New representation of the Hubbard model

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A representation of the t–J Hamiltonian in terms of localized pseudospins and spinless fermions is found. This representation is used for a qualitative analysis of the quasiparticle spectrum, superconductivity, and nuclear relaxation at a low current-carrier density.

1. In the limit $U \gg t$ the Hubbard model is described by a reduced so-called t–J Hamiltonian[1]

$$H_{t-J} = \frac{1}{2} J \sum_{ij} (\vec{\sigma}_i \vec{\sigma}_j) - t \sum_{ij\sigma} (1 - n_{i-\sigma}) a_{i\sigma}^{+} a_{j\sigma} (1 - n_{j-\sigma}), \quad J = 4t^2/U, \tag{1}$$

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where $n_{i\sigma}=a_{i\sigma}^{+}a_{i\sigma}$, and the operator $\vec{\sigma}_i$ represents the electron spin density. The idea of separating the spin and charge degrees of freedom is usually implemented through a representation of the electron operators in terms of fermion-boson (or boson-fermion) pseudofields.[2] When this approach is taken, however, technical problems arise because of the need to maintain a local conservation of the number of pseudoparticles, in order to prevent nonphysical states at each site. We would like to have a representation of the type in (1), in which the operators describing the spin and charge degrees of freedom are not coupled by auxiliary equations. Extremely attractive from this standpoint at a low carrier density is the following new representation of Hamiltonian (1):

$$H=\frac{1}{2}J\sum_{ij}(\vec{S}_i\vec{S}_j)(1-n_i)(1-n_j)-2t\sum_{ij}(\vec{S}_i\vec{S}_j+\frac{1}{4})c_i^{+}c_j. \quad (2)$$

Here $n_i=c_i^{+}c_i$, where c_i^{+} is the spinless fermion operator which creates a hole (or a pair) with a charge of $+e$ $(-e)$, depending on the filling $N_e/N=1\mp\delta$, and $\vec{S}_i$ is a local pseudospin — 1/2. The fermions in (2) describe the physical motion of a charge, and the real spin at the singly occupied sites is expressed in terms of the pseudospin by means of $\vec{S}_i(1-n_i)$. (In the course of the motion of a fermion, a pseudospin "converts" into a real spin and vice versa.) It is a simple matter to verify that, regardless of the orientation of the pseudospins, the charge transport in (2) is carried out in a manner which conserves the projection of the real spin and with an amplitude t, as in the original model. That this is true can also be seen from the circumstance that (2) commutes with the total spin of the system, $\Sigma\vec{S}_i(1-n_i)$. With regard to the extra pseudospins at the few fermion-occupied sites, we note that they do not introduce an extra energy; they merely ensure the conservation of the real spin during the motion of the fermion.

Hamiltonian (2) makes it possible to calculate physical quantities by the standard methods, not complicated by coupling equations.

2. Let us examine the low-density limit $\delta<\delta^*$ (δ^* will be defined below). Starting from the Néel state $(T=0)$, and expressing $H(2)$ in terms of sublattice-symmetric magnons in the linear approximation, we find

$$H=\omega_{\vec{p}}^{0}b_{\vec{p}}^{+}b_{\vec{p}}+\varsigma_{\vec{k}}^{0}c_{\vec{k}}^{+}c_{\vec{k}}+H_{int},$$
$$\omega_{\vec{p}}^{0}=\frac{z}{2}\tilde{J}(1-\gamma_{\vec{p}}^{2})^{1/2},\ \ \tilde{J}=J(1-\delta)^2, \quad (3)$$
$$\varsigma_{\vec{k}}^{0}=z\tilde{t}(1-\gamma_{\vec{k}})-\mu,\ \ \tilde{t}=t<2\vec{S}_i\vec{S}_j+\frac{1}{2}>\sim -0,16t.$$

The interaction has the structure

$$H_{int}=\{\Gamma_n(\vec{k},\vec{p},\vec{q})b_{\vec{p}}^{+}b_{\vec{p}+\vec{q}}+\frac{1}{2}\Gamma_a(\vec{k},\vec{p},\vec{q})(b_{\vec{p}}^{+}b_{-\vec{p}-\vec{q}}^{+}+b_{-\vec{p}}b_{\vec{p}+\vec{q}})\}c_{\vec{k}+\vec{q}}^{+}c_{\vec{k}}. \quad (4)$$

