

## Class of variational singlet wave functions for the Hubbard model away from half filling

P. W. Anderson

*Joseph Henry Laboratories of Physics, Princeton University, Princeton, New Jersey 08544*

B. S. Shastry\*

*AT&T Bell Laboratories, 1D-234 Murray Hill, New Jersey 07974*

D. Hristopulos

*Joseph Henry Laboratories of Physics, Princeton University, Princeton, New Jersey 08544*

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We present a class of variational wave functions for strong-coupling Heisenberg Hubbard models. These are written in the form of three factors—a pair of determinants and a Jastrow function—and are made out of orbitals, *a la* Hartree-Fock theory, which solve a fictitious one-body problem. The wave functions respect various constraints known from general principles and appear to be potentially useful in understanding the possible behavior of the models in quantitative terms.

### I. INTRODUCTION

It is the purpose of this paper to introduce a new class of variational wave functions for the problem of the  $s = \frac{1}{2}$  (quantum) Heisenberg model with mobile vacancies. Such a model is currently the focus of great interest, following the proposal of Anderson<sup>1</sup> that the high- $T_c$  materials are described by it. Although considerable insight into the model has been gained from “mean-field” theories,<sup>2-4</sup> there is a need to assess the relative stabilities of various proposed “phases”—and it is here that we need to appeal to more reliable quantitative tests. The class of wave functions that we introduce are rich enough to encompass the various possibilities uncovered by the mean-field theories, and further to respect several rigorous constraints that the ground-state wave function must satisfy for finite-sized systems. We hasten to add

that we have *not* computed the energies of the various wave functions that we propose here, but we present some evidence for our belief that these must be competitive in energy.

The problem we address consists of electrons with spin up and down respecting the constraint that no double occupation is allowed. For orientation consider the Hamiltonian

$$H = -tP \sum_{(ij)} (C_{i\sigma}^\dagger C_{j\sigma} + \text{H.c.}) P + \frac{1}{2} \sum_{(ij)} \mathbf{S}_i \cdot \mathbf{S}_j J_{ij}, \quad (1)$$

where  $P$  is the projection operator that annihilates doubly occupied sites and the spin operators obey an exclusion principle in real space vis a vis the “holes” (i.e., each site has either an up electron, a down electron, or a “hole”). The relevant states in the Hilbert space on which it acts are spanned by wave functions of the following kind:

$$|\psi\rangle = \sum_{r_1 \dots r_M, s_1 \dots s_Q} \psi(r_1, r_2, \dots, r_M | s_1, s_2, \dots, s_Q) S_{r_1}^- S_{r_2}^-, \dots, S_{r_M}^- C_{s_1}^\dagger C_{s_2}^\dagger, \dots, C_{s_Q}^\dagger |F\rangle, \quad (2)$$

where  $s_r^- \equiv C_{r_1}^\dagger C_{r_1}$ , and  $|F\rangle$  is the reference ferromagnetic state  $\prod_n C_{n_1}^\dagger |0\rangle$ . The above state represents a configuration with  $Q$  holes,  $M$  down-spin electrons and  $N-M-Q$  up-spin electrons. ( $N$  is the total number of sites.) The wave function  $\psi$  is a function of only the coordinates of the holes ( $s_1, \dots, s_Q$ ) and the down electrons ( $r_1, \dots, r_M$ ) and provides the most compact description of the configuration as long as  $Q < N/2$  (since the up electrons are present at all sites not contained in  $\{r\}$  or  $\{s\}$ ). The function  $\psi$  must, in addition, obey several conditions of exclusion: it should vanish when (for any  $i$  and  $j$ )  $r_i = r_j$  or  $s_i = s_j$  or  $r_i = s_j$ . The symmetry of the  $c$ 's and the symmetry of the  $s^-$ 's under exchange forces  $\psi(r_1, \dots, r_M | s_1, \dots, s_Q)$  to be symmetric under the ex-

change of any  $r_i$  with  $r_j$ , and antisymmetric under the exchange of  $s_i$  with  $s_j$ . To this list of constraints we must add the condition of “highest weight,” i.e.,  $S_{\text{total}}^+ |\psi\rangle = 0$ , since the Hamiltonian is rotationally invariant and hence we only need to generate states with a given total spin  $S$  and  $S_z = S$  (the lower  $S_z$  states follow by acting with  $S_{\text{total}}^-$ ). Thus, to generate a singlet state with  $Q$  holes ( $N$  and  $Q$  even) we should pick  $M = (N - Q)/2$ . This condition readily translates into the following constraint on  $\psi$ :

$$\sum_{r_1} \psi(r_1, \dots, r_M | s_1, \dots, s_Q) = 0, \quad (3)$$

where  $r_2, \dots, r_M, s_1, \dots, s_Q$  are held fixed and  $r_1$  is summed over the entire lattice.

