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Gutzwiller projection for bosons

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We apply Gutzwiller's variational method to the interacting Bose lattice gas. In contrast with the Fermi case, the Gutzwiller wave function for bosons can be treated with no further approximation in several limits. Furthermore, this wave function can be shown to be exact for large dimensionality, and also in arbitrary dimension for suitably chosen short-range interactions. At densities commensurate with the lattice, a superfluid-insulator transition is found. These results are compared with the fermionic case, and are applied to several interacting-boson systems.

I. INTRODUCTION

Gutzwiller's variational method[1] is a simple yet powerful technique for studying strongly correlated Fermi systems. In this approach, a variational state for an interacting system is constructed from the corresponding noninteracting ground state by systematically reducing the amplitudes of configurations with large potential energies. Unfortunately, in the case of interacting fermions even this modest program cannot be carried out analytically without further approximations. We present here a natural generalization of Gutzwiller's ansatz to the interacting Bose lattice gas, which can be treated exactly since boson operators on different sites commute.

The simplest model of interacting particles on a lattice is the "Hubbard model," introduced by Gutzwiller, Hubbard, and Kanamori:[2]

$$\mathcal{H} = -t \sum_{<ij>} a_i^\dagger a_j + \sum_i V(n_i), \tag{1}$$

where the sum is performed over all pairs of nearest-neighbor sites, $n_i \equiv a_i^\dagger a_i$ is the number operator at site i, and $V(n)$ is a potential energy which penalizes multiple occupancy of a given site. This is the usual spin-$\frac{1}{2}$ Hubbard model if $a^\dagger$ is the two-component spinor $(c_\uparrow^\dagger, c_\downarrow^\dagger)$ and $V(n) = Un(n-1)/2$. We discuss here the case in which $a^\dagger$ creates a spinless boson.

The Gutzwiller variational ansatz for spin-$\frac{1}{2}$ fermions is

$$|\Psi_g\rangle = \prod_i [1-(1-g)n_{i\uparrow}n_{i\downarrow}]|G\rangle, \tag{2}$$

where $|G\rangle$ is the Fermi sea at the density under consideration and g is a variational parameter which ranges from 0 (forbidding double occupancy) to 1 (leaving the wave function unchanged). This ansatz can be trivially generalized to apply to bosons (and fermions with spins greater than one-half) by rewriting (2) as

$$|\Psi_g\rangle = \prod_i \gamma(n_i)|G\rangle, \tag{3}$$

where $\prod_i \gamma(n_i)$ is a factor which suppresses the amplitude of configurations with large potential energies and $|G\rangle$ is the corresponding noninteracting ground state. We will consider $\gamma(n) = g^{n(n-1)/2}$, which closely parallels the original Gutzwiller ansatz, but any function which progressively suppresses multiple occupancy is expected to give qualitatively similar physics.

For a Bose system, the noninteracting ground state $|G\rangle$ is a macroscopically occupied single-particle state:

$$|G\rangle = (a_{\mathbf{k}=\mathbf{0}}^\dagger)^N |0\rangle, \tag{4a}$$

where $a_{\mathbf{k}=\mathbf{0}}^\dagger = \sum_i a_i^\dagger$ creates an (unnormalized) zero-momentum plane wave state and $|0\rangle$ is the vacuum. Alternately, one may work in the grand canonical ensemble, where the ground state is a coherent state of definite phase rather than particle number:

$$|G\rangle = \exp[\sqrt{\lambda} a_{\mathbf{k}=\mathbf{0}}^\dagger]|0\rangle = \prod_i \exp[\sqrt{\lambda} a_i^\dagger]|0\rangle. \tag{4b}$$

The second equality holds because the boson creation operators at different sites commute. Thus both the noninteracting ground state (4b) and the variational wave functions constructed from it via (3) can be written as a product of single-site wave functions. It is this property which permits an exact treatment of the Gutzwiller wave function for bosons.

