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Resonating-valence-bond state with fermionic charges and bosonic spins: Mean-field theory

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We consider a representation of the Hubbard model, in which the charge carriers are fermions and the spin carriers are bosons. We show that there exists a mean-field solution with a condensate of spin singlets and we characterize the low-temperature behavior of the quasiparticles. Finally, we calculate the tunneling spectrum for a normal-metal–resonating-valence-bond (RVB) state tunnel junction and suggest the tunneling experiment as a probe of the statistics of the RVB quasiparticles.

It has been suggested by Read and Chakraborty[1] that the charge carriers of the resonating-valence bond (RVB) model are fermions and that the spin carriers are bosons. This is in contrast to the commonly held view, first proposed by Kivelson, Rokhsar, and Sethna,[2] where the situation is just the opposite: bosonic charges and fermionic spins. Read's and Chakraborty's argument is that in order to get the lowest energy of a hole in a RVB state (using the prescription of Sutherland[3] to choose the relative phases of the singlets) it is necessary to assign to each hole a "vortex" in the gauge field, so that the self-overlap of the state is unchanged by the presence of the hole. It turns out that the interchange of two holons gives a factor π in the overall phase.

We will use the "slave boson" approach to derive a mean-field theory for this particular choice of statistics. The basic idea is that with this method the correct statistics for the quasiparticles can be brought in from the start.

Our starting point is analogous to that of Zou and Anderson[4] (see also Kotliar and Liu[5]) who introduce a new set of operators

$$c_{i\uparrow}=e_i^\dagger s_{i\uparrow}+s_{i\downarrow}^\dagger d_i\,,\quad c_{i\downarrow}=e_i^\dagger s_{i\downarrow}-s_{i\uparrow}^\dagger d_i\,, \tag{1}$$

where in contrast to the Zou-Anderson work we choose the e's and d's to be *fermions* and the s's to be *bosons*. The introduction of these operators will bring us out of the physical subspace. This is defined by the requirement

$$e_i^\dagger e_i+s_{i\uparrow}^\dagger s_{i\uparrow}+s_{i\downarrow}^\dagger s_{i\downarrow}+d_i^\dagger d_i=1\,, \tag{2}$$

since we will interpret $e_i^\dagger$ as a creation operator for an empty i site, $d_i^\dagger$ as creating a doubly occupied i site, and $s_{i\sigma}^\dagger$ as creating a spin σ on site i. It is easy to show that in the physical subspace the electron operators will satisfy the usual commutation relations.

The Hubbard-Hamiltonian in the large-U limit will take the form

$$H=-t\sum_{i,j,\sigma}s_{i\sigma}^\dagger e_i e_j^\dagger s_{j\sigma}-J\sum_{\langle i,j\rangle}b_{ij}^\dagger b_{ij}\,, \tag{3}$$

($J=4t^2/U$). Here the first term describes the hopping of electrons, where the presence of e_i and $e_j^\dagger$ makes sure that the site to which the electron is hopping is really empty and that the site it is leaving becomes empty. In the second term the operator $b_{ij}^\dagger$ creates a pair of spins on the sites i and j which are in the singlet combination

$$b_{ij}^\dagger=\frac{1}{\sqrt{2}}(s_{i\uparrow}^\dagger s_{j\downarrow}^\dagger-s_{i\downarrow}^\dagger s_{j\uparrow}^\dagger)\,. \tag{4}$$

This last term can, in turn, be rewritten in the more conventional Heisenberg form

$$b_{ij}^\dagger b_{ij}=-\mathbf{S}_i\cdot\mathbf{S}_j+\tfrac{1}{4}n_i n_j\,, \tag{5}$$

where $n_i=n_{i\uparrow}+n_{i\downarrow}$. We will use the first form because it is the singlets that are important in a RVB state.

Consider next the partition function

$$Z=\mathrm{Tr}(e^{-\beta(H-\mu\hat{N})}P)\,, \tag{6}$$

P is an operator that projects onto the physical subspace. Since the Hamiltonian will never take us out of this subspace ($[P,H]=0$), we will only need this one P. Mathematically, P is represented by a set of Kronecker-deltas:

$$P=\prod_i\int_{-\pi/\beta}^{\pi/\beta}\frac{d\beta\lambda_i}{2\pi}\exp[i\beta\lambda_i(e_i^\dagger e_i+s_{i\uparrow}^\dagger s_{i\uparrow}+s_{i\downarrow}^\dagger s_{i\downarrow}-1)]\,. \tag{7}$$