## II. VARIATIONAL WAVE FUNCTIONS

We now present our variational wave functions which fulfill all the above constraints and yet retain sufficient flexibility as we demonstrate below. We first consider an auxiliary problem of establishing a suitable basis in the Hilbert space. We choose some Hermitian one-particle problem—typically a hopping problem—and solve for the eigenfunctions, thus:

$$\sum_j h_{ij}^0 \phi_{\nu}(r_j) = \lambda_{\nu} \phi_{\nu}(r_i). \quad (4)$$

The eigenfunctions  $\phi_{\nu}$  form a complete orthonormal basis set which are  $N$  in number. Thus

$$(\phi_{\nu_i}, \phi_{\nu_j}) \equiv \sum_r \phi_{\nu_i}^*(r) \phi_{\nu_j}(r) = \delta_{ij},$$

where the sum is over the appropriate lattice. The definition of  $h_{ij}^0$  in Eq. (4) is unspecified at this stage and provides us with great flexibility. We define  $\{t_{\alpha}\}$  for  $1 \leq \alpha \leq M + Q$

$$\begin{aligned} (t_1, \dots, t_M) &= (r_1, \dots, r_M), \\ (t_{M+1}, t_{M+2}, \dots, t_{Q+M}) &= (s_1, s_2, \dots, s_Q). \end{aligned} \quad (5)$$

Further partition the eigenfunctions  $\{\phi_{\nu}\}$  into two sets  $\{\psi_{\nu_i} | 1 \leq i \leq M\}$  and  $\{\chi_{\nu_{\alpha}} | 1 \leq \alpha \leq M + Q\}$  with no common element. Our variational wave function is

$$\begin{aligned} \psi_{\text{var}}(r_1, r_2, r_M | s_1, \dots, s_Q) \\ = \left[ \prod_{i < j} f(s_i - s_j) \right] \det[\psi_{\nu_i}(r_j)] \det[\chi_{\nu_{\alpha}}^*(t_{\beta})]. \end{aligned} \quad (6)$$

Here  $f(s)$  is an even function of its argument and will be specified later. It is easily seen that the antisymmetry with respect to  $s$ 's stems from the second determinant and the symmetry with respect to the  $r$ 's stems from their "residing" in both determinants. The hard-core constraints are all built into the determinants. The only constraint needing some thought is the highest weight condition—we must verify that we annihilate  $\psi$  by summing  $r_1$  over the entire lattice keeping all other coordinates fixed. This follows readily when we expand the determinants and find that a typical sum looks like  $[\phi_{\nu_{P_i}}(r_i) \chi_{\nu_{Q_{\alpha}}}^*(r_1)]$  into functions of  $(r_2, \dots, \text{etc.})$ , where  $P$  and  $Q$  are some permutations of appropriate indices. However, the sum over the square bracket is precisely  $(\chi_{\nu_{Q_{\alpha}}}^*, \phi_{\nu_{P_i}})$ , which vanishes since  $\phi$ 's and  $\chi$ 's are distinct eigenfunctions of a one-body Hermitian Hamiltonian.

The freedom inherent in our variational wave functions stems from the various partitions of the complete set into two subsets, and more fundamentally, from the complete freedom in choosing the one-body Hamiltonian to "organize" the Hilbert space via Eq. (4). We give below several examples of  $h_{ij}^0$  and the resulting functions. Let us note that wave functions of this nature were discussed by Shastry<sup>5</sup> who considered the case with no holes and with  $h_{ij}^0$  taken as the tight-binding model. The projected Gutzwiller states considered by Gros, Rice, and Joynt<sup>6</sup> and Shiba<sup>7</sup> are particular cases of this class.