Wave functions constructed from (3) and (4) are of the "Jastrow"[3] form, i.e., can be written as a product of functions of the interparticle separation $\Pi_{<i,j>}\chi(\mathbf{r}_i - \mathbf{r}_j)|G\rangle$, where i and j run over all pairs of particles. Jastrow wave functions have been extensively studied[4] in the context of ^{4}He, treating $\chi(\mathbf{r})$ variationally. The Gutzwiller ansatz assumes the computationally simple case of $\chi(0) = g$ and $\chi(\mathbf{r}) = 1$ for $\mathbf{r} \neq 0$. This form of χ can describe arbitrary on-site correlations. The presence of linearly dispersing phonon modes, however, requires[5] that $\chi(r)$ tend to $1 - \text{const}/r^2$ as $r \to \infty$, which is not contained in the simple Gutzwiller form. Thus long-wavelength density fluctuations are not properly taken into account by the Gutzwiller ansatz. We note that off-diagonal long-range order is a generic feature of boson-Jastrow wave functions[6] since these states are obtained by modifying the magnitudes but not the phases of free boson states which possess long-range phase coherence. This feature of boson-Jastrow wave functions in general (and the boson-Gutzwiller ansatz in particular) is analogous to the preservation of the discontinuity in the momentum distribution at the Fermi surface[1] in the fermion-Gutzwiller wave function.

Although originally proposed as a variational wave function, the relevance of Gutzwiller states to interacting Fermi systems has been strengthened by the discovery that the completely projected, half-filled, one-dimensional Fermi sea is the exact ground state of an antiferromagnetic spin model with algebraically decaying interactions.[7] It has also been shown[8] that the approximation Gutzwiller introduced for calculating expectation values within the ansatz (2) is equivalent to a saddle-point approximation to a path integral formulation of the Hubbard model. This result and its generalization to include antiferromagnetism becomes exact in the limit of infinite dimensionality.[9] We discuss below the connection between the Bose-Gutzwiller wave function and the exact solution of the Hamiltonian (1) in the limit of large dimensionality.

Using the generalization [(3) and (4b)] discussed above we apply the method of Gutzwiller to lattice bosons interacting via the boson Hubbard model (1). The Bose-Gutzwiller ansatz reduces to a product of single-site wave functions, so that the expectation value per site of the Hubbard Hamiltonian (1) in this variational state is simply

$$\langle H\rangle = -zt\langle a^\dagger\rangle\langle a\rangle + \frac{U}{2}\langle n(n-1)\rangle, \tag{5}$$

where z is the mean number of neighbors per lattice site and $\langle\cdots\rangle$ is evaluated in the single-site state

$$|\Psi\rangle = \sum_n g^{n(n-1)/2}\frac{\lambda^{n/2}}{\sqrt{n!}}|n\rangle. \tag{6}$$

The problem becomes tractable in three interesting limits: (a) for dilute bosons and arbitrary U, when only the first three terms in (6) need be retained; (b) for large U, at a density between two integer densities m and $m+1$, when only the terms corresponding to these two integers need be kept; and (c) at integer densities near the superfluid-solid transition, where number fluctuations are suppressed, so that only $m-1$, m, and $m+1$ need be considered. Below, these variational results are applied to the dilute interacting Bose gas, spin-$\frac{1}{2}$ XY models (ferromagnetic and antiferromagnetic), and liquid helium-4, respectively.

II. THE DILUTE BOSE GAS: PERTURBATION THEORY VERSUS GUTZWILLER

Our understanding of interacting Bose systems is based upon Bogoliubov's[10] analysis of a dilute, weakly interacting Bose gas using the canonical transformation method. Alternately, the same results can be obtained by the summation of an infinite set of "ladder" diagrams[11] in perturbation theory. Although they are generally incalculable for dense or strongly interacting bosons, the general features of (a) a nonzero condensate and (b) a linear dispersion for phonon excitations (corresponding to a finite compressibility) are expected to persist even when perturbation theory is inapplicable.