(Being in the large-U limit, the states with double occupancy, i.e., the d_i's, can be neglected.) With this representation the partition function can be written

$$Z=\prod_i\int_{-\pi/\beta}^{\pi/\beta}\frac{d\beta\lambda_i}{2\pi}Z(\lambda_1,\ldots,\lambda_N)\,, \tag{8}$$

with

$$Z(\lambda_1,\ldots,\lambda_N)=\mathrm{Tr}(e^{-\beta H_{\mathrm{eff}}})\,, \tag{9}$$

and

$$H_{\mathrm{eff}}=H-\mu\hat{N}-i\sum_i\lambda_i(e_i^\dagger e_i+s_{i\uparrow}^\dagger s_{i\uparrow}+s_{i\downarrow}^\dagger s_{i\downarrow}-1)\,. \tag{10}$$

The strategy is now to do a conventional Hartree-Fock factorization on the effective Hamiltonian, and after self-consistency has been obtained to do the λ_i integrals in a steepest descent calculation, i.e., to find the minimum of the free energy, $F=-1/\beta\ln Z(\lambda_1,\ldots,\lambda_N)$. In this last step we will assume that the minimum is obtained when all λ_i are identical and purely imaginary, i.e., $\lambda_i=i\lambda$. In this way λ will act as a chemical potential.

Let us start with the holon sector, which is the part of the mean-field Hamiltonian describing the e fields. It is given by

$$H_{\mathrm{hol}}=\sum_k\left(t\sum_\tau e^{-ik\tau}\rho_\tau^B+\mu+\lambda\right)e_k^\dagger e_k\,. \tag{11}$$

Here τ represents the nearest-neighbor directions. ρ_τ^B is the Hartree term for the bosons

$$\rho_\tau^B = \sum_\sigma \langle s_{i\sigma}^\dagger s_{i+\tau\sigma} \rangle . \tag{12}$$

As we shall see below this term is negative, independent of τ, and with an absolute value less than unity. This results in a band for the fermions which has a minimum for $k=(0,0)$. With the definitions $\epsilon_k = -2t\rho^B[2-\cos(k_x)-\cos(k_y)]$ and $\mu_F = -(4t\rho^B+\mu+\lambda)$ we write $H_{\rm hol} = \sum_k (\epsilon_k - \mu_F) e_k^\dagger e_k$.

We now turn to the spin sector and use the definition of an RVB state as a condensate of singlet pairs, corresponding to a nonvanishing value for $\langle b_{ij}^\dagger \rangle$. With the introduction of the mean fields

$$\Delta_\tau = J\langle b_{i,i+\tau} \rangle , \quad \rho_\tau^F = \langle e_i^\dagger e_{i+\tau} \rangle , \tag{13}$$

the mean-field Hamiltonian for the spin sector becomes

$$H_{\rm spin} = \sum_{k,\sigma} (\omega_k - \mu_B) s_{k\sigma}^\dagger s_{k\sigma} - \sum_k (\Delta_k^* s_{k\uparrow}^\dagger s_{-k\downarrow}^\dagger + \Delta_k s_{-k\downarrow} s_{k\uparrow}) , \tag{14}$$

where we have introduced the dispersion

$$\omega_k = [2t\rho^F + (J/2)\rho^B][2+\cos(k_x)+\cos(k_y)] ,$$

and the effective chemical potential

$$\mu_B = 2[2t\rho^F + (J/2)\rho^B] + (J/4)(1-\delta) - \lambda .$$

The two chemical potentials μ_F and μ_B for the charges and the spins that we have introduced can be varied independently, since they are built out of the two independent parameters λ and the chemical potential μ for the electrons. The k-space order parameter Δ_k is given by

$$\Delta_k = -\frac{i}{\sqrt{2}} \sum_\tau \Delta_\tau \sin(k\tau) . \tag{15}$$

This is nonvanishing because the real-space order-parameter Δ_τ satisfies $\Delta_{-\tau} = -\Delta_\tau$ which is easily seen from (13). In this paper we will study the case where $\Delta_x = \Delta_y$ and discuss other choices of relative phases in a later publication.