We should note that the spin-spin correlations are closely related to density-density correlations for "hard-core bosons" described by their coordinates in (6) via the correspondence  $S_i^z \rightarrow (\rho_i - \frac{1}{2})$  and  $S_i^+ \rightarrow b_i^+$ . Thus, we may view  $\psi_{\nu}$  as the wave function for a collection of (hard-core) bosons and fermions which have strong on-site repulsion. The modulus squared of the wave function is interpretable as the Boltzmann weight of a configuration of the bosons and fermions. It is worth noting that the modulus square of a determinant is expressible as another determinant as follows:

$$\|\det \phi_i(r_j)\|^2 = \det M_{ij} \geq 0,$$

where

$$M_{ij} \equiv G(r_i, r_j) = \sum_k \phi_k^*(r_i) \phi_k(r_j).$$

The "orbitals" can thus be eliminated in favor of the "Green's function"  $G(r_i, r_j)$ .

The most interesting "sector" from our point of view is the singlet state, wherein we have  $M = (N - Q)/2$ . In this case the choice of  $\psi$ 's determines completely the  $\chi$ 's which are  $M + Q = (N + Q)/2$  in number and hence must be the complementary sets. We now focus on the half-filled case and discuss three different kinds of basis.

## III. SPECIAL CASES

### A. Free particles

This case corresponds to the one studied in Refs. 3–5 and the  $\phi$ 's are simply the plane-wave solutions of a tight-binding Hamiltonian. The singlet wave function which shows considerable promise corresponds to choosing  $\psi$ 's to be the  $N/2$  wave vectors comprising the Fermi surface of a half-filled noninteracting model. For the hypercubic lattice, we have the complementary set of wave vectors (entering  $\det \chi$ ) obtainable from the earlier ones by shifting through  $\mathbf{Q} = \pi, \pi(1, 1), \pi(1, 1, 1)$  in one, two, and three dimensions. Thus,

$$\psi_A(r_1, \dots, r_M) = \exp \left[ i \mathbf{Q} \cdot \sum_i \mathbf{r}_i \right] \|\det e^{ik_i r_j}\|^2. \quad (7)$$

This wave function is real and has the Marshall<sup>8</sup> sign in all dimensions. (This fact seems unknown to many workers in the field.) In fact, this wave function is intimately related to the  $s$ -wave solution of Baskaran, Zou, and Anderson (BZA),<sup>2</sup> but has a net momentum  $\mathbf{Q}$  ( $N/2$ ) rather than zero.

### B. Density wave

We set up the one-body Hamiltonian by choosing a staggered one-body potential energy which takes values  $\pm \lambda_0$  on the two sublattices  $A$  and  $B$ . The tight-binding model is defined by the recursion relations for this amplitude

$$\lambda \psi(r) = - \sum_{\delta} \psi(r + \delta) + \lambda_0 \psi(r) (\delta_{r,A} - \delta_{r,B}),$$

where  $\lambda$  is the eigenvalue and  $\delta$  is the set of nearest-

neighbor vectors. These equations are solved by

$$\psi(r) = e^{ik \cdot r} (\Phi_A \delta_{r,A} + \Phi_B \delta_{r,B}) .$$

The amplitudes satisfy the two equations  $(\lambda - \lambda_0)\Phi_A = -\psi_k \Phi_B$  and  $(\lambda + \lambda_0)\Phi_B = -\psi_k \Phi_A$ , where

$$\psi_k = \sum_{\alpha=1}^d \cos k_{\alpha} .$$

Thus, the eigenvalues are  $\lambda = \pm \lambda_k$ ,  $\lambda_k = (\lambda_0^2 + \psi_k^2)^{1/2}$ . For the bonding states  $\lambda = -\lambda_k$ , we have

$$\Phi_A^{(-)} : \Phi_B^{(-)} = \psi_k : (\lambda_0 + \lambda_k) ,$$

and for the antibonding states  $\lambda = +\lambda_k$ ,

$$\Phi_A^{(+)} : \Phi_B^{(+)} = -(\lambda_0 + \lambda_k) : \psi_k .$$

A complete set of states is obtained by confining ourselves to the  $N/2$   $k$  values for which  $\psi_k > 0$  and retaining the two solutions  $\lambda = \pm \lambda_k$ . The variational wave function for the half-filled case is now

$$\psi_B(r_1, \dots, r_M) = \det \psi_{k_1}^{(-)}(r_j) [\det \psi_{k_j}^{(+)}(r_j)]^* .$$

