Variational Monte Carlo Calculations for the t'-J Model with Fermi Holes and Boson Spins

N. E. Bonesteel[(a)] and J. W. Wilkins
Department of Physics, The Ohio State University, Columbus, Ohio 43210
(Received 27 September 1990)

We have performed variational Monte Carlo calculations for the two-dimensional t'-J model (t' is an effective, sublattice-preserving hopping amplitude) using new wave functions which describe *fermionic* holes hopping in a background liquid of singlet bonds represented by products of *bosonic* spin operators. The variational energies we obtain from these wave functions can be directly compared with those of other proposed wave functions. We find that our energies are lowest in the $t'/J \ll 1$ limit.

PACS numbers: 74.65.+n, 75.10.Jm

Strong correlations in the copper-oxide superconductors have motivated theorists to study a variety of "strong-coupling" fermion models. One of the simplest of these is the t-J model describing holes undergoing nearest-neighbor hops (with amplitude t) in a spin-$\frac{1}{2}$ antiferromagnet (with exchange coupling J). The two-dimensional square-lattice version of the t-J model may describe the essential low-energy physics of a single copper-oxide sheet in a high-T_c superconductor.[1,2] If so, the ratio of t and J is probably intermediate,[3] with $t/J \sim 4$—a difficult regime theoretically.

Recent mean-field work on the $t/J \ll 1$ regime[4] has suggested that the ground state (if one excludes the possibility of phase separation by adding long-range Coulomb repulsion, see below) is a so-called commensurate-flux-phase (CFP) state, a generalization of the $\frac{1}{2}$-flux state of Affleck and Marston.[5] These states are characterized by a fictitious "flux" parameter which is taken to be uniform throughout the lattice with a flux density commensurate with the number of electrons per site. Among the interesting properties of the CFP states is that they exhibit a spontaneously broken time-reversal symmetry for any finite doping. Such a broken symmetry is a prerequisite for some of the more exotic superconducting mechanisms, e.g., the anyon superfluid model,[6,7] and so this result provides strong motivation for further study of the $t/J \ll 1$ limit, despite its unphysical nature.

In this Letter we present a new class of variational wave functions with significantly lower magnetic energies (J) than the CFP states. These new wave functions describe *fermionic* holes hopping (slowly) in a background liquid of singlet pairs represented by products of *bosonic* spin operators. By construction each hole is constrained to a single sublattice and is described by a t'-J model (where $t' \sim t^2/J$ is an effective sublattice-preserving hopping parameter). In the case where it can be checked, the magnetic energy of the new wave function is substantially lower ($\sim 40\%$) than that of the corresponding CFP state[8] *clearly indicating that the CFP states are not stable in the $t/J \ll 1$ limit.* This result is especially significant because our wave functions are real and thus time-reversal invariant—a result at variance with the anyon mechanism.

It is reasonable to assume that in the $t/J \ll 1$ limit of the t-J model coherent hole motion proceeds via two successive nearest-neighbor hops followed by a spin flip ($S_i^- S_j^+$) which heals the ferromagnetic "wake" left by the hole. The intermediate state in this process involves a misoriented spin and so costs energy $\sim J$; thus the effective next-nearest-neighbor hopping amplitude t' is of the order t^2/J. The effective low-energy Hamiltonian is then the t'-J model

$$H = -\sum_{i,j} t'_{ij}(1-n_{i,-\sigma})c^\dagger_{i\sigma}c_{j\sigma}(1-n_{j,-\sigma}) + J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j + V_C . \quad (1)$$

The matrix t'_{ij} contains the sublattice-preserving second- and third-neighbor hopping matrix elements: t'_d and t'_c. When (1) is "derived" from the t-J model the diagonal hopping amplitude t'_d is twice the collinear hopping amplitude t'_c, and both are positive. The third term in (1), V_C, is the long-range Coulomb interaction without which the t'-J model almost certainly phase separates into hole-rich and electron-rich phases in the $t'/J \ll 1$ limit.[9] By including long-range repulsion between electrons these phase-separated states can be ruled out as unphysical. From a variational point of view the problem then becomes to find a *homogeneous* wave function with optimal t'-kinetic and magnetic energies—the expectation values of the first and second terms in (1), respectively. [It is also possible that (1) has crystalline ground states for certain commensurate filling fractions—we will not consider that possibility here.]

