PHYSICAL REVIEW B VOLUME 37, NUMBER 13 1 MAY 1988

Hole propagation in correlated spin systems

Robert Joynt
Department of Physics, University of Wisconsin–Madison, 1150 University Avenue, Madison, Wisconsin 53706
(Received 14 December 1987)

An approximation method is presented for the calculation of the Green's function for a single hole moving in a correlated spin background. General formulas are obtained for calculating the moments of the Green's function, generalizing the Brinkman-Rice method to a general spin state. Numerical results are presented for a one-dimensional Gutzwiller resonating-valence-bond (RVB) state. In the two-dimensional case, the bandwidth is derived. The kinetic energy of a single hole in a correlated antiferromagnet or Gutzwiller RVB state is higher than in a Néel antiferromagnet.

The discovery of high-temperature superconductors[1] has touched off a theoretical debate on what theoretical model best describes the materials. One intriguing possibility is that a two-dimensional Hubbard model with large intra-atomic repulsion U and a nearly half-filled band may be appropriate.[2] Each site is then occupied by a hole or a spin. The superconductivity in this model would be the result of hole pairing induced by singlet spin bonds[3] or Bose condensation of bound hole-spin quasiparticles.[4,5]

A central question in this physical picture is whether a hole in this spin background can propagate freely or not. If it can, then one is justified in treating the holes as quasiparticles and proceeding to determine their statistics, possible pairing interaction, etc. If, on the other hand, hole motion is purely diffusive, the issues surrounding superconductivity from hole-hole coherence must be handled more carefully. A second issue is the question of the kinetic energy of a single hole in correlated spin states. For example, the ground state of the two-dimensional Heisenberg Hamiltonian has long been thought to be a correlated state with antiferromagnetic long-range order.[6,7] Recent calculations by Gros[8] on a d-wave resonating-valence-bond (RVB)-type state have called this into question. Doped systems with finite hole concentration also have kinetic energy and it is then also possible that a normal Gutzwiller RVB state[9] is lowest in energy. To resolve these questions, it is necessary to understand the relation between the hole energy and the nature of the spin background. Mean-field theories,[10] which take the hole energy to be independent of the background, are not suitable for dealing with this question.

In this paper, I focus on the problem of a single hole. I follow the moment method of Brinkman and Rice[11] (BR) to calculate the single-particle Green's function (GF). These authors calculated the GF for ferromagnetic, Néel, and random spin configurations and the calculations for the Néel state have recently been refined in connection with superconductivity by several authors.[12] Our interest here is in correlated spin states which are *not* eigenstates of the spin projection on an axis at any site.

The single-hole GF is defined as

$$G_{ij}(\omega)=\left\langle\psi\left|c_i^{\dagger}\frac{1}{\omega-H}c_j\right|\psi\right\rangle , \tag{1}$$

where $|\psi\rangle$ is a spin state, i.e., contains no holes. H is taken to be the kinetic energy operator.

$$H=-\sum_{\langle i,j\rangle,s}(1-n_{i,-s})c_{is}^{\dagger}c_{js}(1-n_{j-s})+\text{H.c.} , \tag{2}$$

with a hopping matrix element equal to one. The operators $(1-n)$ merely ensure that H never creates any doubly occupied sites. For generality, the spin-spin interactions which stabilize $|\psi\rangle$ are not included in H. This means, however, that as the hole moves the spin configuration is not allowed to relax. In the Hubbard model, this is a good approximation only if $U\gg 1$, where U is the intra-atomic Coulomb repulsion.

The expression (1) may now be expanded:

$$G_{ij}(\omega)=\frac{1}{\omega}\sum_n(-\omega)^{-n}\langle c_i^{\dagger}H^n c_i\rangle . \tag{3}$$

All expectation values are in the state $|\psi\rangle$. The nth moment is determined by a path of n steps leading from site i to site j. In the BR calculation, the matrix element could be calculated by geometrical reasoning: If the motion of the hole disturbed (left unchanged) the spin configuration, the answer is zero (one). In our case, the spin configuration is not an eigenfunction of the z component of spin on the sites, and we must do the fully quantum-mechanical calculation of the operator product along a path from i to j in the state $|\psi\rangle$. This may be carried out at low order in n by using the fermion anticommutation relations, the identities $c_{i\uparrow}^{\dagger}c_{i\uparrow}=\frac{1}{2}(1+\sigma_i^z)$, $c_{i\downarrow}^{\dagger}c_{i\downarrow}=\frac{1}{2}(1-\sigma_i^z)$, $c_{i\uparrow}^{\dagger}c_{i\downarrow}=\sigma_i^{+}$, $c_{i\downarrow}^{\dagger}c_{i\uparrow}=\sigma_i^{-}$, and the fact that $\langle n_i\rangle=1$. σ_i^{α} is the α th Pauli matrix on the site i. For example, if i and j are nearest neighbors, the ω^{-2} term in Eq. (1) is given by

$$-\omega^{-2}\sum_{a,b}\langle c_{ia}^{\dagger}c_{ib}c_{jb}^{\dagger}c_{ja}\rangle=-\tfrac{1}{2}\omega^{-2}\langle 1+\sigma_i\cdot\sigma_j\rangle . \tag{4}$$