Note, however, that

$$e^{i\mathbf{Q} \cdot \mathbf{r}} \psi_k^{(+)}(r) \propto \psi_k^{(-)}(r + \hat{n}) ,$$

where  $\hat{n}$  is a unit translation vector [say  $a$ ,  $a(1,0)$ ,  $a(1,0,0)$  in one, two, and three dimensions]. Therefore, denoting  $f(r_1, \dots, r_M) \equiv \det \psi_{k_1}^{(-)}$ , we thus find

$$\psi_B(r_1, \dots, r_M) = \exp \left[ i\mathbf{Q} \cdot \sum_i r_i \right] f(r_1, \dots, r_M) f^*(r_1 + \hat{n}, r_2 + \hat{n}, \dots, r_M + \hat{n}) . \quad (8)$$

Note that  $f$  can be chosen real since all wave vectors appear with their negatives in the (lower) bonding band, and hence  $\psi_B$  is also real, and has the "correct" Marshall sign.

This wave function  $\psi_B$  is instructive, since it is actually a singlet, and is translationally invariant for any finite-sized system. The first determinant breaks translation invariance, which is restored by the second one. The wave function  $\psi_B$  possesses oscillatory spin-density correlations which appear to decay exponentially, and the decay length decreases rapidly with increasing  $\lambda_0$ .<sup>9</sup>

### C. Flux phases

This case is perhaps the most fascinating one and has a particular appeal and "naturalness" in two dimensions that we now consider. The Hamiltonian  $h_{ij}^0$  is chosen to be that of the tight-binding model in the presence of a uniform magnetic field  $B$  pointing along the normal to the plane. This is a problem considered by Hofstadter<sup>10</sup> for arbitrary values of the flux through a square. We illustrate the case of the square lattice with a flux  $\pi$  (in units of  $\hbar c/e$ ) through each square. Such a flux is natural within the mean-field theory where it is recognizable as the flux or  $s + id$  phase.<sup>3,4</sup> This flux, we believe, is optimal for small concentration of holes  $\delta$ , but expect that with increasing  $\delta$  the optimal flux should be reworked. In particular, we expect commensuration effects to be very important, and that there should be plateaus of stability of flux for rational  $\delta$ .<sup>11</sup>

The simplest illustration of our ideas is for the case of flux  $\pi$  which can be realized in a tight-binding model with recursion relations

$$\lambda \psi(n, 2\nu + 1) = -t \sum_{\sigma=\pm 1} [\psi(n + \sigma, 2\nu + 1) + \psi(n, 2\nu + 1 + \sigma)] , \quad (9)$$

$$\lambda \psi(n, 2\nu) = -t \sum_{\sigma=\pm 1} [\psi(n, 2\nu + \sigma) - \psi(n + \sigma, 2\nu)] . \quad (10)$$

These relations correspond to the Landau gauge with  $\mathbf{A} = (-y|B|, 0, 0)$  with

$$Ba^2 = \frac{1}{2} \hbar c / e ,$$

and

$$\tilde{t}_{ij} = t \exp \left[ -i \left[ \frac{2\pi e}{\hbar c} \right] \int_i^j \mathbf{A} \cdot d\mathbf{l} \right] .$$

We denote the "sublattice"  $\hat{A}$  as all sites in odd numbered rows, i.e.,  $(n, 2\nu + 1)$  and  $\hat{B}$  as all sites in even numbered rows  $(n, 2\nu)$ . The obvious solution reads

$$\psi(n, m) = (\Phi_A \delta_{r,A} + \Phi_B \delta_{r,B}) e^{ik_x n + ik_y m}$$

with

$$(\lambda + 2t \cos k_x) \Phi_A = -2t \cos k_y \Phi_B$$

and

$$(\lambda - 2t \cos k_x) \Phi_B = -2t \cos k_y \Phi_A .$$

The eigenvalues are thus  $\lambda = \pm \lambda_k$ , where

$$\lambda_k = 2t (\cos^2 k_x + \cos^2 k_y)^{1/2} .$$

Correspondingly, the amplitudes

$$\Phi_A^{(+)} : \Phi_B^{(+)} = [\cos k_x \mp (\cos^2 k_x + \cos^2 k_y)^{1/2}] : \cos k_y .$$