Because we are interested in the $t'/J \ll 1$ regime our approach has been to construct variational wave functions which optimize the magnetic energy—whatever the cost to the t'-kinetic energy. Accordingly, we follow Liang, Doucot, and Anderson[10] (LDA) who constructed a class of wave functions for the insulating antiferromagnet which included states with excellent energies [the best being $E_{\mathrm{LDA}} = -0.3344(1)J$/bond versus the "exact" result[11] $E = -0.33459(5)J$/bond]. A simple gen-

eralization of the Liang-Doucot-Anderson wave functions to the doped case utilizes the Schwinger-boson–slave-fermion representation in which the physical electron operator $c_{i\sigma}^{\dagger}$ is factorized into $f_i b_{i\sigma}^{\dagger}$ with f_i a spinless-fermion annihilation operator and $b_{i\sigma}^{\dagger}$ a spin-indexed boson creation operator. The strict no-double-occupancy (Gutzwiller) constraint is then enforced by requiring that all physically acceptable states $|\psi\rangle$ satisfy $(f_i^{\dagger}f_i + b_{i\uparrow}^{\dagger}b_{i\uparrow} + b_{i\downarrow}^{\dagger}b_{i\downarrow})|\psi\rangle = 0$ for all lattice sites i. In terms of the bosonic singlet-bond creation operator $B_{ij}^{\dagger} = (1/\sqrt{2})(b_{i\uparrow}^{\dagger}b_{j\downarrow}^{\dagger} - b_{i\downarrow}^{\dagger}b_{j\uparrow}^{\dagger})$ our ansatz wave function may be written as

$$|\{\lambda\};\{\mathbf{k}\}\rangle = \sum_{\alpha,\{\mathbf{r}\}} \omega(\alpha)\,\mathrm{Det}[\exp(i\mathbf{k}_i\cdot\mathbf{r}_j)]\,|\alpha;\{\mathbf{r}\}\rangle\,, \qquad (2)$$

where[12] $\omega(\alpha) = \prod_{l=1}^{q}\lambda(|i_{\alpha_l} - j_{\alpha_l}|)$ and

$$|\alpha;\{\mathbf{r}\}\rangle \equiv f_{\mathbf{r}_1}^{\dagger}\cdots f_{\mathbf{r}_m}^{\dagger} B_{i_{\alpha_1},j_{\alpha_1}}^{\dagger}\cdots B_{i_{\alpha_q},j_{\alpha_q}}^{\dagger}|0\rangle$$

with $m = N\delta$, $q = N(1-\delta)/2$ (δ is the fraction of holes doped into the system and N the total number of sites), and α denotes the singlet-bond configuration. The coordinates $\{\mathbf{r}\}$ label the hole positions while i_α and j_α label spin positions. The "vacuum" state $|0\rangle$ is defined by requiring that $f_i|0\rangle = 0$ and $b_{i\sigma}|0\rangle = 0$ for all i and σ, and the function $\lambda(m)$ and the set of $\mathbf{k}$ states should be chosen to optimize the energy of (2). We divide the square lattice into two Néel sublattices, A and B, and the sum in (2) is then over all singlet-bond states satisfying the Gutzwiller constraint (every site on the lattice has either a single Schwinger boson or a Fermi hole operator, and not both) and in which all the i_α's and j_α's are in the A and B sublattices, respectively. This last requirement constrains the allowed configurations in (2) to have equal numbers of holes on the A and B sublattices, and so the matrix element of the nearest-neighbor electron hopping operator in (2) is zero. Because of this, (2) cannot be used to estimate the kinetic energy of the t-J model; however, it is ideal for the t'-J model.