For i,j next-nearest neighbors, the first nonvanishing term is order ω^{-3}, and there is normally more than one path from i to j. The contribution from a path $i\rightarrow k\rightarrow j$ is

$$\tfrac{1}{4}\omega^{-3}\{1+\langle\sigma_i\cdot\sigma_k+\sigma_i\cdot\sigma_j+\sigma_j\cdot\sigma_k\rangle+i\langle\sigma_i\cdot(\sigma_k\times\sigma_j)\rangle\} . \tag{5}$$

In a term from a path of length n, all rotationally invariant spin-correlation functions up to order σ^{n+1} appear, and the complexity of such functions increases rapidly with n. An exception occurs for any path having retraced

steps. The retracing preserves the state and the expectation value is the same as for the shorter path with the retraced steps deleted.[7] To calculate expectation values at high order, we make the approximation of neglecting all terms involving cross products of σ's. Such terms may be expected to be small for the states we will consider, with spins tending to be parallel or antiparallel. The symmetry of the operator product, together with the fact that the expectation value is always unity for $|\psi\rangle$, a ferromagnetic state, leads to the result that

$$\langle c_i^\dagger H^n c_j\rangle = 2^{-n}\sum_{\text{paths}}\sum_{\substack{l=0\\ \text{even}}}^{n}\langle(\sigma_{i_1}\cdot\sigma_{i_2})(\sigma_{i_3}\cdot\sigma_{i_4})\cdots(\sigma_{i_{l-1}}\cdot\sigma_{i_l})\rangle \tag{6}$$

for paths with no self-intersections. Here, the sum is over paths of length n, and the $l=0$ terms in the sum is equal to one. The σ subscripts label sites in increasing order along the path from $i_1=i$ to $i_l=j$. The number of terms in the sum over l is 2^n. In one dimension (1D), the simple topology allows explicit calculation—any path from i to j is the product of the direct path and retracings. Every expectation value at a given order in $G_{ij}(\omega)$ is the same, and is precisely (6) with i_l increasing along the chain. The 1D GF is, therefore, $G_{ij}(\omega)=M_{ij}G_{ij}^0(\omega)$, where M_{ij} is the envelope function given by (6) and

$$G_{ij}^0(\omega)=\int_{-\pi}^{\pi}[\omega+2\cos(k)]^{-1}e^{-ik(i-j)}dk$$

is the free (ferromagnetic) GF. For random spins, $M_{ij}=2^{-|i-j|}$. To compute M_{ij}, we factor the spin products: $\langle(\sigma_1\cdot\sigma_2)(\sigma_3\cdot\sigma_4)\rangle\approx\langle\sigma_1\cdot\sigma_2\rangle\langle\sigma_3\cdot\sigma_4\rangle$, and similarly for higher-order functions. The pair correlation function for all separations has been calculated by Gebhard and Vollhardt[13] for the 1D $U=\infty$ Gutzwiller wave function. They find $\langle\sigma_i\cdot\sigma_j\rangle=4(-1)^r\mathrm{Si}(\pi r)/\pi r$, where $r=|i-j|$ and Si is the sine-integral function. With this input, M_r may be computed numerically which I have done for r up to 24. The results are shown in Fig. 1. $|M_r|$ behaves roughly as $(0.576)^r$. Its falloff is, therefore, exponential, just as in the random case, though slightly slower. In addition, and more important for later considerations, it oscillates with a period of roughly 5.

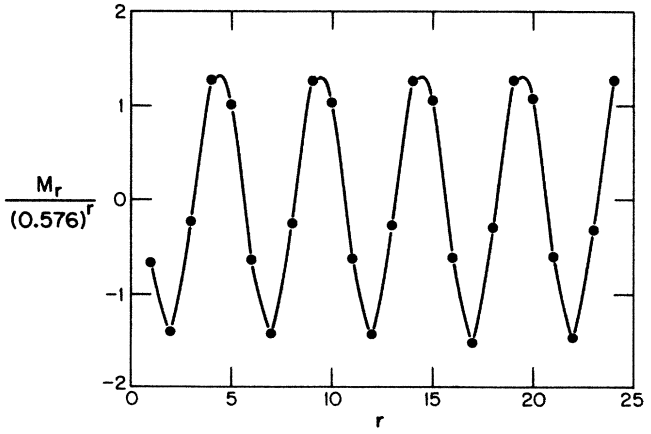

FIG. 1. Plot of the dimensionless function M_r, which determines the spatial decay of the single-hole Green's function in one dimension. M_r has been normalized to remove the exponential falloff $\sim(0.576)^r$. The oscillations arise from the antiferromagnetic correlations in the Gutzwiller RVB state.