Noting that  $k_y$  and  $k_y + \pi$  lead to the same solution, we obtain the complete set of solutions by restricting to the "first Brillouin zone" (BZ)  $-\pi < k_x \leq \pi$ ,  $-\pi/2 < k_y \leq \pi/2$  containing one-half the  $k$  values, and retaining the two bands with  $\lambda = \pm \lambda_k$ .

The singlet wave function obtained by choosing  $\psi_k$  to be  $\phi_k^{(-)}$  is

$$\psi_C(r_1, \dots, r_M) = [\det \phi_{k_1}^{(-)}(r_j)] [\det \phi_{k_1}^{(+)}(r_j)]^* . \quad (11)$$

Notice, however, that

$$e^{iQr}\phi_k^{(+)} \propto \phi_{k+Q}^{(-)}(r),$$

where the wave vector  $k+Q$  is brought into the first BZ by adding an appropriate reciprocal-lattice vector.

Using this we find

$$\psi_C(r_1, \dots, r_m) \exp \left[ iQ \sum_i r_i \right] \left| \det \phi_{k_i}^{(-)}(r_j) \right|^2. \quad (12)$$

Note that  $\psi_C$  is also a real wave function with the Marshall sign; we thus see that all the functions  $\psi_A$ ,  $\psi_B$ , and  $\psi_C$  are singlet and satisfy the Marshall sign and hence cannot be orthogonal to each other nor to the exact ground state of the Heisenberg model for a finite-sized system. Further, the wave function  $\psi_C$  should, in the thermodynamic limit, be equal to the Gutzwiller projection of the Bardeen-Cooper-Schrieffer (BCS) BZA (Ref. 2) state with  $s+id$  symmetry.<sup>3,4</sup> Its energy—as found by Gros<sup>6</sup>—is  $\sim -0.32$  per bond (with the Hamiltonian  $S_i \cdot S_j$  per bond) and quite competitive with more elaborate calculations, and also much better than the  $s$  wave (which should correspond to  $\psi_A$ ) with no flux which has an energy  $\sim -0.27$  per bond.

#### IV. TRIANGULAR LATTICE

Another instructive example of the efficacy of the flux phases is the triangular lattice. Here, we could try the wave function, at half filling, to be essentially as in  $\psi_A$ , with the two determinants made up of the set of  $N/2$  lower and  $N/2$  upper momentum eigenfunctions (i.e., bipartitioning the eigenfunctions using  $\epsilon_{k_j} > \epsilon_{k_j}$ ). The variational energy per bond was evaluated<sup>9</sup> for a  $6 \times 6$  lattice and yields  $\epsilon \sim -0.112$ /bond. Here the single-particle energies for the tight-binding model read

$$\epsilon_k = 2t[\cos k_x + \cos k_y + \cos(k_x + k_y)]$$

(viewing the triangular lattice as a square with all diagonals in the northeast direction), and the density of states is very skewed and asymmetric about zero energy—unlike in bipartite lattices.

However, our construction (at half filling) requires a bipartitioning of the set of eigenfunctions and it would appear advantageous to choose a  $h^0$  that has a symmetric spectrum (about zero energy). We show below that at a flux of  $\pi/2$  through each triangle is specially suited for this. The recursion relations for the amplitudes [analogous to Eqs. (9) and (10)] are

$$\begin{aligned} \lambda \psi(n, m) = & t[\psi(n, m+1) + \psi(n, m-1) \\ & + e^{-i\pi m} \psi(n+1, m) + e^{i\pi m} \psi(n-1, m) \\ & + e^{-i\pi m} e^{-i\pi/2} \psi(n+1, m+1) \\ & + e^{i\pi m} e^{-i\pi/2} \psi(n-1, m-1)], \quad (13) \end{aligned}$$

where the hopping elements are worked in the Landau gauge (with a flux  $\pi/2$  through each triangle). These can be solved in the usual way with

$$\begin{aligned} \psi(n, m) = & \exp(ik_x n + ik_y m) \\ & \times [\phi_A(k) \delta_{m, \text{even}} + \phi_B(k) \delta_{m, \text{odd}}]. \end{aligned}$$