At density ρ per site, Bogoliubov's theory yields a condensate fraction

$$f \equiv \frac{\langle a^\dagger\rangle^2}{\rho} \approx 1 - \frac{A}{\rho}(\rho u)^{d/2} - \frac{B}{\rho}(\rho u)^2, \tag{7}$$

and an energy per site of

$$E(\rho) \approx \frac{\rho^2 U}{2} + \rho U[C(\rho u)^{d/2} + D(\rho u)^2], \tag{8}$$

where the zero of energy is chosen so that the free Bose gas has energy $E=0$, and where the dimensionless interaction strength

$$u = \frac{U}{2zt} \tag{9}$$

is defined as the ratio of the on-site potential U to the characteristic kinetic energy $2zt$, which is the bandwidth for a bipartite lattice with z nearest neighbors per site. The constants A, B, C, and D are lattice dependent. These expressions are valid when the typical interparticle spacing is much larger than the scattering length, permitting the neglect of three-particle scattering and allowing the depletion of the condensate to be assumed small.

In comparison, Bose-Gutzwiller variational wave functions for dilute Bose gases yield (to lowest order in ρ)

$$f = 1 - \rho\left(\frac{u}{1+u}\right)^2 \tag{10}$$

and

$$E(\rho) = \frac{\rho^2 U}{2}\left(\frac{1}{1+u}\right). \tag{11}$$

The optimal Gutzwiller parameter is $g = 1/(1+u)$, resulting in an on-site density-density correlation $\langle n(n-1)\rangle$ of $\lambda^2 g \approx \rho^2 g$. The Gutzwiller results depend on dimension and lattice structure only through the mean coordination number z.

It is instructive to compare the momentum distributions $n_{\mathbf{k}} = \langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}}\rangle$ of the two approaches. Both calculations yield delta function peaks at $\mathbf{k}=\mathbf{0}$, corresponding to a nonzero condensate fraction. In the Bogoliubov solution the uncondensed particles have $n_{\mathbf{k}}$ varying as k^{-4} for large momenta, while the Gutzwiller distribution is independent of k. Thus the Gutzwiller wave function does not correctly describe long-wavelength correlations, as noted above. A related problem with the boson-Gutzwiller ansatz is presented by the single-mode approximation for the phonon excitation energy, which is found to be quadratic in wave number rather than linear.

III. INFINITE U: FULLY PROJECTED STATES

The case of an infinite Hubbard U (i.e., hard-core bosons) can be solved[12] in the dilute continuum via an expansion in ρa^d, where a is the scattering length; the results correspond to perturbation theory using a pseudopotential to eliminate singularities due to the hard core. The corresponding ground-state wave function[13] never yields a vanishing on-site density-density correlation. The (admittedly simplistic) Gutzwiller variational wave functions do not suffer from this constraint, and can easily be applied to the dense hard-core regime.

Consider the case of density ρ lying between the two integers m and $m+1$, with a large Hubbard U. The appropriate wave function (3) and (4a) is then the fully projected state $|\Psi_{g\to 0}\rangle$, which consists of the equal-amplitude superposition of *all* configurations with m or $m+1$ bosons per site distributed such that the average density is ρ. Without loss of generality we specialize to the case of density between 0 and 1. Expectation values in this fully projected state can be easily computed via combinatorial methods. Alternately we may use the grand canonical state (3) and (4b) which corresponds to the (normalized) single-site wave function $(1-\rho)^{1/2}|0\rangle + \rho^{1/2}|1\rangle$. No variational parameters remain, i.e., $g = 0$. The condensate fraction becomes simply $f = 1-\rho$ and the energy per site $E = -zt\rho(1-\rho)$. In the limit of large U the compressibility remains finite even at densities near one particle per site, as in the Fermi case, and is given by $\kappa = (\rho^2\partial^2 E/\partial\rho^2)^{-1} = 1/(2zt\rho^2)$. The "particle-hole" symmetry relating density ρ and $1-\rho$ is preserved in the Gutzwiller approach.

The fully projected wave function is the equal-amplitude superposition of states $|\mathcal{C}\rangle$ in which each site is either empty or singly occupied and the overall density of occupied sites is ρ: $|\Psi_{g\to 0}\rangle = \sum |\mathcal{C}\rangle$. (Only these configurations survive the complete Gutzwiller projection.) A simple method[14] can be used to construct a short-ranged Hamiltonian which has this equal-amplitude state as its ground state, as follows. First, recall that the ground state of a Hamiltonian whose off-diagonal matrix elements are all negative is the unique nodeless eigenstate of that Hamiltonian. We now show that the (nodeless) state $\sum |\mathcal{C}\rangle$ is in fact an eigenstate of a Hamiltonian with infinite on-site repulsion and a nearest-neighbor interaction. The kinetic energy operator $\hat{T}$ acting on this state yields $-t\sum \nu(\mathcal{C})|\mathcal{C}\rangle$, where $\nu(\mathcal{C})$ is the number of nonmultiply occupied configurations which can be reached from $\mathcal{C}$ by hopping a single particle. Therefore $\nu(\mathcal{C})$ counts the number of empty sites in configuration $\mathcal{C}$ which are adjacent to an occupied site:

$$\nu(\mathcal{C}) = \tfrac{1}{2} \sum_{<ij>} [n_i(1-n_j) + n_j(1-n_i)], \tag{12}$$

where the sum is over pairs of nearest-neighbor sites. If we then consider a potential energy term $\hat{V}(\mathcal{C}) = +t\nu(\mathcal{C})$ (corresponding to a nearest-neighbor interaction in addition to the infinite on-site repulsion), the equal-amplitude state will be an eigenstate (with zero energy) of the operator $\hat{T}+\hat{V}$. Thus the equal-amplitude state is the ground state of this short-ranged Hamiltonian.

IV. THE SPIN-$\frac{1}{2}$ XY MODEL

Following Matsubara and Matsuda,[15] we may represent spin-$\frac{1}{2}$ magnets as lattice hard-core Bose gases: down spins correspond to unoccupied sites and up spins correspond to occupied sites. The nearest-neighbor XY model then precisely corresponds to (1), with $t = -J_{xy}$ and $U = \infty$. The appropriate Gutzwiller states are the fully projected states discussed in the previous section.

Consider first the ferromagnetic XY model on an L site lattice. The corresponding noninteracting boson ground state is obtained by macroscopically occupying the $\mathbf{k} = 0$ single particle state, as in (4a). Let the occupation of this state be denoted by N. Completely projecting out multiple occupancy ($g = 0$) we arrive at the equal-amplitude superposition of all spin configurations with N up spins. We find that the minimum energy is achieved for $N = L/2$. This spin state is simply the result of applying the total spin lowering operator $L/2$ times to the ferromagnetic state with all L spins up. Its long-range magnetic order in the xy plane corresponds to the superfluidity of the related boson state.

On a bipartite (e.g., square) lattice, the ferromagnetic and antiferromagnetic XY models are related by a transformation which rotates the spins on one of the sublattices by π about the $\mathbf{y}$ axis. Equivalently, one may macroscopically occupy the $\mathbf{k} = (\pi,\pi)$ free particle state, which is the lowest energy free particle state for $J > 0$ [$t < 0$ in (1)]. The analysis of the previous paragraph then applies with only minor modifications, and the best variational state of the form (3) and (4a) is again a superposition of all spin configurations $\mathcal{C}$ having $L/2$ spins up. In this superposition, configuration $\mathcal{C}$ has amplitude $(-1)^{\mu(\mathcal{C})}$, where $\mu(\mathcal{C})$ is the number of up spins on one of the two sublattices. This amplitude explicitly satisfies the Marshall sign rule,[16] a requirement for the true antiferromagnetic XY ground state. Our variational state has perfect long-range staggered magnetic order in the xy plane. This state has been considered previously[17] in variational studies of the square lattice spin-$\frac{1}{2}$ XY model, and its energy $E = -J$ per site is quite close to numerical estimates[18] ($E \approx -1.08J$ per site). Of course, much more sophisticated variational wave functions of the Jastrow form have been applied to models mentioned here. What is remarkable about the simple Gutzwiller ansatz is its quite reasonable performance despite the absence of any variational parameters.

V. THE SUPERFLUID-SOLID TRANSITION

At integer fillings, an interacting Bose lattice gas undergoes a transition from a superfluid to a solid as the on-site repulsion U is increased, similar to the Mott metal-insulator transition for fermions. This transition has recently been studied in low-dimensional Bose-Hubbard models using quantum Monte Carlo techniques.[19,20] In contrast with the spin-$\frac{1}{2}$ Fermi gas on a bipartite lattice, which is an insulator at half-filling for arbitrary positive U due to the formation of a commensurate spin density wave, the corresponding Bose gas remains a conductor up to a critical interaction strength U_c. The difference is the absence of occupied states at momenta $\pm\pi/2$ in the weakly interacting Bose gas, which renders the system insensitive to umklapp scattering at small U.

