Gutzwiller wave function for a model of strongly interacting bosons

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We study a model of strongly interacting lattice bosons with a Gutzwiller-type wave function that contains only on-site correlations. The variational energy and the condensate fraction associated with the variational wave function are exactly evaluated for both finite and infinite systems and compared with exact quantum Monte Carlo results in two dimensions. This ansatz for the wave function gives the correct qualitative picture of the phase diagram of this system; at commensurate densities, this system enters a Mott-insulator phase for large values of the interaction.

Strongly interacting boson systems have been extensively studied for a long time. Apart from the usual λ transition between the superfluid and the normal liquid at a given temperature, systems of bosons in an external potential may also undergo a superfluid-insulator transition at $T=0$ upon a change of strength in the interaction or the conditions of the environment. Such a phase transition has recently been studied in several works for a model of strongly interacting lattice bosons interacting with a repulsive on-site interaction. The model described by the Hamiltonian

$$H=\frac{-t}{2}\sum_{\langle i,j\rangle}(a_i^\dagger a_j+\text{H.c.})+\frac{U}{2}\sum_i n_i(n_i-1) \qquad (1)$$

is the focus of the present Brief Report. It describes a system of M bosons on a lattice with N sites in d dimensions. This system exhibits a superfluid phase for all values of the interaction U and noncommensurate densities; i.e., $\rho=M/N$ not an integer. Indeed, some particles can always gain kinetic energy at no cost in potential energy by hopping to sites occupied by a smaller number of particles. At commensurate densities (i.e., integer ρ), the model also exhibits a superfluid phase at small U/t since the penalty in potential energy is not large enough to offset the gain in kinetic energy that delocalizes the particles. However, for large enough interaction, this is no longer true, and the system is trapped into a Mott-insulator state. Accordingly, there exist two transitions from the superfluid phase to the Mott-insulator phase: (i) when U/t approaches some critical value U_c/t at commensurate (integer) densities n_c and (ii) when the density ρ approaches n_c at large on-site repulsion U/t.

A scaling theory of these transitions has been worked out by Fisher *et al.*[1] They have shown that transition (i) is in the universality class of the $(d+1)$-dimensional XY model, whereas (ii) is described correctly by mean-field theory in any dimension.

Apart from considerations of universal quantities, the explicit phase diagram of this system is of interest. These questions have recently been addressed in exact path-integral Monte Carlo (PIMC) simulations in both one and two dimensions.[2,3] More general, if approximate, information is provided by mean-field theory, in which the location of the phase boundaries can also be determined. A mean-field-theory treatment of this model has been indicated in the work by Fisher *et al.*[1]

In this work we present an exact variational calculation with a Gutzwiller-type wave function

$$\Psi(n_1,n_2,\ldots,n_N)=\prod_{i=1}^{N} f(n_i)\,\delta\left[\sum_{i=1}^{N} n_i-M\right], \qquad (2)$$

for both finite and infinite lattices. This wave function does not incorporate any information on the geometry or dimensionality of the lattice and is therefore also mean field in nature. In particular, it does not include long-range correlations arising from zero-point phonons: These must be described by a Jastrow factor of the type $\exp[\sum_{i<j} g(r_i-r_j)]$ multiplying Eq. (2), with $g(r)$ decaying as r^{-2} for large r.[4] This term would ensure a correct behavior of the structure factor $S(k)$ for small k and hence the correct spectrum for low-energy excitations. However, inclusion of this factor ruins the appealing feature of Eq. (2), namely, that it leads to an explicit solution for all values of the interaction U/t and density ρ.