The matrix elements have the behavior $\Gamma_n,\Gamma_a\Rightarrow 0$ as $\vec{p}\Rightarrow 0\xi,\vec{Q}$; where $\vec{Q}=(\pm\pi,\pm\pi)$. Here z is the number of nearest neighbors, the lattice is either quadratic or cubic, and the lattice constant is unity. The weak seed fermion dispersion in (3) is simply the result of the mean field. It is subsequently canceled by the eigenenergy part. As a result, we have $\epsilon_{\vec{k}} \simeq \epsilon_{\vec{k}+\vec{Q}}$. The coherent motion of a fermion results from quantum fluctuations of spins involving the simultaneous excitation of two magnons. In the lowest-order self-consistent approximation, the fermion eigenenergy is

$$\Sigma_\omega(\vec{k}) = \frac{1}{2}\sum_{\vec{p}\vec{q}} \Gamma_a^2(\vec{k}\vec{p}\vec{q}) \int dx \rho_x(\vec{k}+\vec{q}) \left\{ \frac{\theta(x)}{\omega - x - \omega_{pq} + i\gamma} + \frac{\theta(-x)}{\omega - x + \omega_{pq} + i\gamma} \right\}, \quad (5)$$

where $\omega_{pq} = \omega_{\vec{p}} + \omega_{\vec{p}+\vec{q}}$, and $\rho_x(\vec{k})$ is the spectral density of the fermion Green's function $G_x(\vec{k}) = (x - \zeta_k^0 - \Sigma_x(\vec{k}))^{-1}$. Near $p \sim 0, \vec{Q}$, the magnon energy is $w_p \simeq vp$, where the velocity renormalized by the charge fluctuations is $v \simeq v_0(1-\beta)^{1/2}$, and

$$\beta = (2z)^{3/2}(t^2/v) \sum_{kq} \int^{0} dx \int_{0} dy \rho_x(\vec{k}) \rho_y(\vec{k}+\vec{q})/(y - x + \omega_{\vec{q}}). \quad (6)$$

It can be seen from (5) that in the case $\omega \ll \omega_{\max} \simeq v(z/2)^{1/2}$ the damping Σ''_ω approaches zero (more rapidly than w^2), while at $w > w_{\max}$ it is large and depends only weakly on w. Consequently, for a qualitative analysis we can set

$$\rho_\omega(\vec{k}) = Z_0 \delta(\omega - \varsigma_k)\theta(\omega_{max} - \omega) + \rho_{inc}\theta(\omega - \omega_{max}), \quad (7)$$

where the incoherent part is $\rho_{\text{inc}} \sim 1/2\Gamma$, where $\Gamma = \Sigma''(\omega \gg \omega_{\max})$. From (5)–(7) we then find

$$v = v_0 \tau^{1/2}, \quad Z_0 = \left(1 - \frac{\partial \Sigma\omega}{\partial \omega}\right)_0^{-1} \simeq (J/t)\tau^{1/2}, \quad (8)$$

$$\varsigma_k = |\vec{k} - \vec{Q}/2|^2/2m - \mu, \quad m^{-1} \simeq Z_0 \frac{\partial^2 \Sigma_\omega(\vec{k})}{\partial k^2} \simeq J\tau^{1/2}, \quad \Gamma \simeq 2\sqrt{\pi}t,$$

$$\tau = 1 - \delta/\delta^*, \quad \delta^* = (J/4t)/[1 + \frac{1}{\sqrt{\pi}} \ln(2t/J)].$$

The presence of the Fermi surface near $\vec{Q}/2$, the value of the residue of the Green's function of the quasiparticles, Z_0, and the value of their mass m agree with the existing results in the case $\delta \Rightarrow 0$, found previously by other methods. A new result is the value of the critical carrier density δ^*, at which the Néel state becomes unstable ($\delta^* \simeq 0.04$ at $t/J = 3$). The effective interaction between quasiparticles turns out to be greatest (and attractive) at a large momentum transfer $\sim \vec{Q}$. Since we need the opposite situation (a stronger forward scattering, for a Cooper instability to occur when the carriers do not have a spin structure, there is no superconductivity at $\delta < \delta^*$.