A spatial Fourier analysis of $G_{ij}(\omega)$ will be presented in a future publication. It is already clear from the qualitative behavior of G that its poles lie well off the real axis except for a limited range of wave vectors corresponding to the oscillations of M_r. The electrons propagate in a diffusive manner with a relatively short coherence length.

A more physically interesting case is that of hole motion in two dimensions. I consider only the square lattice. Here, closed loops, i.e., paths with self-intersections, are possible and the number of paths to be considered grows rapidly with the moment to be computed. The simplest approximation is to treat the lattice as a Cayley tree to eliminate loops, which is very accurate for a Néel antiferromagnet.[11] Consider first the diagonal GF, $G_{ii}(\omega)$. As BR point out, $G_{ii}(\omega)$ is independent of spin configuration in this approximation. Since $G_{ii}(\omega)$ determines the bandwidth of the hole, this implies that the kinetic energy of a hole in the Gutzwiller RVB (for example) state would be the same as that in the Néel state. The differences in the two states arise when closed loops which return to the origin are considered. On the square lattice, the simple four-step loop leads to nonzero contribution at order ω^{-5}. The matrix element for a general spin state for this path may be calculated. If the spins are labeled 1, 2, 3, 4 clockwise around the square, then

$$\langle c_1 H^4 c_1^\dagger\rangle\equiv m=\tfrac{1}{4}[1+\langle\sigma_2\cdot\sigma_3\rangle+\langle\sigma_2\cdot\sigma_4\rangle+\langle\sigma_3\cdot\sigma_4\rangle-i\langle\sigma_2\cdot(\sigma_3\cdot\sigma_4)\rangle]\ .$$

For the two-dimensional d-wave state, or the Gutzwiller-RVB state, the spin correlations can be calculated numerically.[12] The result, together with results for the antiferromagnet, is listed in Table I.

TABLE I. List of characteristics of various two-dimensional spin states on the square lattice. The normal RVB state is that defined in Refs. 2 and 9. The d-wave state is the nominally superconducting state defined in Ref. 8. The Oitmaa-Betts state is a correlated antiferromagnet as described in Ref. 6. The second and third columns give the nearest-neighbor and second-neighbor spin correlation, whereas m, listed in the fourth column, also contains a contribution from the second-neighbor correlation. The fifth column gives the kinetic energy of a single hole in the corresponding state. This is calculated using the square loop approximation, explained in the text. The spin correlations for the RVB states are taken from variational Monte Carlo calculations of C. Gros, R. Joynt, and T. M. Rice (unpublished). The correlations for the Oitmaa-Betts states are taken from Ref. 6.

State	$\langle\sigma_i\cdot\sigma_j\rangle_1$	$\langle\sigma_i\cdot\sigma_j\rangle_2$	m	Kinetic energy
Ferromagnet	1	1	1	−3.97
Normal RVB	−1.10	0.56	−0.16	−3.37
d-wave RVB	−1.28	0.44	−0.28	−3.29
Néel	−1	1	0	−3.46
Oitmaa-Betts	−1.31	0.78	−0.21	−3.34

We now take a clue from the one-dimensional case and assume that the exponential falloff and oscillation in sign of the matrix elements for larger loops allows us to keep only the contributions from the squares. The longer loops will be subject to destructive interference. This is the fundamental approximation of this paper.

We now follow BR and write $G_{ii}(\omega)=1/\omega(1-\xi)$, where ξ is the sum of all paths which return for the first time to their starting point only at the end of the path. $\xi=(4/\omega^2)[1-(3+2m)/\omega^2]$ includes 12 branched retraced paths and 8 loops and is correct to order ω^{-4}. This reasoning may be continued[14] and leads at infinite order to

$$\xi=\frac{2}{3}\left\{1-\frac{2m}{\omega^2}-\left[\left(1-\frac{2m}{\omega^2}\right)^2-\frac{12}{\omega^2}\right]^{1/2}\right\}.$$

The density of states for hole excitations is $\rho(\omega)=(1/\pi)\mathrm{Im}G_{ii}(\omega-i\delta)$ and the band edge is given by setting the argument of the square root to zero. The results are shown in the table.