Brinkman and Rice[21] have shown that within the Gutzwiller ansatz *and* in Gutzwiller's statistical approximation, a half-filled band of spin-$\frac{1}{2}$ fermions becomes insulating at a critical value of the interaction parameter. At this U_c, the Gutzwiller variational parameter is driven to zero: for $U \geq U_c$ the best variational wave function of the Gutzwiller form (2) has exactly one particle per site. Accompanying the vanishing of g is a diverging effective mass, a vanishing compressibility, and a vanishing quasiparticle residue (computed from the discontinuity in the momentum distribution function at the Fermi surface). When the energy of the fermion-Gutzwiller wave function is evaluated exactly,[22] however, the best variational wave function always has *nonzero* g of order t/U, and has a discontinuity at the Fermi surface. Thus the transition found by Brinkman and Rice is an artifact of Gutzwiller's statistical approximations for evaluating the free energy.

As in the analogous fermionic transition, the Bose solid-superfluid transition occurs only when the density of particles is commensurate with the lattice. The boson-Gutzwiller ansatz admits a simple calculation of the superfluid-solid transition which can be carried out without recourse to further approximations. Unlike the fermion case, the boson-Gutzwiller ansatz alone *does* yield a finite-U transition. We consider an integer density lattice gas near its Mott transition. (Without loss of generality, let $\rho = 1$.) Since number fluctuations are suppressed near U_c, we are justified in retaining only states with 0, 1, or 2 particles per site, i.e., taking the limit $g \to 0$, $g\lambda = \text{const}$ in (3) and (4b). For U approaching U_c from below, the condensate fraction, energy per site, and on-site density-density correlations are

$$f = \frac{\alpha^2}{2}\left[1 - \left(\frac{u}{u_c}\right)^2\right] , \tag{13}$$

$$E = \frac{-zt\alpha^2}{4}\left(1 - \frac{u}{u_c}\right)^2 , \tag{14}$$

and

$$\langle n(n-1)\rangle = \frac{1}{2}i\left(1 - \frac{u}{u_c}\right) , \tag{15}$$

where $\alpha = (1+\sqrt{2})/2$. (Note that the condensate fraction plays the role of the quasiparticle weight in the fermion case.) In the Gutzwiller approximation, the critical interaction strength u_c is given by $u_c = U_c/2zt = \alpha^2 \approx 1.45$. For comparison, quantum Monte Carlo calculations in one dimension yield[19] $u_c = 1.2$ and in two dimensions give[20] $u_c = 2.1$. As u_c is approached from below, the compressibility vanishes linearly as

$$\kappa = \frac{\sqrt{2}}{4zt}\left(1 - \frac{u}{u_c}\right) . \tag{16}$$

Above U_c, the optimal Gutzwiller parameter g is zero. The variational wave function is then the insulating state with precisely one boson per site, so that $E = f = \langle n(n-1)\rangle = 0$. For large U, this insulating state has a charge gap $\Delta \equiv E_{N+1} + E_{N-1} - 2E_N$ of $U - zt$. Approaching U_c from above, this "Mott gap" collapses as

$$\Delta = 2\sqrt{2\sqrt{2}zt}(u - u_c)^{1/2} . \tag{17}$$

Not surprisingly, our factorizable variational states yield mean-field exponents for the superfluid-solid transition, rather than the correct $d+1$-dimensional XY behavior.[23]

VI. CONNECTION WITH MEAN-FIELD THEORY

In the fermionic case the Gutzwiller approach to the Hubbard model involves two approximations: (a) the Gutzwiller ansatz itself and (b) the Gutzwiller statistical approximation for evaluating the energy of the trial wave function. Considerable effort has been devoted to finding limits in which these approximations become exact. Only recently, Metzner and Vollhardt[9] have shown that step (b) in the Gutzwiller approach is exact in the limit of infinite dimensionality. The ansatz (2) itself does not seem to become exact in any limiting situation. In contrast, the generalized Gutzwiller ansatz (3) and (4) for the *bosonic* case is exact in the limit of infinite dimensions, i.e., the infinite range hopping model where i and j of Eq. (1) runs over all possible pairs of lattice sites has a ground state of the form (3). The function $\gamma(n)$ is determined by the condition that the state $\sum_n \gamma(n)|n\rangle$ is the ground state of the single-site mean-field Hamiltonian h_{MF} given by

$$h_{\text{MF}} = -\frac{zt}{2}(\langle a\rangle a^\dagger + a\langle a^\dagger\rangle) + V(a^\dagger a) . \tag{18}$$

