Superconducting Instabilities in the Large-$U$ Limit of a Generalized Hubbard Model

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We study a generalized Hubbard model in the $U = \infty$ limit with use of the slave-boson technique. The $N = \infty$ theory describes a Fermi liquid with a strongly renormalized effective mass. The $1/N$ corrections give rise to different superconducting instabilities depending on the band structure and the filling factor. For low densities there is a $p$-wave instability while close to half filling in the cubic lattice we find a $d$-wave instability. We also calculate Fermi-liquid parameters.

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The study of superconductivity in strongly correlated systems has been the subject of current intense theoretical interest, and is motivated by the discovery of unconventional superconductivity in the rare-earth-based copper oxides and in heavy-fermion materials. There is a growing suspicion that Hamiltonians with purely repulsive interactions have superconducting ground states, and these ideas have received support from recent model calculations. The $d$-wave superconducting instabilities were suggested in the context of the Anderson lattice based on antiferromagnetic spin-fluctuation exchange. The large-$N$ expansion led to a similar conclusion but in this analysis the pairing mechanism was given by charge fluctuations. In the context of the Hubbard model, $d$-wave and extended $s$-wave superconducting instabilities were found in an RPA treatment of the small-$U$ limit of the Hubbard model. In this paper we address the infinite-$U$ limit of this model. We define a generalized Hubbard model describing $N$-fold-degenerate bands, which we treat systematically by a large-$N$ expansion. The mean-field theory of the model describes a strongly correlated Fermi liquid. Fluctuations around mean-field theory give rise to a residual interaction between the quasiparticles. We calculate the Fermi-liquid properties of the system. At low densities there is an attraction in the $p$-wave channel, while the interaction is repulsive in the $s$- and $d$-wave channels. Close to half filling, one $d$-wave channel becomes attractive and the other channels are repulsive.

The model under consideration is given by the Hamiltonian

$$H = -\frac{t_0}{N} \sum_{\langle ij \sigma \rangle} f_{i \sigma}^* b_{j \sigma} b_{j \sigma} + \varepsilon_0 \sum_{\langle i \sigma \rangle} f_{i \sigma}^* f_{i \sigma},$$

constrained to the subspace of states with quantum number $Q_i = q_0 N$, $Q_i = \sum_{\langle i \sigma \rangle} f_{i \sigma}^* f_{i \sigma} + b_{i \sigma}^* b_{i \sigma} = q_0 N.$

$\sigma$ is a degeneracy index running from 1 to $N$. The $N = 2$ case corresponds to particles with spin. $f_{i \sigma}$ is a fermion operator and $b_{i \sigma}$ is a slave boson which keeps track of empty sites. $\varepsilon_0$ is a site energy and $t_0 K_{ij}/N$ a hopping matrix element with $K_{ii} = 0$. In the following calculations we will assume a cubic lattice, with $K_{ij} = 1$ if site $j$ is a nearest neighbor of site $i$, and $K_{ii} = 0$ otherwise. A series of models are defined by the parameter $q_0$. If $q_0 = 1/N$, the $N = 2$ case is strictly equivalent to the $U = \infty$ one-band Hubbard model, while for arbitrary $N$, the model describes $N$-fold-degenerate correlated bands. As in the heavy-fermion problem, we will keep $q_0$ finite, therefore relaxing the single-occupancy constraint, to obtain a systematic loop expansion, and set $q_0 = 1/N$, $N = 2$ at the end of the calculations. Our result can be viewed as an exact systematic treatment of a slightly unrealistic model or as an approximate treatment of the infinite-$U$ Hubbard model which is consistent with all the conservation laws.

The mean-field theory of this model can be studied with use of a variety of techniques. To study (1) and (2) beyond mean-field theory, it is advantageous to use the functional integral formulation of the model. The partition function is given by

$$Z = \int [Df] [Df^*] [Db] [Db^*] [D\lambda] \exp \left( - \int d\tau S(\tau) \right),$$

with

$$S(\tau) = \sum_{i} \left[ b_{i \sigma}^\dagger \left( \frac{\partial}{\partial \tau} - i\lambda_i \right) b_{i \sigma} + i\lambda_i q_0 N + \sum_{\sigma} f_{i \sigma}^\dagger \left( \frac{\partial}{\partial \tau} + (\varepsilon_0 - i\lambda_i - \mu) \right) f_{i \sigma} - \frac{t_0}{N} \sum_{\langle i \sigma \rangle} f_{i \sigma}^\dagger b_{i \sigma}^\dagger f_{j \sigma},$$

where $\mu$ is a chemical potential which is adjusted to have $\delta$ particles per spin per site, while $\lambda_i$ is a Lagrange multiplier enforcing the constraint.