We use two variational approaches: a *general* minimization with respect to the $\{f(n), n=0,1,\ldots\}$ and a simplified approach in which $f(n)$ is *parametrized* according to

$$f(n)\sim \exp(-\kappa n^2/2)/\sqrt{n!}\,, \qquad (3)$$

and where the optimal parameter κ minimizing the ener-

gy is sought. This parametrization corresponds (in position representation) to a wave function with a contact term $\Psi(r_1,r_2,\ldots,r_M)=\exp[-\kappa/2\sum_{i<j}\delta(r_i-r_j)]$. As we shall see, the two approaches are equivalent for all intents and purposes: They give the same asymptotic behavior $[U/t\to U_c/t=d(\sqrt{n_c}+\sqrt{n_c+1})^2]$ for commensurate densities $\rho=n_c$ and at $U/t=\infty$ for incommensurate densities, and agree closely in the numerical values for the energy and momentum condensate. As the critical value U_c/t (at $\rho=n_c$) is approached from below, there is a second-order phase transition from the superfluid into a Mott insulator with an energy per particle, $E\sim-(U_c-U)^2$, below the transition and $E=0$ above it. As the parameterized form of the wave function is considerably simpler to evaluate for the finite systems (which we can then compare to the exact numerical calculations), we shall base much of our detailed calculations on this version.

We are also able to calculate the condensate fraction associated with the wave function (the Fourier transform at $k=0$ of the one-body density matrix), $n(k=0)$. One obtains $n(k=0)\sim U_c-U$ below the transition and $n(k=0)=0$ above it. For incommensurate densities the condensate fraction is strictly positive for any value of U, demonstrating that the system is always superfluid. We given an explicit formula for $n(k=0)$ as a function of the density ρ.

We have in addition performed high-precision simulations of the two-dimensional model ($d=2$) using a zero-temperature diffusion Monte Carlo scheme[5] [it is for this reason that we use a canonical formulation in Eq. (2)]. This allows us to compare the variational energy (at finite N) with the exact energy at all values of the parameters, especially away from the critical point where the solution is expected to be accurate. The exact energy for a system with 16 bosons ($\rho=1$, $d=2$), e.g., is found to be off by about 20% at $U/t=6$, by 5% at $U/t=4$, and by 1.5% at $U/t=2$. The critical interaction $U_c/t=6+4\sqrt{2}\sim11.66$ (at density $\rho=1$, in two dimensions) compares well with the value of $U_c/t\sim8.5$ found in a previous work[2] from two-dimensional PIMC simulations.

We now present the calculations for this model. The norm of the wave function is given by

$$\langle\Psi|\Psi\rangle=\prod_{i=1}^{N}\left[\sum_{n_i}f^2(n_i)\right]\delta\left[\sum_{i=1}^{N}n_i-M\right]. \tag{4}$$

This can be written as

$$\langle\Psi|\Psi\rangle=\int_{-\pi}^{\pi}\frac{d\lambda}{2\pi}\exp Ng(f,\lambda), \tag{5}$$

$$g(f,\lambda)\equiv-i\lambda\rho+\ln\left[\sum_{n=0}^{\infty}f^2(n)\exp(i\lambda n)\right]. \tag{6}$$

Similarly, we find, for the potential and kinetic energies,

$$\langle\Psi|\begin{Bmatrix}E_{\rm pot}\\ \\ E_{\rm kin}\end{Bmatrix}|\Psi\rangle=N\int_{-\pi}^{\pi}\frac{d\lambda}{2\pi}\exp[Ng(f,\lambda)]\begin{Bmatrix}\tilde{E}_{\rm pot}(f,\lambda)\\ \\ \tilde{E}_{\rm kin}(f,\lambda)\end{Bmatrix}, \tag{7}$$

with

$$\tilde{E}_{\rm pot}(f,\lambda)=\frac{U}{2}\frac{\sum n(n-1)f^2(n)\exp(i\lambda n)}{\sum f^2(n)\exp(i\lambda n)} \tag{8}$$

and

$$\tilde{E}_{\rm kin}(f,\lambda)=-dt\exp(i\lambda)\frac{[\sum\sqrt{n+1}f(n)f(n+1)\exp(i\lambda n)]^2}{[\sum f^2(n)\exp(i\lambda n)]^2}. \tag{9}$$

For the given wave function, the condensate fraction is proportional to the kinetic energy per particle. We find that $n(k=0)=-1/(dN)E_{\rm kin}$.

