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Variational calculations for the Sutherland model

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A system of fermions or bosons interacting in one dimension via a two-body potential of the form $V(r)=g/r^2$ is known to have a ground state of Jastrow type. The boson system is explored in this paper within the hypernetted-chain scheme to study the various ground-state properties, and the results are compared with the exact results available for this system. The results are expected to have important bearing on spin correlations in the Gutzwiller state.

Recently, there has been an upsurge of interest in the Gutzwiller type of wave functions to describe strongly correlated electron systems.[1-7] The accurate Monte Carlo calculations[1-3] of the various ground-state properties of interacting fermions on a one-dimensional lattice have also been supplemented by analytic results,[4] in particular, on spin correlation functions. The latter work has recently motivated Shastry[5] and Haldane[6] to explore the Gutzwiller wave function as a spin wave function. Shastry and Haldane observed the following interesting results: The $s=\frac{1}{2}$ one-dimensional (1D) isotropic Heisenberg antiferromagnet with an exchange coupling falling off as the inverse square of the distance between sites has a singlet ground state of Jastrow form. This state was also found to be identical to the Gutzwiller wave function for the Hubbard chain and also to the 1D version of the resonating-valence-bond (RVB) state of Anderson.[3,7] The Shastry-Haldane work was based on what we call the *Sutherland model* in the present work.

Sutherland[8] investigated the ground state for a system of bosons (or fermions) interacting in 1D via a two-body potential of the form $V(r)=g/r^2$. The interesting result of that investigation was that the ground-state wave function was found to be of Jastrow form. He also noticed that the square of the wave function is identical with the probability distribution function from the theory of random matrices.[9,10] This identification then allowed for the exact determination of the pair-correlation functions, one-particle density matrices, and the momentum distribution functions for a few values of the parameter g (in fact, only for $g=-\frac{1}{2}$, 0, and 4). The Shastry-Haldane work is a discretized form of the continuum 1D Bose model of Sutherland. Their result corresponds to the case of $g=4$. Other interesting facts about the g/r^2 potential have been discussed at length by Sutherland in Ref. 8.

While the simple model of Sutherland is quite remarkable because in this case the ground state is exactly known and it provides the exact results for the various ground-state properties mentioned above, calculation of these quantities for values of g other than the ones stated above, or for higher dimensions, and extension to multicomponent systems is, however, not possible. On the other hand, for the Jastrow wave functions, a natural and quite reliable calculational scheme is the hypernetted-chain (HNC) scheme, where such a generalization, if required, could be achieved. In this paper, we have applied the HNC procedure in the continuum limit to obtain the ground-state properties mentioned above for various values of g. The primary aim of the present work is to assess the reliability of the approximate scheme compared with the exact result. A discrete version of the present work, which should be comparable with the Shastry-Haldane work, is currently under investigation and will be published later.

Let us first consider the pair-correlation functions. The case of $g=0$ corresponds to free fermions (one spin state) or bosons with an infinite hard core. The pair-correlation function is then simply (in the following, the particle density is taken to be $d=1$)

$$G(r)=1-[s(r)]^2,\quad s(r)\equiv\frac{\sin\pi r}{\pi r}, \tag{1}$$

and is plotted in Fig. 1. For $g>0$, we have solved the HNC equations following Ref. 11. The method is briefly described as follows: The ground-state wave function is written in the Jastrow form as

$$\Psi=\exp\left[\frac{1}{2}\sum_{i<j}u(r_{ij})\right], \tag{2}$$

where $u(r)$ is assumed to be a real function of r and vanishes for larger r. The expectation value of the Hamiltonian (in this case, the Sutherland Hamiltonian) is then ex-

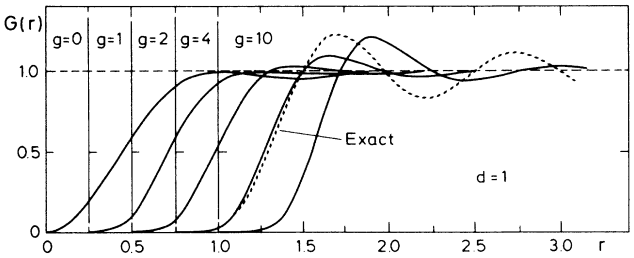

FIG. 1. Pair-correlation functions for various values of the parameter g obtained within the HNC scheme. The dashed curve marked *exact* is the exact result for $g=4$ from Ref. 8.