The amplitudes are

$$[\phi_B(k):\phi_A(k)] = \left[ \frac{\lambda}{2t} - \cos k_x \right] : [\cos k_y - i \cos(k_x + k_y)], \quad (14)$$

where the eigenvalues  $\lambda = \pm \lambda_0(k)$

$$\lambda_0(k) = 2t[\cos^2 k_x + \cos^2 k_y + \cos^2(k_x + k_y)]^{1/2}. \quad (15)$$

The zone is halved in the usual way  $-\pi < k_x \leq \pi$  and  $-\pi/2 \leq k_y \leq \pi/2$ . The fascinating feature of (15) is that the allowed energies form two very symmetric bands  $t[-2\sqrt{3}, -\sqrt{3}]$  and  $t[\sqrt{3}, 2\sqrt{3}]$ , and further, the spectrum has a gap  $2\sqrt{3}t$ . Thus, the flux  $\pi/2$  restores the particle-hole symmetry in that the spectrum has a symmetry  $\lambda \rightarrow -\lambda$ . We choose the two determinants to be those corresponding to the two sets of eigenvalues and would expect the energy to be rather competitive and better than the previous case at any rate. A calculation on the  $6 \times 6$  lattice<sup>9</sup> confirms this expectation and yields  $\epsilon \sim -0.159$ /bond.

Several remarks are in order here. The wave function in this case can be written as

$$\psi = \exp \left[ i(\pi, \pi) \sum_i r_i \right] [\det \psi_{k_i}^{(-)}(r_i)]^2, \quad (16)$$

where the orbitals are in the lower subband (on using

$$[\psi_{-k}^{(+)}(r)]^* = e^{i\pi(n+m)} \psi_{k+\pi(1,1)}^{(-)}(r)$$

to express the positive-energy determinant in terms of the lower one). However, the determinant in (16) is *not real* in spite of being a filled subband. The reason, of course, is that we have introduced a nontrivial flux  $\pi/2$  per triangle which is to be distinguished from  $-\pi/2$ . Thus,  $\psi$  and its complex conjugate are distinct wave functions with, of course, the same energy expectation value. Thus, the time reversal invariance breaking that is masked in the square lattice (by  $e^{i\pi} = e^{-i\pi}$ ) is unveiled in the frustrated triangular lattice for flux  $\pi/2$ . In fact, if we switch on a small diagonal bond in the square lattice with a hopping strength  $\delta t$ , then the flux  $\pi/2$  phase immediately becomes viable and the eigenvalues are as in (15) with  $\delta^2$  as the coefficient of  $\cos^2(k_x + k_y)$ . A similar flux  $\pi/2$  state is discussed in a recent work by Wen, Wilczek, and Zee<sup>12</sup> who work at the BZA level with a square lattice containing both classes of diagonal bonds.

The other remark concerns the close similarity between our estimate of energy ( $\sim -0.159$ ) and that for the triangular lattice of Laughlin and Kalmeyer<sup>13</sup> who work with a Laughlin-Jastrow wave function to again find ( $\sim -0.159$ /bond). This curious coincidence could be the consequence of the possibility that the Laughlin-Jastrow wave function is the best approximant to our determinants in a certain technical sense.<sup>14</sup> It should also be noted that the energy of the wave function is not as good as the best available variational estimates<sup>15</sup> ( $\sim -0.179$ ).

### V. AWAY FROM HALF FILLING

The above examples show that the flux states are very appealing and yet are unable to be variationally the best available wave functions in most cases treated above. Frustration induced by exchange interactions does not, in most cases, “stabilize” the flux states. However, the main frustrating term in the problem is the hole kinetic energy which prefers some sort of ferromagnetism<sup>16</sup> but may not be representable in terms of a static distribution of frustrated exchange bonds. We can introduce correlations among the holes via the hitherto unspecified function  $f$ . We suggest  $f(r)=[d(r)]^{2\nu}$ , with

$$d(r) = \left[ \sin^2 \frac{\pi}{L} x + \sin \frac{\pi}{L} y \right]^{1/2},$$

the “distance” variable, and  $\nu$  a parameter (either positive or negative). This term gives the probability distribution for a configuration—an extra term

$$\sim +4\nu \sum_{i < j} \ln |s_i - s_j|,$$

which is analogous to an electrostatic repulsion (or attraction) for  $\nu > 0$  ( $< 0$ ).