For finite systems the integrals [Eqs. (5) and (7)] have to be calculated explicitly. In the $N\to\infty$ limit, of course, the integrals are given by the values of the integrands at their saddle point $\bar{\lambda}$, which is located at $\bar{\lambda}=0$, provided that $\rho=\sum_{n=0}^{\infty}nf^2(n)/\sum_{n=0}^{\infty}f^2(n)$ [cf. Eq. (6)]. Under this condition [and considering properly normalized wave functions $\sum_{n=0}^{\infty}f^2(n)=1$], the energy per particle is given by

$$E=-\frac{dt}{\rho}\left[\sum_{n=0}^{\infty}\sqrt{n+1}f(n)f(n+1)\right]^2+\frac{U}{2\rho}\sum_{n=0}^{\infty}n(n-1)f^2(n). \tag{10}$$

From this equation we can now obtain the optimal values of the parameters $f(n)$, $n=0,\ldots,\infty$, by solving for $\partial E/\partial f(n)=0$ (under the constraints stated above). This can easily be done by iteration.

Equation (10) can also be solved asymptotically in the limit $U/t\to U_c/t$, for commensurate densities n_c, and $U/t\to\infty$ (for incommensurate densities). In fact, we can show that a self-consistent ansatz for $f(n)$ close to the transition is given by $f(n_c)=\sqrt{1-2\epsilon}$ and $f(n_c\pm1)=\sqrt{\epsilon}$ with $\epsilon\ll1$ and $f(n_c\pm2)\ll\sqrt{\epsilon}$, etc. In this limit the energy [Eq. (10)] reduces to

$$E=-\frac{dt}{n_c}\epsilon(1-2\epsilon)(\sqrt{n_c}+\sqrt{n_c+1})^2+\frac{U}{2n_c}[2\epsilon+n_c(n_c-1)]. \tag{11}$$

A simple derivation of E with respect to ϵ shows that the probability ϵ to have $n_c\pm1$ particles on one site vanishes at the critical interaction $U_c/t=d(\sqrt{n_c}$

$+\sqrt{n_c+1})^2$. Close to the transition ($\Delta = U_c/t - U/t$), the energy is given by

$$E(\Delta) = \frac{-\Delta^2}{4n_c U_c} . \tag{12}$$

For $U > U_c$ we find that $E_{\rm kin} = 0$, $E_{\rm pot} = U/2(n_c - 1)$.

Our complete results for the commensurate case $\rho = 1$ are presented in Figs. 1–3. In Fig. 1 we show the evolution of the probability to have a site occupied by n particles, $f^2(n)$, with U/td for $n = 0,1,2,3,4$ [cf. Eq. (10)]. Note that $f^2(n)$ quickly becomes extremely small for $n \geq 3$.

In Fig. 2 we show the energy per particle of the system as a function of the variational parameter κ for different values of the interaction ($U/td = 1,3,5,7$) for a finite lattice with size $N = 16$ [from Eq. (7)] and for the infinite lattice [from Eqs. (8) and (9)]. The optimal value of the parameter, $\kappa_{\rm opt}$, is marked also. The variational energy $E(\kappa_{\rm opt})$ is on this scale indistinguishable from the one given by the more general $E[\{f(n)\}_{\rm opt}]$.

The inset in Fig. 2 gives the value of $\kappa_{\rm opt}$ as a function of U, as determined numerically, both for the finite and infinite systems, where it diverges as $\kappa_{\rm opt} \sim \ln(U_c/t - U/t)$.

Figure 2 contains one more important piece of information. The horizontal lines underneath each curve for the finite system give the *exact* value of the ground-state energy for the corresponding two-dimensional (2D) system (with $N = 16$), as determined with a pure-diffusion Monte Carlo method.[5] For example, we find a ground-state energy per particle of $E = -0.511 \pm 0.002$ at $U/t = 6$ (in 2D), whereas the variational energy is $E_{\rm var} = -0.401$ for the optimal solution $\{f(n)\}$ and $E_{\rm var} = -0.388$ for the wave function parametrized according to Eq. (3). The agreement of the variational energy with the exact solution is good, considering the simplicity of the wave function.

In Fig. 3 we show the values of the momentum condensate for this case of $\rho = 1$, both for the finite case $N = 16$ and in the infinite system and compare them to the *exact* superfluid density at $N = 16$ (cf. Ref. 2). The numerical calculation of the momentum condensate, although in principle possible,[6] has not been carried out for this model, in contrast to the (more interesting) superfluid density.