pressed in terms of the radial distribution function $G(r)$ as ($\hbar^2/m=1$)

$$E=\frac{1}{8}N\int dr\frac{\partial u(r)}{\partial r}\frac{\partial G(r)}{\partial r}+\frac{1}{2}N\int dr\,V(r)G(r)\,. \tag{3}$$

The HNC scheme then relates $u(r)$ with $G(r)$ (ignoring the *elementary* or *bridge* diagrams) in the following manner:

$$u(r)=\ln G(r)-G(r)+1+\frac{1}{2\pi}\int\left[1-\frac{1}{S(k)}\right]e^{i\mathbf{k}\cdot\mathbf{r}}\,, \tag{4}$$

where $S(k)$ is the static structure function. Substituting Eq. (4) in Eq. (3), one obtains the energy expression in terms of $G(r)$ only. The optimal pair-correlation function is then obtained by minimizing the energy with respect to arbitrary variations of $G(r)$, and solving the Euler-Lagrange equation numerically.[11] This procedure has been extended also to incorporate different species of particles.[12] The results for $G(r)$ from the above-mentioned procedure are plotted in Fig. 1 for $g=1$, 2, 4, and 10. With increasing g, we obtain more structures in $G(r)$ with an overshoot developing for $g\geq 2$, indicating that the system is gradually transformed into an ordered (short-range) state. For $g=4$, the exact result obtained by Sutherland,

$$G(r)=1-[s(r)]^2-\left[\int_0^{2r}s(z)dz\right]\left[\frac{1}{2}\frac{ds(2r)}{dr}\right]\,, \tag{5}$$

is also plotted in Fig. 1. The comparison between the HNC and the exact result is quite good for small interparticle separation. However, Sutherland noted that for increasing values of g (the interaction, thus, becoming more repulsive), the system is more nearly ordered on a lattice. This is not well reproduced by the uniform density calculation of HNC. The discrete version of the present HNC scheme should be more appropriate to compare at this value of g. For large values of g (e.g., for $g=10$), the HNC result also indicates the ordering (short range) of the system, where a large overshoot in the correlation function and the subsequent structures start to appear.

The one-particle density matrix is defined as

$$n(r-r')=\frac{N}{\mathcal{N}}\int dr_1\ldots dr_{N-1}\Psi^*(r_1,\ldots,r_{N-1},r')\times\Psi(r_1,\ldots,r_{N-1},r)\,, \tag{6}$$

where $\mathcal{N}$ is the normalization integral. The density matrix is normalized such that $n(0)=d$ where d is the particle density. The momentum distribution function $n(k)$, which is the average number of particles with momentum $\mathbf{k}$, is just the Fourier transform of $n(r)$. It is normalized in the manner $\int n(k)\,dk=d$.

In contrast to the pair-correlation functions discussed above, the momentum distributions and the density matrices, in fact, depend on the statistics of the particles. In the case of $g=0$, one obtains for the free fermions,

$$n(r)=\frac{\sin(\pi dr)}{\pi r}\,,\quad n(k)=\begin{cases}\dfrac{1}{2\pi}, & |k|<\pi d\,,\\ 0, & |k|>\pi d\,.\end{cases} \tag{7}$$

For particles obeying Bose statistics, Sutherland[8] found that there is no Bose condensation into a single momentum state. Also, the momentum distribution diverges as $1/\sqrt{|k|}$ at the origin.

For $g=4$, the exact results for $n(r)$ and $n(k)$ were derived for bosons by Sutherland[8] as

$$n(r)=\frac{\mathrm{Si}(2\pi dr)}{2\pi r}\,,\quad \mathrm{Si}(r)\equiv\int_0^r\frac{\sin y}{y}dy\,, \tag{8}$$

$$n(k)=\begin{cases}\dfrac{1}{4\pi}\ln(2\pi d/|k|), & |k|\leq 2\pi d\,,\\ 0, & |k|\geq 2\pi d\,.\end{cases}$$

The momentum distribution function, therefore, exhibits a weak (logarithmic) singularity at zero momentum.