In principle this defines the best trial wave function for a given Hamiltonian, but it is difficult to solve in practice except when the potential energy assumes the simplified form $V(n) = \infty$ for $n > 2$.

Why does the boson-Gutzwiller state experience a fluid-insulator transition at a finite interaction strength, while the fermion-Gutzwiller state does not? The reason for this difference lies in the properties of the free particle states which are used in the construction of these wave functions. In both cases, at commensurate densities and for large U, the determining factor is whether or not a *partially* projected wave function ($g \neq 0$), which is described by a small density of empty and doubly occupied sites in a sea of singly occupied sites, can realize a lower energy than the *fully* projected wave function ($g = 0$), which consists of precisely one particle per site. In particular, the energy of the partially projected state will be lower (even for large U) if the empty and doubly occupied sites are correlated so that the matrix elements connecting states with two singly occupied sites and states with nearby empty and doubly occupied sites are enhanced relative to a random distribution of such sites, i.e., if the system can realize an energy gain of order t^2/U by having g different from zero.

The question of the correlation between the nonsingly occupied sites in partially projected states is related to density fluctuations in the corresponding free particle states, which is in turn determined by the compressibilities of these states. Since the free Fermi sea has a nonzero compressibility we expect that empty and doubly occupied sites in the related projected state will be more likely to occur near one another, leading to a small ($g \approx t/U$) nonzero projection even for large U. On the other hand, the free Bose gas is infinitely compressible. In the nearly completely projected Bose wave function at a density of one particle per site, the nonsingly occupied sites will be completely uncorrelated, so that there is no energetic reason (within the framework of the Gutzwiller variational states) for retaining such sites for large U.

VII. HELIUM-4

Anderson and Brinkman[24] have suggested that liquid ^{3}He can be viewed as a "nearly localized Fermi-liquid," i.e., a strongly correlated liquid close to its solidification point. This physical picture has been elaborated and quantified by Vollhardt *et al.*,[25] using the results Brinkman and Rice obtained with the Gutzwiller approximation. To compute the properties of a strongly interacting Fermi fluid, such as ^{3}He, the liquid is modeled by a lattice gas of fermions at a density of one per unit cell. (This is not to suggest that ^{3}He, is a lattice system; rather, one imagines coarse graining the helium liquid to obtain an effective lattice model with parameters t and U which are related to the bare kinetic and interaction energies.) The Fermi liquid parameters $m^*, F_o^s, F_o^a, \ldots$, corresponding to a given U/t and filling factor are then computed.

Even though the boson-Hubbard model lacks some essential features of ^{4}He, such as an attractive long-range van der Waals attraction, it is nevertheless amusing to compare the results of the simple calculation given above with experiment in ^{4}He. For simplicity let us assume U is large so that we can use fully projected states. Using the experimentally determined zero temperature condensate fraction $f \approx 0.10 \pm 0.02$ we find that $\rho \approx 0.9$. From the experimentally determined chemical potential $\mu = -7.1$ K we determine that $zt \approx -9.0$ K. The Gutzwiller prediction for the sound velocity is then 1.8×10^4cm/sec, which compares favorably with the experimental value of $c = 2.4 \times 10^4$ given the simplicity of our approach. The agreement is much less dramatic than in the spin-$\frac{1}{2}$ fermion case, with its multitude of "Fermi liquid" parameters, since the spinless boson gas has only these two "Bose liquid" parameters. Given a model for U and ρ as a function of pressure, one could study the dependence of c and f on pressure at zero temperature along the lines of Ref. 25.

Note added: After completing this work we received a prepublication copy of work by Krauth, Caffarel, and Bouchaud[26] describing similar boson-Gutzwiller calculations.

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