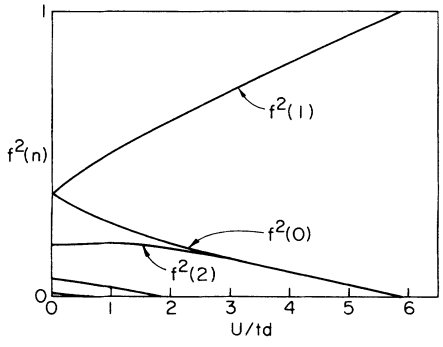

FIG. 1. Probability $f^2(n)$ of a site to be occupied by n particles vs interaction U/td for $n = 0,1,2,3,4$.

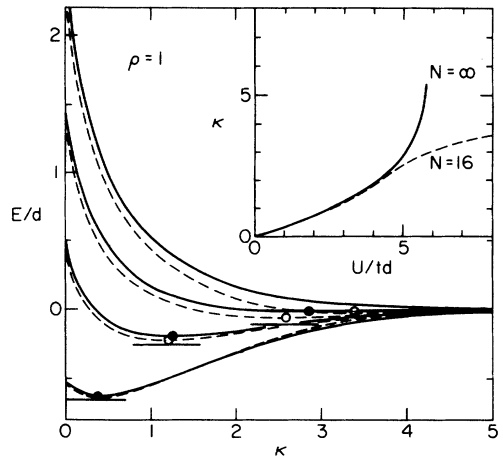

FIG. 2. Variational energy (scaled by the dimension of the lattice) E/d vs variational parameter κ at density $\rho = 1$ for $U/td = 1,3,5,7$ (from below). $N = \infty$ (solid line, solid circles) and $N = 16$ (dashed line, open circles). The exact ground-state energies for $N = 16$ in two dimensions are indicated by horizontal lines. The inset gives the optimal values of the variational parameter, $\kappa_{\rm opt}$, as a function of U/td for both $N = 16$ and ∞.

As is well known,[7,8] there is no direct relationship between the two quantities away from the small-U/t region, where the agreement is excellent. In general, the fact that $n(k) > 0$ only allows us to conclude that the trial wave function describes a superfluid. For $N = \infty$, $n(k)$ goes to zero as $(U_c - U)/4dtn_c$ at the transition into the insulating state. In two dimensions the transition takes place at an interaction strength of $U_c/t = 11.66$, which compares well with the exact value from the PIMC simulations, which yield $U_c/t \sim 8.5$. The critical exponent, of course, coincides with the mean-field one and cannot be expected to coincide with that (~ 0.669) predicted by the scaling theory of Fisher *et al.*[1]

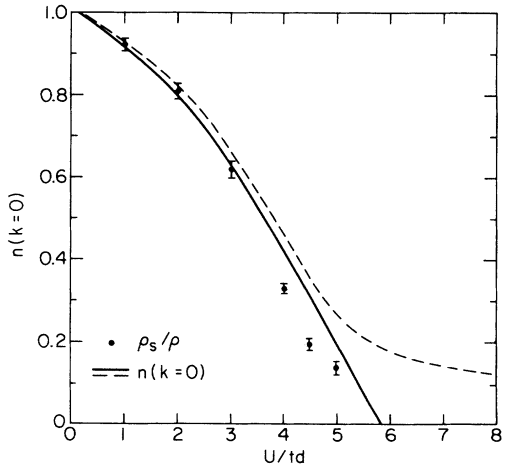

FIG. 3. Variationally calculated values of the momentum condensate $n(k = 0)$ vs interaction (scaled by the dimension) U/td for density $\rho = 1$. $N = \infty$ (solid line) and $N = 16$ (dashed line). Also shown are the exact values of the superfluid density ρ_s/ρ for the system with $N = 16$ in 2D.