It is interesting to note that the density matrix in Eq. (8) is identical to the spin correlations for the spin-singlet Gutzwiller-RVB state for the Heisenberg model

$$\langle S_0^z S_n^z\rangle=\frac{\mathrm{Si}(\pi n)}{4\pi n}(-1)^n\,. \tag{9}$$

As Shastry pointed out,[5] this equality is a consequence of the *singlet* nature of the ground state ($\langle S_0^z S_n^z\rangle=\langle S_0^x S_n^x\rangle$), which implies that the spin correlation function is one-half of the one-body density matrix. The equivalence also suggests that for the correlation functions, the discrete nature of the particle position is not important.

The HNC procedure for evaluation of the density matrix and the momentum distribution function that we have followed in the present work is given in detail in Ref. 13. This method has the interesting quality of having the correct normalization, as compared to the methods developed earlier,[14] and is known to be reasonably accurate for liquid ^{4}He. The accuracy can be improved by introducing the elementary diagrams. In this approach, the density matrix is calculated from the radial distribution functions of a binary mixture.[12] The method was first proposed by Reatto and co-workers,[15] who noticed that the one-particle density matrix is proportional to one of the three radial distribution functions of a binary mixture comprising of two particles $\{1,1'\}$ in the bath of $(N-1)$ particles $\{2,\ldots,N\}$.

For a two-component system, the ground-state wave function can be written in the Jastrow form[12] as

$$\Psi(\mathbf{r}_{1,1},\ldots,\mathbf{r}_{1,N_1};\mathbf{r}_{2,1},\ldots,\mathbf{r}_{2,N_2})=\exp\frac{1}{2}\left[\sum_{i<j}^{N_1}u_{11}(|\mathbf{r}_{1,i}-\mathbf{r}_{1,j}|)+\sum_{i<j}^{N_2}u_{22}(|\mathbf{r}_{2,i}-\mathbf{r}_{2,j}|)+\sum_{\substack{i=1,N_1\\ j=1,N_2}}u_{12}(|\mathbf{r}_{1,i}-\mathbf{r}_{2,j}|)\right]\,,$$

where $u_{\alpha,\beta}(r)$ are the correlation functions between the three particle pairs, the pair-distribution functions can be written as[12]

$$G_{\alpha,\beta}(r)=\frac{N_\beta(N_\alpha-\delta_{\alpha\beta})}{\rho_\alpha\rho_\beta}\frac{\int\Psi^2 d\mathbf{r}_{(i_\alpha,i_\beta)}}{\int\Psi^2 d\mathbf{r}_1\ldots d\mathbf{r}_N},\quad \alpha,\beta=1,2\,, \tag{10}$$

where $d\mathbf{r}_{(i_\alpha,i_\beta)}$ denotes $d\mathbf{r}_1\ldots d\mathbf{r}_N$ with $d\mathbf{r}_{i_\alpha}$ and $d\mathbf{r}_{i_\beta}$ omitted, and ρ_α is the partial density of the species α. If we consider the choice

$$\begin{aligned} u_{\alpha\alpha}(r)&=u(r)\,,\\ u_{\beta\beta}(r)&=0\,,\\ u_{\alpha\beta}(r)&=\tfrac{1}{2}u(r)\,, \end{aligned} \tag{11}$$

the density matrix is then written in terms of $G_{\beta\beta}$ as[13]

$$n(r)=\frac{G_{\beta\beta}(r)}{G_{\beta\beta}(0)}\,. \tag{12}$$

The momentum distribution function is then obtained by performing a Fourier transform on $n(r)$. The numerical Fourier transform requires special care because the density-matrix decays as $1/r$ for large r. The partial pair correlations are obtained by solving the two-component HNC equations in the zero-concentration limit[16] (the contributions from the elementary diagrams are ignored in the present calculation).

In Fig. 2, we have presented the one-particle density matrix $n(r)$ as obtained via the HNC approximation for $g=4$ and $d=1$. The normalization condition is trivially satisfied because of Eq. (12). The overall agreement with the exact result [Eq. (8)] is quite good. The discrepancy between the two results can be greatly reduced by introducing the elementary diagrams. In the case of liquid ^{4}He, the contribution from the elementary diagrams to $n(r)$ was found to be quite significant.[13] Similar calculations in the present model would be very interesting and will be published later. It should be noted, however, that both the exact and HNC results agree closely in the large-r limit.