It is convenient to use the radial gauge where the phase of the boson field is absorbed in the Lagrange multiplier $\lambda$, and its radial parts define the field $r_i$. After integration over the Fermi field an effective action is obtained:

$$S(\tau) = \sum_{i} \left\{ r_i (\partial/\partial \tau - i\lambda_i) r_i + i\lambda_i q_0 N \right\} - N T \text{Tr} \ln \left( \partial/\partial \tau + (\varepsilon_0 - i\lambda_i - \mu) \right) \delta_{ij} - \left( t_0/N \right) r_i K_{ij} r_j.$$
In the large-$N$ limit the functional integral can be evaluated by the saddle-point method. Equation (5) has a static space-independent saddle point $r_\alpha = \sqrt{N} r_\alpha$, $\delta \lambda_i = \lambda_0$. The saddle-point equations $\delta S/\delta r_0 = 0$ and $\delta S/\delta \lambda_0 = 0$ define $r_0$ and $\lambda_0$, given by

$$q_0 = r_0 + i a/(2\pi)^4 \int d^d k f(E_k - \mu),$$

$$\lambda_0 r_0 = \left[ a/(2\pi)^4 \right] \int d^d k f(E_k - \mu) \epsilon_k,$$

where $a$ is a lattice constant. The kinetic energy is $\epsilon_k = -t_0 \delta K(k)$. $K(k)$ is the Fourier transform of $K_{ij}$, and $E_k = \epsilon_k + (\epsilon_0 - \lambda_0)$ is the energy of a renormalized band of quasiparticles. The chemical potential $\mu$ is fixed so as to leave $\delta$ particles per spin per site, $\delta = [N/V d^d k f(E_k - \mu)]$. This leaves the Fermi momentum $k_F$ unrenormalized as required by Luttinger's theorem. $r_0 = \delta q_0 - \delta$ gives a reduction of the bandwidth as the fermion concentration $\delta$ is increased. The instability point $\delta = q_0$ is reached when the number of particles per spin per site equals its maximum allowed value. $\lambda_0$ is the average bare kinetic energy.\(^7\)

The $1/N$ corrections to the $N = \infty$ results are obtained by our expanding around the mean-field solution. Setting $r_\alpha = r_0 (1 + \delta r_\alpha)\), $\delta \lambda_i = \lambda_0 + i \delta \lambda_i$, we find the partition function to order $1/N$:

$$Z = \exp \left[ -\beta S_0 \right] \frac{1}{\Omega_{\delta}} \int \left[ D \delta r \right] \left[ D \delta \lambda \right] \exp \left[ -\frac{1}{\Omega_{\delta}} \sum \delta S(\omega) \right]$$

where the sum is over the boson Matsubara frequency $\omega$ and

$$\frac{\delta S(\omega)}{\Omega_{\delta}} = \frac{NTV}{2} \int d^d q \delta R^* (q, \omega) \delta \lambda (q, \omega)$$

with $V$ the volume of the system and

$$L_{rr} = -\frac{a^d}{2(2\pi)^d} \int d^d k \left[ 2f(E_k - \mu)(\epsilon_k + q - \epsilon_k) + f(E_k + q - \mu) - f(E_k - \mu) \right] (\epsilon_k + q + \epsilon_k)^2/(\epsilon_k + q - \epsilon_k - i\omega),$$

$$L_{\lambda r} = L_{\lambda \lambda} = \frac{a^d}{2(2\pi)^d} \int d^d k \left[ f(E_k + q - \mu) - f(E_k - \mu) \right] (\epsilon_k + q + \epsilon_k)/(\epsilon_k + q - \epsilon_k - i\omega),$$

The propagator $L_{\lambda \lambda}$ is the polarization bubble calculated with the renormalized band energy $E_k$. $L_{\lambda r}$ contains the deviation from $q_0$ filling and a polarizability bubble weighted by the renormalized kinetic energy $\epsilon_k$, and $L_{r r}$ describes the average shift of the kinetic energy. The limiting values of the propagator for $\omega = 0$, $q \to 0$, are $L_{\lambda \lambda} = \rho/2$, $L_{\lambda r} = (q_0 - \delta) - \rho_{\text{eff}}$, and $L_{r r} = \rho\rho_{\text{eff}}$ with $\rho$ the density of states per spin at the Fermi surface. Notice that the fluctuation matrix of inverse propagators $L$ in Eq. (8) is not Hermitian, and, therefore, the stability of the mean field is not directly related to the positivity of its eigenvalues; hence the positivity of its trace and its determinant is not a suitable condition for its stability. Moreover, as pointed out by Ramakrishnan,\(^8\) $L_{r r} < 0$ and the functional integral of Eq. (8) is not well defined. In fact, in Eq. (8) and in the perturbation theory around the mean field, the functional integral of the $\lambda$ field has to be understood as an iterated integral. Integration over the $\lambda$ field first is equivalent to enforcing the constraint of Eq. (2). The coefficient of the remaining integral is $\det(L)/L_{\lambda \lambda}$ since $L_{\lambda \lambda} > 0$, the real stability condition is then the positivity of the determinant $L_{rr} L_{\lambda \lambda} - L_{\lambda r}^2$, which in the $q = 0$, $\omega = 0$ limit is easily seen to be equal to $\rho^2 \rho_{\text{eff}}^2$, the total derivative of the effective action with respect to $r$ at constant $q_0$, where the $\lambda$ field is adjusted to obey the constraint of Eq. (2). This positivity requirement is at all wave vectors $q$ and hence the stability of the mean-field theory is established.