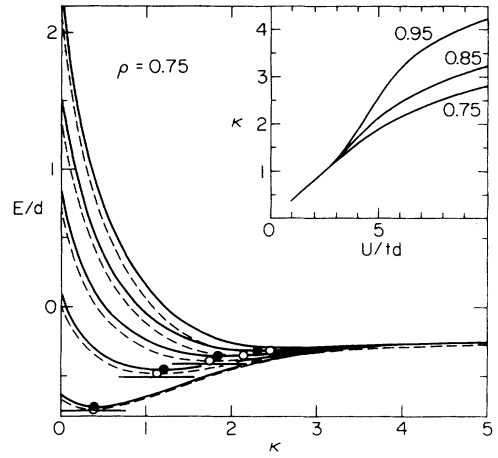

FIG. 4. Variational energy E/d vs κ at density $\rho=0.75$ for $U/td=1,3,5,7,9$ (from below). $N=\infty$ (solid line, solid circles) and $N=16$ (dashed line, open circles). The exact ground-state energies for $N=16$ in two dimensions are indicated by horizontal lines. The inset gives the optimal values of the variational parameter, $\kappa_{\rm opt}$, as a function of U/td at $N=\infty$ for densities $\rho=0.75,0.85,0.95$.

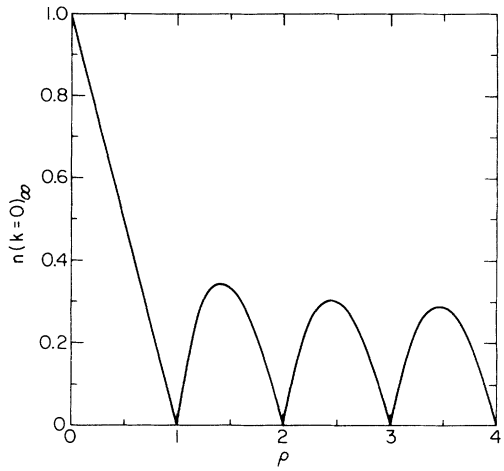

FIG. 5. Variationally calculated momentum condensate $n(k=0)$ vs density ρ.

At a general incommensurate density ρ $(n_c-1<\rho<n_c)$ and $U/t=\infty$, we can again perform an asymptotic analysis with a self-consistent ansatz $f(n_c-1)=a$ and $f(n_c)=(1-a^2)^{1/2}$. A calculation analogous to the one presented for the commensurate case now yields

$$\tilde{E}_{\rm pot}(\kappa)\rightarrow\frac{U(n_c-1)(2\rho-n_c)}{2\rho}\ , \tag{13}$$

$$\tilde{E}_{\rm kin}(\kappa)\rightarrow-dt\frac{n_c(n_c-\rho)[\rho-(n_c-1)]}{\rho}\ . \tag{14}$$

Complete results for the incommensurate case $\rho=0.75$ are given in Fig. 4. In the main picture we show again the energy per particle as a function of the variational parameter κ for different values of the interaction $(U/td=1,3,5,7,9)$ for a finite lattice with size $N=16$ and for the infinite lattice. The optimal value of the parameter, $\kappa_{\rm opt}$, and the *exact* ground-state energies for $N=16$ (in 2D) are also marked. The inset in Fig. 4 gives the value of $\kappa_{\rm opt}$ as a function of U/td for the infinite system (the asymptotic behavior is $\kappa\sim-\ln[2d(1-\rho)]+\ln(U_c-2d)$).

Finally, we show in Fig. 5 the variationally calculated momentum condensate $n(k=0)$ at $U/t=\infty$ as a function of ρ at $N=\infty$. From Eq. (14) we can see that $n(k=0)=n_c(n_c-\rho)[\rho-(n_c-1)]/\rho$. For large values of the density $(n_c-1<\rho<n_c$, with $n\rightarrow\infty)$, the momentum condensate is therefore given by the formula $n(k=0)\sim(n_c-\rho)[\rho-(n_c-1)]$, with a *finite* maximum value of $n(k=0)=\frac{1}{4}$ for $\rho=n_c-\frac{1}{2}$.

In conclusion, we have given a complete treatment of the problem of strongly interacting lattice bosons in terms of a Gutzwiller variational wave function. It will be interesting to see whether this approach can be extended successfully to provide a suitable starting point for calculations on more difficult problems, such as the one of disordered bosons.[9,1]

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