As for the Liang-Doucot-Anderson wave functions, to which our wave functions reduce when $\delta = 0$, if $\lambda(m) \geq 0$ for all m (the only case we have considered) then the spin part of (2) satisfies Marshall's sign,[10,13] i.e.,

$$\mathrm{sgn}(\langle 0|f_{\mathbf{r}_1}\cdots f_{\mathbf{r}_m} b_{i_1\uparrow}\cdots b_{i_q\uparrow} b_{j_1\downarrow}\cdots b_{j_q\downarrow}|\{\lambda\};\{\mathbf{k}\}\rangle)$$

$$= \mathrm{sgn}(\mathrm{Det}[\exp(i\mathbf{k}_i\cdot\mathbf{r}_j)])(-1)^{P(j_1,\ldots,j_q)}\,, \qquad (3)$$

where $P(j_1,\ldots,j_q)$ is equal to the total number of down spins on the A sublattice. While it is well known that the ground state of the pure Heisenberg model satisfies Marshall's sign, away from half filling the ground state of (1) is *not* required to satisfy Marshall's sign. Nonetheless, we expect that Marshall's sign will be approximately satisfied when the magnetic energy dominates[14] and it is for this reason that we believe that (2) is a sensible variational ansatz for the t'-J model in the $t'/J \ll 1$ regime. We emphasize also that requiring Marshall's sign for the spins forces Fermi statistics on the holes, as was first noted in Ref. 15.

If $\lambda(m)$ is taken to be independent of m then (2) describes holes hopping in a (singlet-projected) classical Néel state.[16] The holes then behave as noninteracting spinless fermions with dispersion

$$\epsilon(\mathbf{k}) = -2t_c'(\cos 2k_x + \cos 2k_y) - 4t_d' \cos k_x \cos k_y\,.$$

When $t_d' = 2t_c'$ the minimum-energy hole states are degenerate along the half-zone boundary ($k_x = \pm k_y \pm \pi$). Quantum spin fluctuations are introduced into (2) by allowing $\lambda(m)$ to decay as m increases.[10] The $\lambda(m)$ values we have used are those which optimize the energy at half filling, the optimal values obtained by LDA:[10] $\lambda(3)/\lambda(1) = 0.125$, $\lambda(m)/\lambda(3) = 0.25(m/5)^{-4}$ for $m \geq 5$; for these values (2) has long-range Néel order at half filling.[10,17] Spin fluctuations renormalize the effective hopping matrix elements for the holes; we find for the $\lambda(m)$ values just given that t_d' is more strongly renormalized than t_c'. Thus the occupied $\mathbf{k}$ states we have used in (2) fill the band structure described by $\epsilon(\mathbf{k})$ with $t_c' \gtrsim 2t_d'$ for which the one-hole ground-state degeneracy is lifted, with the minimum hole energy being at $(0,\pi)$ and $(\pi,0)$. This shift may be an artifact of our wave function, though a similar shift [from $(\pm\pi/2, \pm\pi/2)$ to $(0,\pi),(\pi,0)$] has been seen in exact diagonalization studies of the t-J model when t/J becomes less than some critical value.[18]

We now describe the method used to compute the energies of (2). Consider two singlet-bond states: a bra state $\langle\beta;\{\mathbf{r}\}|$ and a ket state $|\alpha;\{\mathbf{r}\}\rangle$. Each of these states has a corresponding singlet-bond configuration which is produced by drawing lines between the pairs of sites which are connected by singlet bonds. When the two configurations corresponding to states $\langle\beta;\{\mathbf{r}\}|$ and $|\alpha;\{\mathbf{r}\}\rangle$ are laid on top of one another a "transition graph" is produced.[19] This transition graph is always made up of closed loops with each loop consisting of alternating α and β bonds. We define the number of loops in this transition graph to be $N_{\alpha\beta}$. The overlap is then given by[19]

$$\langle\beta;\{\mathbf{r}\}|\alpha;\{\mathbf{r}\}\rangle = 2^{N_{\alpha\beta} - N(1-\delta)/2} \qquad (4)$$

(the convention that bonds always connect opposite sublattices in the way defined above ensures that $\langle\beta;\{\mathbf{r}\}|\alpha;\{\mathbf{r}\}\rangle > 0$), and the matrix element of a dot product of spin operators by[19]

$$\langle\beta;\{\mathbf{r}\}|\mathbf{S}_i\cdot\mathbf{S}_j|\alpha;\{\mathbf{r}\}\rangle = \begin{cases} (-1)^{|i-j|}\frac{3}{4}\langle\beta;\{\mathbf{r}\}|\alpha;\{\mathbf{r}\}\rangle & \text{if } i \text{ and } j \text{ share a loop,} \\ 0, & \text{otherwise.} \end{cases} \qquad (5)$$