3. In the case $\delta > \delta^*$ our analysis is based on the phenomenological assumption that the static correlation function at $R \gg 1$ in a rotationally invariant spin-liquid phase with a short-range antiferromagnetic order is

$$< \vec{S}_{\vec{i}} \vec{S}_{\vec{i}+\vec{R}} > \simeq (-1)^{\vec{R}} < \vec{S}_i \vec{S}_i > \exp(-p_0 R)/\pi R, \quad p_0 \simeq (\delta - \delta^*)^{1/2}. \quad (9)$$

The corresponding structure of the spin Green's function D can be found by writing for it (for example) equations of motion with a Heisenberg interaction and then carrying out a decoupling with the help of (9) in a second step. We then find

$$D_\omega(\vec{p}) = A\frac{1-\gamma_{\vec{p}}}{\omega^2 - \omega_{\vec{p}}^2}\ , \quad \omega_{\vec{p}} \simeq \begin{cases} vp, & p \sim 0; \\ v(p_0^2 + p'^2)^{1/2}, & \vec{p} \sim \vec{Q} - \vec{p}\ '. \end{cases} \tag{10}$$

Using the normalization condition $A \simeq 2J$, we find $\langle \vec{S}_i \vec{S}_{i+1} \rangle = -0.30$ at $p_0 \ll 1$. A propagator similar to (10), with a gap spectrum at $p = Q$, was postulated in Ref. 3. We can of course talk only in terms of a pseudogap, which is apparently most prominent in the superconducting phase, in which charge fluctuations are suppressed. It would nevertheless be interesting to carry out a qualitative analysis at $\delta > \delta^*$ on the basis of assumption (9).

Singling out the mean-field part of (2), we find

$$H_{int} = -\Gamma(\vec{k}, \vec{p}, \vec{q})(\vec{S}_{-\vec{p}} \vec{S}_{\vec{p}+\vec{q}}) c_{\vec{k}+\vec{q}} c_{\vec{k}},$$

$$\Gamma(\vec{k}, \vec{p}, \vec{q}) = zt\{\gamma_{\vec{p}-\vec{k}} + \gamma_{\vec{p}+\vec{q}+\vec{k}} + (J/2t)(1-\delta)(\gamma_{\vec{p}} + \gamma_{\vec{p}+\vec{q}})\}. \tag{11}$$

The basic component of the fermion energy is

$$\Sigma_\omega(k) = \frac{3}{4}\sum_{pq} \alpha_{\vec{p}} \alpha_{\vec{p}+\vec{q}} \Gamma^2(\vec{k}, \vec{p}, \vec{q}) \int dx \rho_x(\vec{k}+\vec{q}) \left(\frac{\theta(x)}{\omega - x - \omega_{pq} + i\gamma} + \frac{\theta(-x)}{\omega - x + \omega_{pq} + i\gamma}\right) \tag{12}$$

and in the interaction between carriers,

$$V(\omega, q) = -\frac{3}{2}\sum_{p} \alpha_{\vec{p}} \alpha_{\vec{p}+\vec{q}} \Gamma^2(\vec{k}\vec{p}\vec{q}) \omega_{pq}/(\omega_{pq}^2 - \omega^2) \tag{13}$$

it is determined by the region $\vec{p} \sim \vec{Q}$, $q \sim 0$, since we have $\alpha_p = 2\sqrt{2}(p_0^2 + p'^2)^{-1/2}$ at $\vec{p} \sim \vec{Q} - \vec{p}'$, and $\alpha_p = p/2\sqrt{2}$ at $p \sim 0$. This behavior reflects the anomalously large susceptibility $\chi_s(q) \simeq \{J[p_0^2 + z(1+\gamma_q)]\}^{-1}$ of a nearly antiferromagnetic liquid near $\vec{p} \sim \vec{Q}$: $\chi_s \vec{Q}) \sim 1/J\delta$. The matrix element $\Gamma(kpq)$ is at its maximum at $k \sim 0$; at values of J/t, which are not too small, we would expect the Fermi surface to lie near the center of the Brillouin zone. Using the approximation with $\omega_{max} \simeq 2\omega_g = 2vp_0$, analogous to (7), we find

$$Z_0 = (\pi\tilde{J}/4t)/|3\ln p_0|^{1/2}, \quad \varsigma_k = k^2/2m - \mu, \quad m^{-1} \simeq \tilde{J}/|\ln p_0|^{1/2}. \tag{14}$$

