_{\rm Mott}(n_0)\rangle^{(0)} \\ |\Psi_{\rm Def}(n_0)\rangle^{(0)}_{\rm hole} &= \frac{1}{\sqrt{n_0}} \sum_i f_i b_i |\Psi_{\rm Mott}(n_0)\rangle^{(0)} \end{aligned} \tag{3}$$

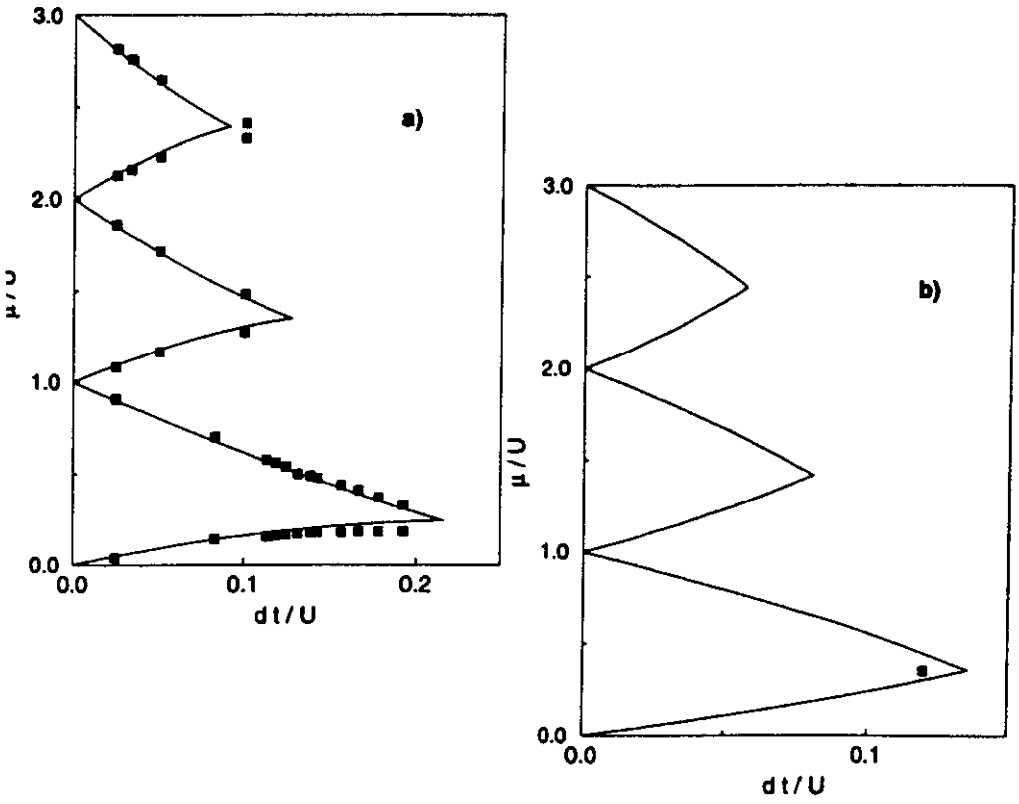

FIGURE 1. Phase diagram of the Bose Hubbard model in one (left) and two (right)dimension. The squares (left) are the results of the Quantum Monte Carlo calculation by Scalettar et al. for the one dimensional Bose Hubbard model. The square (right) is the result of the Quantum Monte Carlo calculation of Trivedi et al. The hopping matrix element is scaled by the dimension d.

where the f_i is the eigenvector of the hopping matrix t_{ij} with the lowest eigenvalue. The energies of these state can be calculated with Rayleigh-Schrödinger perturbation theory. The result of the a third order perturbation calculation specialized to the hypercubic lattice in one and two dimensions is shown in the Figure 1.

We have repeatedly compared a strong-coupling expansion to the numerical QMC simulations for the incompressible-compressible phase boundary of the bose Hubbard model. A mean-field treatment of the bose Hubbard model (e.g.[1,9]) cannot capture the physics of the one dimensional system which is completely dominated by fluctuations. The dimensionality only enters as a trivial prefactor in integrals over the phase space. For this reason, mean-field theories will always give a concave shape

to the Mott-insulator lobes independent of the dimension. A strong-coupling expansion, on the other hand, easily distinguishes the shape difference from one dimension to higher dimensions and shows that a proper treatment of density fluctuations is critical in determining the Mott-insulator to superfluid transition. In conclusion we have described an analytical method to accurately calculate the phase diagram of the bose Hubbard model in any dimension. Extensions of these techniques to include disorder will be presented separately.

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