The numerical result for the momentum distribution function $n(k)$ is shown in Fig. 3 for $g=4$ within the HNC scheme. The exact result in Eq. (8) is also plotted here for comparison. Again, the overall agreement is quite good. The vanishing of the exact result at $k=2\pi$ is not reproduced by the HNC result; it is, however, very small for $k\gtrsim 2\pi$. The discrepancy is, of course, related to that for $n(r)$ at small distance. The agreement between the two results for $n(k)$ is expected to improve if we consider the contributions from elementary diagrams. As a final check, the normalization condition is $\int n(k)dk=0.98$, close to unity. The reason for the slight deviation from unity is purely numerical error.

In closing, we wish to emphasize that, in this paper, we intended to introduce the hypernetted-chain scheme, a well-established procedure for calculating the ground state (and also the low-lying excitations), in a system where a few exact results are available. The pair-correlation function obtained at $g=4$ in this approximate scheme is found to compare reasonably well with the exact result available. The results are presented for various values of g merely to demonstrate the flexibility of the approach while being reasonably accurate. For the correlations in the spin-singlet Gutzwiller-RVB state, the important quantity is the one-body density matrix, which in the present scheme is in very good agreement with the exact result for $g=4$. The momentum distribution function also shows the correct behavior, except in the region of k, where the exact result for $n(k)$ goes to zero. In this region, corrections to the HNC approximation are important. Similar reasoning explains the discrepancy in the density matrix. Work of similar type for a discrete model will be reported in a separate publication. Finally, the approximation scheme discussed in this paper can also be ex-

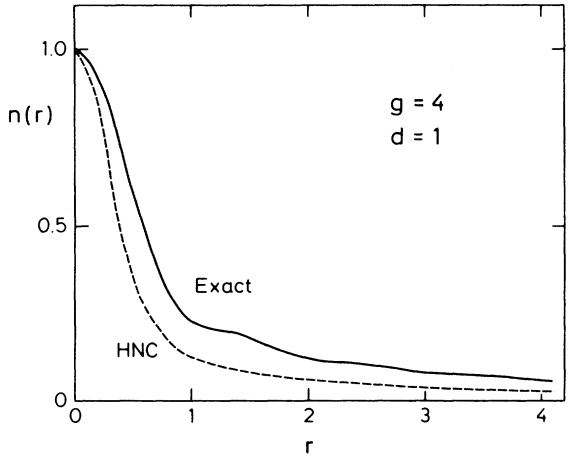

FIG. 2. The one-particle density matrix for $g=4$ obtained within the HNC scheme (dashed curve) and compared with the exact result from Ref. 8.

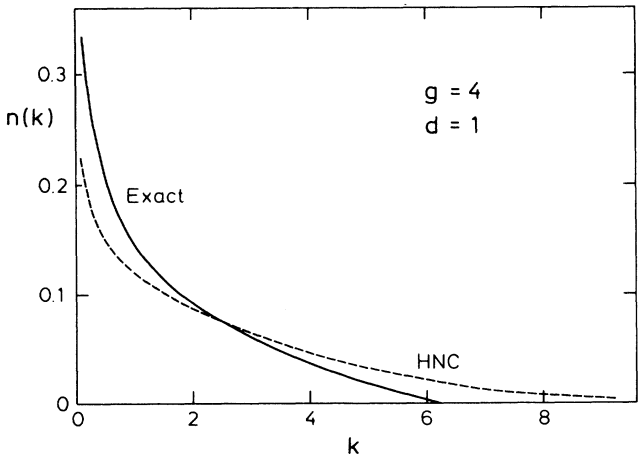

FIG. 3. The momentum distribution function for $g=4$ in the HNC procedure (dashed curve) as compared with the exact result of Ref. 8.

tended to Fermi systems. Noticing that the ground state of an interacting Fermi system in 1D is of Jastrow type,[8] we expect that the Fermi-HNC scheme in Ref. 12 should be particularly appropriate. These studies will be reported in future publications.

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