At $\delta > \delta^*$, the quasiparticle description is thus limited to the narrower region $\omega < \omega_g \sim J(\delta - \delta^*)^{1/2}$ and has an additional logarithmic "weight increase" of the fermion. The low-energy quasiparticle Hamiltonian is

$$H = \sum_k \varsigma_{\vec{k}} c^+_{\vec{k}} c_{\vec{k}} + \sum_{kk'} V(\vec{k}\vec{k}') c^+_{\vec{k}'} c^+_{-\vec{k}'} c_{-\vec{k}} c_{\vec{k}}. \tag{15}$$

Here the interaction in the Cooper channel, put in an antisymmetric form and renormalized to the quasiparticle weight, is

$$V(\vec{k}, \vec{k}') = -\frac{(\pi z J)^2}{2v|\ln p_0|}\{(1 - \frac{k^2 + k'^2}{4z})F_a - \frac{\vec{k}\vec{k}'}{2z}F_s\}, \tag{16}$$

where $F_{a,s}$ are the antisymmetric and symmetric parts of the function

$$F^{(d=2)} = (2\pi)^{-1}\{(\vec{k}' - \vec{k})^2 + (2p_0)^2\}^{-1/2} \; , \; F^{(3)} = (2\pi^2)^{-1} \ln \frac{24}{(\vec{k}' - \vec{k})^2 + (2p_0)^2}.$$

In the two-dimensional case, the quasi-Coulomb nature of the attraction results in a p-orbital pairing of fermions at

$$T_c^{(2)} \simeq (4\gamma/\pi)(\delta - \delta^*)^{1/2} v \exp(-1/\lambda),$$
$$\lambda \simeq (a - b\delta)/|\delta \ln(\delta - \delta^*)|^{1/2}, \quad a \simeq 0,30, \quad b \simeq 1,26. \tag{17}$$

With $J \sim 1200K$ and $\delta \sim 0.1$ we have $\lambda \simeq 1/3$, $T_c \simeq 40K$. There is no superconductivity at $\delta > 0.24$, since $\lambda(\delta)$ changes sign at $\delta \simeq 0.24$. Below T_c we have either (a) a gapless A phase with an order parameter $\Delta(k) = \Delta_0 \sin\theta_k$, $2\Delta_0/T_c = (2\Delta/T_c)_{\rm BCS}(2/\sqrt{e})$ $\sim 4{,}3$, or (b) a B phase with $\Delta(k) = \Delta_0 \exp(i\theta_k)$ and an isotropic gap $2\Delta_0/T_c$ $= (2\Delta/T_c)_{\rm BCS}$. A scattering by nonmagnetic impurities suppresses T_c in each of these phases.

4. The hyperfine interaction which determines the nuclear relaxation takes the form $A_{hf}(\vec{I}_i\vec{S}_i(1 - n_i))$ in representation (2). The imaginary part of the one-point spin susceptibility is $\sim (1 - \delta)^2\chi_s'' + (S(S+1)/3)\chi_e''$, where the second term has a Fermi-liquid behavior. The relaxation is dominated, however, by the pseudospin part $\chi_s''(\vec{p} \sim \vec{Q})$. To calculate this part, we introduce a damping $\gamma w(P)$ at the poles of function (10). It is natural to assume that this damping is due primarily to local charge fluctuations: $\gamma(Q) \simeq \Gamma^2(0,Q,0)T\chi_e''(\omega)/\omega$. At $T > T_c$ we then have $\gamma(Q) = \pi T/3$ and $T_1^{-1} \simeq (2A_{hf}^2/J)T^2/(\omega_g^2 + T^2)$. At $T < T_c$ in the A phase, for example, we have $T_1^{-1} = T_1^{-1}(T_c)f(T)$, where

$$f(T) \simeq (4/11)(T/T_c)^4, \quad T \ll T_c$$
$$f(T) \simeq 2(T/T_c)^2/(1 + \exp(\Delta/T)), \quad T \sim T_c. \tag{18}$$

This behavior is similar to that observed for copper nuclei in high-T_c superconductors.

5. The softening of magnons (8) in the region $\delta \sim \delta^*$ and the logarithmic infrared behavior at $\delta > \delta^*$ bear the features of a strong coupling of fermions with a boson field in the region $\delta \geqslant \delta^*$. Our analysis at $\delta > \delta^*$ by perturbation theory with a low-frequency cutoff may be regarded as a parametrization of the problem. There is the possibility that the qualitative results for $\delta > \delta^*$—in particular, on the current-carrier statistics and the superconductivity scenario—will survive in a more accurate theory.

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