The ferromagnetic result for which the exact answer for the kinetic energy is -4 is included in order to show that the inclusion of loops gives very good results accurate to better than 1%, even when there is constructive interference from longer loops. The loop approximation should be better for the antiferromagnetically correlated states. A surprising result is that the kinetic energy of a hole in the Néel state is considerably lower than in correlated states, and may be traced to the fact that $m<0$ in the latter due to stronger nearest-neighbor correlation. Then translation of the system with a hole gives a larger charge in phase to the many-body wave function. The true antiferromagnetic state has less long-range order and the bonds have more singlet character, raising the hole energy. The energy of the hole in the normal Gutzwiller-RVB state is between that in the Néel and in the true antiferromagnetic states. Its nearest-neighbor correlations are less negative, relatively lowering the hole energy, but the hole gets less help from longer-range parallel spins to lessen its energy further. The d-wave superconducting state has higher kinetic energy than all the others. This is to be expected and is due to the broader input momentum distribution, just as in ordinary Bardeen-Cooper-Schrieffer (BCS) superconductivity. Let us discuss case by case the implications of these results for the stability of the various states with holes. The low energy of the hole in a ferromagnet merely confirms a well-known result:[15] in the absence of spin-spin interactions the ferromagnetic state with one hole is stable. If there are antiferromagnetic nearest-neighbor spin-spin interactions, then at half-filling one might expect a state with long-range antiferromagnetic order. It is remarkable that the addition of holes moves the state towards *more* long-range order (Néel state), but this conclusion is inescapable. This indicates that the usual idea that the Néel state should be destroyed most quickly by the addition of holes is not correct. The energies of the correlated antiferromagnet and the d-wave RVB state are already extremely close in the half-filled case. As holes are added, the antiferromagnet may become stable unless longer-range interactions are added. As concerns the competition between normal and d-wave RVB states, it appears that at some finite concentration, the normal state will eventually become lower in energy.

Using the same methods, one can also calculate numerically the results for $G_{ij}(\omega)$ for $i\neq j$. This requires knowledge of longer-range spin correlations and more elaborate path-counting methods and has not yet been undertaken.

In conclusion, I have formulated a method for computing the Green's function for holes in correlated spin systems. This can be used to determine the character of the propagation and the kinetic energy. This is an improvement over mean-field theories which ignore the spin configuration. The kinetic energy, together with spin-correlation energy, determine the delicate relative stability of competing phases in the doped Mott insulator.

I am very grateful to F. C. Zhang, T. M. Rice, and C. Gros for helpful discussions, and to the Zentrum für Theoretische Studien, Eidgenössische Technische Hochschule, Zurich and the Aspen Center for Physics for hospitality during the course of this work. Numerical calculations were performed at the San Diego Supercomputer Center.

[1] J. G. Bednorz and K. A. Müller, Z. Phys. B **64**, 188 (1986).
[2] P. W. Anderson, Science **235**, 1196 (1987).
[3] C. Gros, R. Joynt, and T. M. Rice, Z. Phys. B **68**, 425 (1987). See also Refs. 10 and 12.
[4] S. Kivelson, D. Rokhsar, and J. Sethna, Phys. Rev. B **35**, 8865 (1987).
[5] Z. Zou and P. W. Anderson, Phys. Rev. B **37**, 627 (1988).
[6] J. Oitmaa and D. D. Betts, Can. J. Phys. **56**, 897 (1978).
[7] H. Yokoyama and H. Shiba (to be published). These authors demonstrate the equivalence of the Gutzwiller state at $U=\infty$ and the RVB state as defined in Ref. 2.
[8] C. Gros (unpublished).
[9] C. Gros, R. Joynt, and T. M. Rice, Phys. Rev. B **36**, 381 (1987); for the half-filled case, see T. A. Kaplan, P. Horsch, and P. Fulde, Phys. Rev. Lett. **49**, 889 (1982); P. Horsch and T. A. Kaplan, J. Phys. C **16**, L1203 (1983); Bull. Am. Phys. Soc. **30**, 513 (1985).
[10] M. C. Gutzwiller, Phys. Rev. **134**, A293 (1964); **137**, A1726 (1965); for applications to superconductivity, see G. Baskaran, Z. Zou, and P. W. Anderson, Solid State Commun. **63**, 973 (1987); A. Ruckenstein, P. Hirschfeld, and J. Appel, Phys. Rev. B **36**, 857 (1987).
[11] W. F. Brinkman and T. M. Rice, Phys. Rev. B **2**, 1324 (1970).
[12] J. E. Hirsch, Phys. Rev. Lett. **59**, 228 (1987); Y. Takahashi, Z. Phys. B **67**, 503 (1987); B. Shraiman and E. Siggia, Phys. Rev. Lett. **60**, 740 (1988).
[13] F. Gebhard and D. Vollhardt, Phys. Rev. Lett. **59**, 1472 (1987).
[14] The reasoning is the same as that leading to Eq. (2.26) of Ref. 11.
[15] Y. Nagaoka, Phys. Rev. **147**, 392 (1966). See this reference also for a discussion of the moment expansion of the Green's function.