The spin Hamiltonian $H_{\rm spin}$ can be diagonalized by a Bogoliubov transformation. The quasiparticles, i.e., the *spinons,* are created and annihilated by the operators $\gamma_{k\sigma}^\dagger$ and $\gamma_{k\sigma}$, which are given by

$$s_{k\uparrow} = u_k \gamma_{k\uparrow} + v_k \gamma_{-k\downarrow}^\dagger , \quad s_{-k\downarrow} = v_k \gamma_{k\uparrow}^\dagger + u_k \gamma_{-k\downarrow} , \tag{16}$$

where the quasiparticle energies are

$$E_k = [(\omega_k - \mu_B)^2 - |\Delta_k|^2]^{1/2} , \tag{17}$$

and the coherence factors are $u_k^2 = \frac{1}{2}[(\omega_k - \mu_B)/E_k + 1]$ and $v_k^2 = \frac{1}{2}[(\omega_k - \mu_B)/E_k - 1]$. Finally, there is a condensation energy, so that the diagonalized spin Hamiltonian has the form

$$H_{\rm spin} = \sum_{k,\sigma} [E_k \gamma_{k\sigma}^\dagger \gamma_{k\sigma} - (\omega_k - \mu_B - E_k)/2] . \tag{18}$$

We can now write down the self-consistency equations. First the number of holons should be equal to the doping, i.e.,

$$\delta = \langle e_i^\dagger e_i \rangle = \frac{1}{N} \sum_k n_F(\epsilon_k - \mu_F) . \tag{19}$$

The holon hopping amplitude obeys

$$\rho_\tau^F = \langle e_{i+\tau}^\dagger e_i \rangle = \frac{1}{2N} \sum_k [\cos(k_x)+\cos(k_y)] n_F(\epsilon_k - \mu_F) . \tag{20}$$

In the spin sector we must have that the total number of spin sites should be given by the number of sites with no holons, i.e., $N(1-\delta)$,

$$1-\delta = 2\langle s_{i\sigma}^\dagger s_{i\sigma} \rangle = \frac{1}{N} \sum_k \left(\frac{\omega_k - \mu_B}{E_k} [2n_B(E_k)+1] - 1 \right) . \tag{21}$$

The equation for the spin hopping field ρ_τ^B is

$$\rho_\tau^B = 2\langle s_{i+\tau\sigma}^\dagger s_{i\sigma} \rangle = \frac{1}{2N} \sum_k \frac{\omega_k - \mu_B}{E_k} [\cos(k_x)+\cos(k_y)][2n_B(E_k)+1] . \tag{22}$$

Finally, we have the gap equation for the spinon condensate. It is calculated by forming the combination $(\Delta_x^* + \Delta_y^*)/2 = \Delta_0$ to obtain

$$1 = \frac{J}{2N} \sum_k \frac{[\sin(k_x)+\sin(k_y)]^2}{E_k} [2n_B(E_k)+1] . \tag{23}$$

Equations (19)–(23) determine the unknowns: μ_F, μ_B, ρ_τ^F, ρ_τ^B, and Δ_0. The physics of these equations is dominated by the gap in the spinon spectrum. The minimal value for E_k is found to be

$$E_g = 2\sqrt{2}\Delta_0 \left(\frac{(t_B - \mu_B/2)^2}{t_B^2 + 2\Delta_0^2} - 1 \right)^{1/2} , \tag{24}$$

where $t_B = 2t\rho^F + J/2\rho^B$. From this expression it is seen that there exists a maximal value for the spin chemical potential, and E_g will approach zero as μ_B approaches this maximal value from below.

We will first consider the half-filled band case, where $\delta=0$, at very low temperatures. Here we only need to consider the spin sector. At half-filling the mean-field $\langle s_{i+\tau\sigma}^\dagger s_{i\sigma} \rangle$ vanishes. This is in agreement with the physical fact that in this case a spin cannot hop without violating the constraint (2), all sites having exactly one spin. Consequently, ω_k is zero. However, the spinon quasiparticles can still move because E_k has dispersion. In Eqs. (21) and (23) the temperature-dependent part of the k sums will be totally dominated by the region in k space around the gap, which in this case is located at the k points $(\pi/2,\pi/2)$ and $(-\pi/2,-\pi/2)$. Setting μ_B equal to its maximal value, i.e., $\mu_B = -2\sqrt{2}\Delta_0$, the temperature-dependent k sums can be eliminated from the two equations and we finally obtain the solution for Δ_0,

$$\Delta_0 = J\sqrt{2} \left\{ 1 - \frac{1}{2N} \sum_k \left[1 - \left(\frac{\sin(k_x)+\sin(k_y)}{2} \right)^2 \right]^{1/2} \right\} = 0.8188J . \tag{25}$$

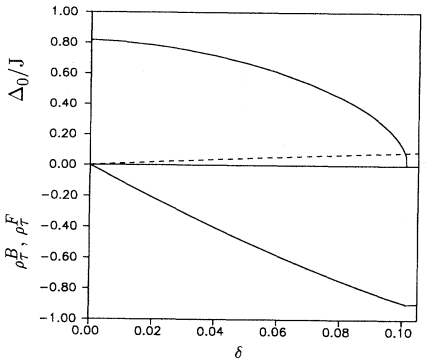

FIG. 1. The RVB order parameter Δ_0 (upper solid line), ρ_τ^B (lower solid line), and ρ_τ^F (dashed line) vs the number of holes per site at zero temperature and $J/t = \frac{1}{10}$.