The extra flexibility offered by the Jastrow function for holes in  $\psi_\nu$  [Eq. (6)] can be used to introduce correlations of considerable variety in the problem. A large and positive  $\nu$ , for instance, would favor a “Wigner crystallization” of the holes.<sup>17</sup> We envisage a program consisting of evaluating the kinetic energy of holes in the various flux phases numerically, in addition to the exchange energy, and varying the set of orbitals (i.e., of flux) to minimize the total energy. Several “natural” possibilities offer themselves—the flux  $\pi$  state near half filling should be favorable.

Another interesting possibility in the case of flux  $\pi/3$  which should be of relevance close to a filling of  $\frac{1}{3}$  (i.e.,  $M=Q=N/3$ ). Here the band splits into three Hofstadter subbands. One proposal is to choose the lowest set of  $N/3$  states in the first determinant and the highest  $\frac{2}{3}N$  states in the second determinant. Such a wave function is clearly a singlet. Another proposal is to choose the orbitals in the second determinant from the bottom

and top bands while keeping the first determinant unchanged. This state is not a singlet (since the orbitals are not exclusive). We can, however, project out the singlet component in this wave function, at least formally. Likewise, in the case of quarter filling we expect a state with flux  $\pi/4$  to be relevant—this state may, in fact, apply to the case of  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  for  $\delta \sim 0$ . A singlet state is obtained by choosing the first determinant to be made of from the lowest of the four bands and the second from the upper three.

Let us also note that the wave function  $\psi_B$  [Eq. (8)] can be modified to give a nonsinglet state with Néel order—to do this, we merely omit the second determinant ( $f^*$ ) and take the modulus squared of the first. This wave function contains a variational “handle” on the Néel order through the parameter  $\lambda_0$ . At  $\lambda_0=0$ , we get back the state Eq. (7), and for large  $\lambda_0$  we have a pure Néel state: the wave function explicitly breaks translation invariance since the orbitals do so. It is not clear whether one can generalize the state usefully to move away from half filling since all the complications of commensurability are likely to be lost. Let us also note that Néel order enters explicitly in this wave function through  $\lambda_0$  (the conjugate field), unlike the case of say  $\psi_A$  [Eq. (7)], which if raised to a sufficiently high power, should display Wigner crystallization of the hard-core bosons (i.e., Néel order) as spontaneously broken symmetry. Such a situation arises<sup>18</sup> in the case of the Jastrow functions in the  $1-d$   $1/r^2$  problem.<sup>19,3</sup>

In addition to the above variational viewpoint, we could also independently examine the nature of various correlation functions in the given (explicit) wave functions numerically. It would be amusing to see if the exotic nature of excitations in the half-filled limit (i.e., of fractional statistics advocated by Laughlin<sup>20</sup> and Wilczek<sup>21</sup>), which are believed to be “inherited” by the dopants, actually comes to be realized in our explicit construction of “doped” wave functions starting from the insulating limit.

Finally we should note that these wave functions can possibly be of use in disordered quantum spin systems<sup>22</sup> where the natural guess<sup>23</sup> would be to choose orbitals that are eigenfunctions of an appropriate random  $M_{ij}$ , leading to the picture of a “valence-bond glass” for strong enough disorder.

\*On leave from Tata Institute of Fundamental Research, Bombay, India.

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<sup>23</sup>In keeping with our discussion of the triangular lattice, we ex-

pect that the appropriate  $M_{ij}$  is  $\sqrt{|J_{ij}|} e^{i\phi_{ij}}$ , where the phase  $\phi_{ij}$  should be chosen so as to bipartition the eigenvalues into two sets that are (nearly) symmetry about zero. These would correspond to the suitable “flux” that corrects for frustration.