The expectation value of a dot product of spin operators may then be written as

$$\langle\{\lambda\};\{\mathbf{k}\}|\mathbf{S}_i\cdot\mathbf{S}_j|\{\lambda\};\{\mathbf{k}\}\rangle=\sum_{\substack{\alpha\beta\\\{\mathbf{r}\}}}\frac{\langle\beta;\{\mathbf{r}\}|\mathbf{S}_i\cdot\mathbf{S}_j|\alpha;\{\mathbf{r}\}\rangle}{\langle\beta;\{\mathbf{r}\}|\alpha;\{\mathbf{r}\}\rangle}P[\alpha,\beta;\{\mathbf{r}\}]\,, \tag{6}$$

where

$$P[\alpha,\beta;\{\mathbf{r}\}]=\frac{1}{\langle\{\lambda\};\{\mathbf{k}\}||\{\lambda\};\{\mathbf{k}\}\rangle}\omega(\beta)\omega(\alpha)\langle\beta;\{\mathbf{r}\}|\alpha;\{\mathbf{r}\}\rangle|\mathrm{Det}\,e^{i\mathbf{k}_i\cdot\mathbf{r}_j}|^2\,. \tag{7}$$

The function $P[\alpha,\beta;\{\mathbf{r}\}]$ is positive definite [because (2) satisfies Marshall's sign] and normalized to unity when summed over all transition graphs. We used the Monte Carlo method with the standard Metropolis updating[20] to calculate (6) and a similar expression for the t'-kinetic energy of (2). Our update scheme combined the "loop-gas" technique of LDA for the boson spins and the "inverse-update" method of Ceperley, Chester, and Kalos[21] for the fermion holes.

Figure 1 shows the magnetic energies we have obtained using our wave functions, as well as the energies of other wave functions and models for comparison. The calculations for our wave functions, and for the uniform-flux states,[8] were performed on 24×24 lattices with periodic boundary conditions. On this graph the magnetic energies of a completely phase-separated state lie on a straight line drawn through $E\sim-0.334J$/bond at half filling and $E=0$ at zero filling. As expected, these phase-separated magnetic energies are lower than those of any other wave function, including ours, clearly showing that the t'-J model (and the t-J model), in the absence of long-range Coulomb interactions, must phase separate in the $t'(t)/J\ll1$ limit.[9] As stated above, our viewpoint is that the addition of long-range repulsion between electrons will make the phase-separated states physically unacceptable, and we include their energies only to provide an absolute lower bound to the magnetic energy.

The next-lowest magnetic energies shown in Fig. 1 are for our wave functions. Just above them are the energies from a broken-bond model (BBM). A broken bond is two neighboring sites i and j which are not both occupied by an electron, i.e., for which $\langle n_i n_j\rangle=0$ rather than 1. Assuming that the half-filled energy per bond, $\sim-0.334J$, is lost for each broken bond then we have

$$E_{\mathrm{BBM}}=\left(-\frac{0.334J}{\mathrm{bond}}\right)\frac{1}{2N}\sum_{\langle ij\rangle}\langle n_i n_j\rangle\,, \tag{8}$$

where the expectation value is taken using our wave functions. The true magnetic energies of our wave functions are *lower* than this naive model, indicating that, although magnetic energy is being lost due to bond breaking as holes are added to the system, some of the remaining bonds are "strengthened." This result is not surprising in light of recent spin-wave calculations which show