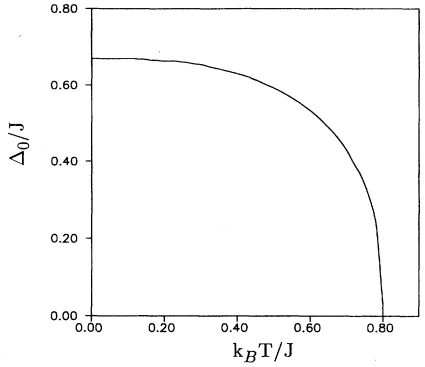

FIG. 3. The temperature dependence of the RVB order parameter showing a second-order phase transition at a critical temperature. ($\delta = 0.05$ and $J/t = \frac{1}{10}$).

Next, we consider the solutions to the mean-field equations, (19)–(23), away from the half-filled band case. We have solved the equations numerically and find that the presence of holes suppresses the strength of the singlet condensate and at a critical filling the RVB order parameter goes to zero. The holon and spinon bandwidths increase with increasing hole concentration. Figure 1 shows Δ_0, ρ_τ^B, and ρ_τ^F versus the doping with $J/t = \frac{1}{10}$ and $T = 0$. The RVB state is characterized by a nonvanishing Δ_0 at $T = 0$ and the $(J/t) - \delta$ phase diagram is shown in Fig. 2.

The temperature dependence of Δ_0 and the gap in the spinon spectrum E_g is shown in Figs. 3 and 4, respectively.

We now turn to the low-temperature limit. The gap vanishes as T approaches zero which means that the chemical potential reaches its maximum value, found by setting $E_g = 0$ in Eq. (24),

$$\mu_{B,\max} = -2[(t_B^2 + 2\Delta_0^2)^{1/2} - t_B] .$$

The temperature-dependent part of the k sums in Eqs. (21), (22), and (23) is in the low-temperature limit dominated by a k-space region in the neighborhood of $k_{\min}$, where $k_{\min}$ is given by $E_{k_{\min}} = E_g$. Since the Bose distribution $n_B(E_k)$ at low temperatures is strongly peaked close to $k_{\min}$ it is a good approximation to replace E_k by the dispersion in the neighborhood of $k_{\min}$,

$$E_k \simeq (E_g^2 + 4\Delta_0^2 |k - k_{\min}|^2)^{1/2} . \tag{26}$$

The gap E_g plays the role as the chemical potential for the spinon quasiparticles and above the critical temperature it equals the absolute value of the chemical potential for the original s particles, see Eq. (1). We can now find the gap analytically from Eq. (21) in the limit $T \to 0$,

$$E_g(T \to 0) = \bar{E}_g = -\frac{1}{\beta} \ln(1 - e^{-\beta E_C}) , \tag{27}$$

where the energy E_C is given by

$$E_C = \frac{\pi}{2}(t_B^2 + 2\Delta_0^2)^{1/2} \times \left[2 - \delta - \frac{1}{N}\sum_k \frac{\omega_k - \mu_{B,\max}}{[(\omega_k - \mu_{B,\max})^2 - |\Delta_k|^2]^{1/2}}\right] . \tag{28}$$

This quantity determines the cross over between a low-temperature regime where the gap is exponential in temperature and a regime where E_g behaves as $T \ln T$ (see Fig. 4). The temperature dependence of $\bar{E}_g$ is shown in

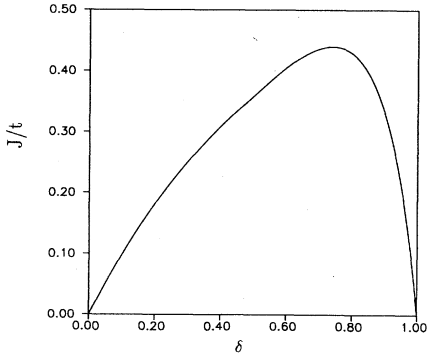

FIG. 2. The phase diagram in the $(J/t) - \delta$ plane: Δ_0 is nonvanishing in the area above the curve.