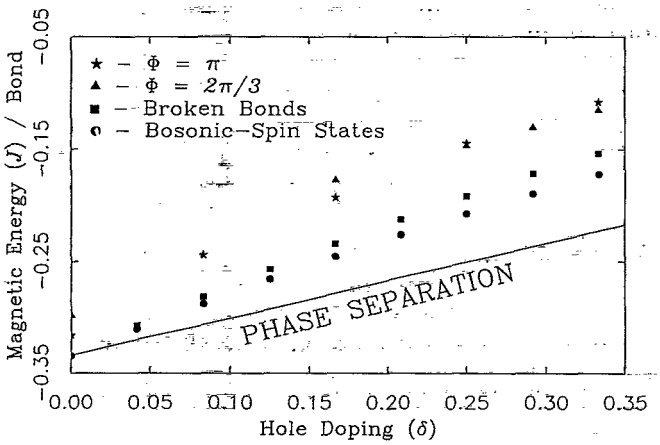

FIG. 1. Magnetic energy per bond vs doping for a phase-separated state (solid line), our wave functions—referred to as bosonic spin states (circles), a simple broken-bond model (squares), and the uniform-flux states (stars and triangles; taken from Ref. 8). The solid line shows the average magnetic energy per bond for a completely phase-separated state. The circles are the energies we have found for wave function (2). The squares are the energies for a simple broken-bond model computed from Eq. (8), and the stars and triangles are the energies of the uniform-flux states with $\Phi=\pi$ and $\Phi=2\pi/3$, respectively (Ref. 8). At $\delta=\frac{1}{3}$ the $\Phi=2\pi/3$ uniform-flux state is an example of a CFP state. Our wave function has significantly lower energy than this state, indicating that the CFP state is unstable in the $t/J\ll1$ limit.

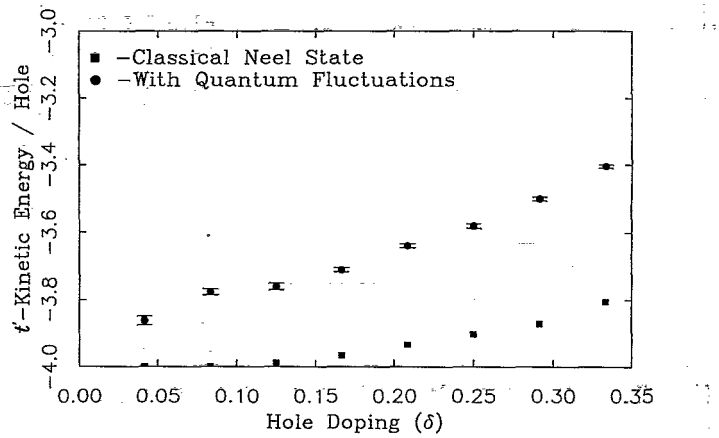

FIG. 2. The t'-kinetic energy per hole vs doping for our wave functions with (circles) and without (squares) quantum spin fluctuations. The occupied hole $\mathbf{k}$ states fill the band described by $\epsilon(\mathbf{k})$ given in the text with $t_d'\gtrsim2t_c'$.

that the local energy near a frozen hole is enhanced over its half-filled value.[22] Finally, the uniform-flux-phase energies calculated by Liang and Trivedi[8] are also shown in Fig. 1. As predicted by the mean-field theories, at $\delta = \frac{1}{3}$ the magnetic energy of the $\frac{1}{3}$-flux (CFP) state is lower than that of the $\frac{1}{2}$-flux state; however, both of these energies are much higher than that of our wave function, as well as of the naive broken-bond model. This indicates that the CFP state cannot be stable, not only in the $t'/J \ll 1$ limit of (1), but also in the $t/J \ll 1$ of the t-J model.

Figure 2 shows the t'-kinetic energy per hole of (2) for two cases: (i) $\lambda(m)$ has the optimal half-filled values given above, and (ii) $\lambda(m)$ is taken to be constant (classical Néel spin background). As δ is increased the t'-kinetic energies per hole for case (i) increase in roughly the same fashion as for case (ii); the added holes fill a spinless Fermi sea where the effective hopping matrix elements are renormalized from their "bare" values. One effect of this renormalization, as discussed above, is that the one-hole minimum is placed at $(0,\pi)$ and $(\pi,0)$. Another is that the total t'-kinetic energy is increased; thus adding quantum spin fluctuations to (2)—i.e., allowing $\lambda(m)$ to vary—lowers the magnetic energy at the cost of increasing the t'-kinetic energy.

To conclude, we have presented a class of variational wave functions suitable for the t'-J model in the $t'/J \ll 1$ limit. These wave functions have excellent magnetic energies, substantially lower than the uniform-flux-phase wave functions (including the case we could check with commensurate flux), thus providing a direct demonstration that the CFP states are unstable for the t-J model when t/J is less than some finite critical value.

We acknowledge useful discussions with D. L. Cox, T.-L. Ho, C. Jayaprakash, S. Liang, M. Ma, S. Sarker, and N. Trivedi. We thank Y. Shapir for sending us a copy of his work. This work was supported by the DOE–Basic Energy Sciences, Division of Materials Research.

---

[a]Present address: Institut für Theoretische Physik, Eidgenössische Technische Hochschule Hönggerberg, CH-8093 Zürich, Switzerland.