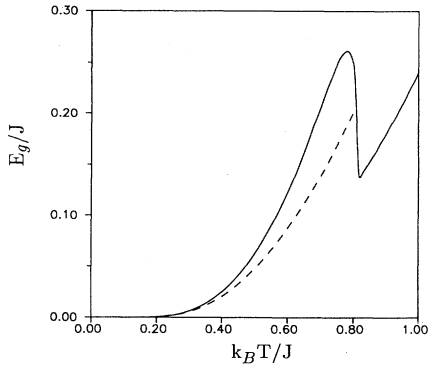

FIG. 4. The temperature dependence of the excitation gap in the spinon spectrum. The numerical result has been compared with the analytic low-temperature expression [Eq. (27)] (dashed line). $\delta = 0.05$ and $J/t = \frac{1}{10}$. E_C found from Eq. (26) is 0.12 J.

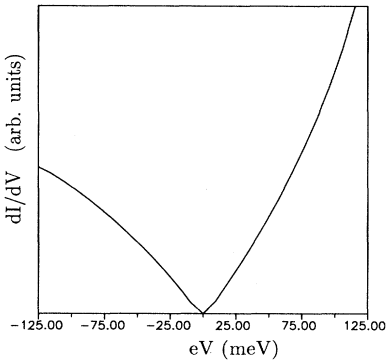

FIG. 5. The differential conductance for a tunnel junction between a normal metal and a RVB state.

Fig. 4 and compared to the full numerical solution. The zero temperature solutions for Δ_0 and t_B is used in the calculation of $\bar{E}_g$.

The separation of the charge and spin degrees of freedom in the RVB state and thereby the departure from a Fermi-liquid state necessarily has physical significance. The clearest example is the current-voltage ($I-V$) characteristic for a normal-metal to RVB state tunnel junction.[6,7] The consequences of the previously proposed representation of the RVB state, i.e., bosonic holons and fermionic spinons, is an asymmetric $I-V$ characteristic.[7] More precisely an Ohmic behavior for one particular polarity of the bias voltage and a current growing quadratic with voltage for the opposite polarity. The latter is due to the extra phase space available when a particle is tunneling from the normal-metal to the RVB metal and the energy of the incoming particle can be distributed between two particles. But this phase space is only present in one tunneling direction because at low temperatures the holons, being bosons, are practically monoenergetic. The reversed situation, i.e., the representation where the holons are fermions and the spinons are bosons, results in a more symmetric characteristic because for both tunneling directions a spinon quasiparticle is injected and in both electrodes the charge carriers are fermions. This may provide a way to distinguish experimentally between the two different realizations of the RVB state.

We now calculate the tunneling current for a tunnel junction using the representation for the RVB state considered above. The experiment directly probes the density of states and the energies involved are in the large voltage limit of the order J. It is in this limit that the mean-field treatment is expected to be best.

To calculate the tunneling current we use the standard tunneling Hamiltonian scheme. The result for zero temperature is

$$\frac{dI}{dV}=\frac{e^2 g_F g_N |T|^2}{\hbar N}\sum_k [v_k^2\theta(eV-E_k) + u_k^2\theta(-eV-E_k)], \quad (29)$$

assuming a constant holon density of states we have integrated out the holons. g_F and g_N is the density of states for holons and for the normal-metal electrons, respectively. $|T|$ is the tunneling matrix element and E_k is given by Eq. (17). The result of the numerical integration of Eq. (29) is shown in Fig. 5 and for both directions it exhibits an increasing conductance with increasing voltage. The conductance is symmetric for small voltages, but becomes asymmetric for larger voltages. It should be noticed that the rise in the conductance only persists up to voltages comparable with the spinon bandwidth ($\sim 4t_B$). In the calculation the parameters Δ_0 and t_B from the $T=0$ mean-field solution are used.

Recent experiments on single-crystal samples[8] or epitaxially grown thin films[9] all show characteristics with increasing differential conductance for increasing bias voltage while the asymmetric background seen in the early experiments seems to disappear with better samples.

In conclusion we have derived a mean-field theory for a RVB state with spinless charge carriers and chargeless spin carriers. We have shown that there exists a condensate of singlet pairs consisting of two bosons, for a wide range of parameters. The equations have been solved for the simplest choice of the symmetry of the order parameter.

During the completion of this work we became aware of a similar work by Yoshioka,[10] who solves the mean-field equations for the half-filled case, and find the same result [Eq. (25)]. The choice of symmetry of the condensate order parameter is also discussed by Yoshioka and in accordance with our findings the different mean-field solutions for the half-filled case are not equivalent, the choice used in the present work being the best. This issue and the local gauge transformation invariance for the half-filled case of the large-U Hubbard model in the bosonic representation will be studied in a forthcoming publication.

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