[1]P. W. Anderson, Science **235**, 1196 (1987).

[2]F. C. Zhang and T. M. Rice, Phys. Rev. B **38**, 4632 (1988).

[3]M. S. Hybertsen, E. B. Stechel, M. Schluter, and D. R. Jennison, Phys. Rev. B **41**, 11068 (1990).

[4]P. Lederer, D. Poilblanc, and T. M. Rice, Phys. Rev. Lett. **63**, 1519 (1989); J. P. Rodriguez and B. Doucot, Europhys. Lett. **11**, 451 (1990). The mean-field calculation in these papers [as well as subsequent numerical work, see S. Liang and N. Trivedi, Phys. Rev. Lett. **64**, 232 (1990)] suggest that the CFP states are stable for $t/J \lesssim 1$; however, the energy difference favoring the CFP states is largest when $t/J \ll 1$. We believe that our results for the latter limit call into question the stability of the CFP states for any value of t/J.

[5]I. Affleck and B. Marston, Phys. Rev. B **37**, 3774 (1988).

[6]R. B. Laughlin, Science **242**, 525 (1988); X. G. Wen, F. Wilczek, and A. Zee, Phys. Rev. B **39**, 11413 (1989).

[7]For discussions of the connection between the CFP states and the anyon superfluid, see Y. Hasegawa, O. Narikiyo, K. Kuboki, and H. Fukuyama, J. Phys. Soc. Jpn. **59**, 822 (1990); P. B. Wiegmann, Phys. Rev. Lett. **65**, 2070 (1990); J. P. Rodriguez and B. Doucot, Phys. Rev. B **42**, 8724 (1990).

[8]Liang and Trivedi (Ref. 4).

[9]V. J. Emery, S. A. Kivelson, and H. Q. Lin, Phys. Rev. Lett. **64**, 475 (1990).

[10]S. Liang, B. Doucot, and P. W. Anderson, Phys. Rev. Lett. **61**, 365 (1988).

[11]N. Trivedi and D. Ceperley, Phys. Rev. B **40**, 2737 (1989); J. Carlson, Phys. Rev. B **40**, 846 (1989).

[12]The distance between points, $|i-j|$, is defined to be the minimum number of nearest-neighbor hops to get from i to j.

[13]E. Lieb, T. Schulz, and D. Mattis, Ann. Phys. (N.Y.) **16**, 407 (1961); W. Marshall, Proc. Roy. Soc. London A **232**, 48 (1955).

[14]In the $t'/J \ll 1$ limit we expect that the normalized ground state of (1), $|\psi_0\rangle$, can be decomposed into two parts, $|\psi_0\rangle = |\psi_M\rangle + |\psi_{\bar{M}}\rangle$, where $|\psi_M\rangle$ satisfies Marshall's sign and $\langle\psi_{\bar{M}}|\psi_{\bar{M}}\rangle \sim t'/J$.

[15]N. Read and B. Chakraborty, Phys. Rev. B **40**, 7133 (1989).

[16]M. Ma, Phys. Rev. B **38**, 6813 (1988).

[17]With these $\lambda(m)$ values fixed, we expect that (2) will lose long-range Néel order at a critical doping δ_c [see Y. Shapir (to be published) for a mean-field discussion of this effect]. To test this we have studied large lattices (120×120) using an approximation in which the hole Slater determinant in (2) is replaced by 1. We find that, at $\delta = \frac{1}{3}$, (2) does not have long-range order (instead, $|\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle| \sim |i-j|^{-\alpha}$ with $\alpha \sim 1$), so that, for the values of $\lambda(m)$ we are using, $\frac{1}{3} > \delta_c > 0$.

[18]Y. Hasegawa and D. Poilblanc, Phys. Rev. B **40**, 9035 (1989).

[19]W. Sutherland, Phys. Rev. B **37**, 3786 (1988); M. Kohomoto and Y. Shapir, Phys. Rev. Lett. **61**, 9439 (1988).

[20]N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. **21**, 1087 (1953).

[21]D. Ceperley, G. V. Chester, and M. H. Kalos, Phys. Rev. B **16**, 3081 (1977).

[22]N. Bulut, D. Hone, D. J. Scalapino, and E. Y. Loh, Phys. Rev. Lett. **62**, 2192 (1989).