The fluctuations around the mean-field theory, i.e., the first $1/N$ correction, give rise to a shift in the static values of the mean-field parameters $r_\alpha, \lambda_0$, and to additional renormalizations of the effective mass. The fluctuating Bose fields also induce an effective interaction between the quasiparticles. Restricting ourselves to the static limit $\omega = 0$, the quasiparticle scattering amplitude on the Fermi surface can be expressed as

$$\Gamma(k, -k | k', k') = v_{\text{eff}} (k' - k) \delta_{\sigma_1 \sigma_2} \delta_{\sigma_3 \sigma_4} - v_{\text{eff}} (k' + k) \delta_{\sigma_1 \sigma_4} \delta_{\sigma_2 \sigma_3},$$

where

$$v_{\text{eff}} = -4 \epsilon_{\text{eff}}^2 D_{rr} + D_{\lambda \lambda} + i 4 \epsilon_{\text{eff}}^2 D_{\lambda r}.$$

$\epsilon_{\text{eff}} = -t_0 (q_0 - \delta) K(k_F)$ is the renormalized kinetic energy of the quasiparticles on the Fermi surface and $D_{rr}(q) = \langle \delta R(-q) \delta R(q) \rangle$, $D_{\lambda r}(q) = \langle \delta R(-q) \delta \lambda(q) \rangle$, $D_{\lambda \lambda}(q) = \langle \delta \lambda(-q) \delta \lambda(q) \rangle$ are the boson propagators. It is easy to see that $v_{\text{eff}}$ is proportional to $\epsilon_{\text{eff}}$, as we approach the half filling, i.e., $\delta = q_0$.\(^{1785}\)
The density-density correlation function is calculated to leading order in $1/N$. We find

$$\Pi(q,\omega) = -4N^2\epsilon_F^2\delta R(q,\omega)\delta R(-q,-\omega),$$  \hspace{1cm} (12)$$

the sum of the polarization bubbles for quasiparticles in the renormalized band structure $E_k$. In the static limit $\omega=0$, $q\to0$, Eq. (12) gives the compressibility $dn/d\mu = 2N(q_0-\delta)/\epsilon_F(q_0-\delta-2\rho\epsilon_F)$. This reflects the fact that away from half filling in the large-$U$ Hubbard model, a small change of chemical potential will result in a small change of the density of carriers which are added to the lower Hubbard band. The enhancement in the quasiparticle density of states is canceled by a large $F_0$ of order $1/(q_0-\delta)$, leaving $dn/d\mu = m^*/(1+F_0)$ unrenormalized. The Gutzwiller approximation to the Hubbard model predicts a vanishing compressibility as $U/t_0$ approaches a critical value $(U/t_0)_c$ from below and $\delta$ tends to 0.5. When $U/t_0$ is greater than $(U/t_0)_c$, $\mu$ is a discontinuous function of density at $\delta=0.5$. Our results imply that when $U/t_0$ is much greater than $(U/t_0)_c$, $dn/d\mu$ goes to a finite value as $\delta$ approaches 0.5 from below, and therefore $dn/d\mu$ is an increasing function of $U/t_0$ above $(U/t_0)_c$.

It is possible to evaluate the expressions for the effective potential in the low-density limit $\delta \ll 1$, where the band structure is approximately spherical. We find for $2D$ with $q < 2\pi\delta(\omega=0)$

$$L_{\omega}(q) = 1/[8\pi t_0(q_0-\delta)],$$  \hspace{1cm} (13a)$$

$$iL_{\omega}(q) = (q_0-\delta) + [2-(qa/2)^2]/3/2\pi,$$  \hspace{1cm} (13b)$$

$$L_{\omega}(q) = (q_0-\delta)^2/16\pi^2/2 \delta [1-\delta/2]\nonumber$$

$$-4[2-2(qa/2)^2/3+(qa/2)^4/15].$$  \hspace{1cm} (13c)$$

As in the heavy-fermion problem, these expressions allow one to evaluate the Fermi-liquid parameters. Of special interest is $A^0$ which appears in the expression for the susceptibility $\chi \sim m^*(1-A^0)$. To leading order in $1/N$,

$$A^0 = -(1/4t_0)\int_{-1}^1 d\cos\theta v_{\text{eff}}(2k_F(1-\cos\theta)).$$

We find that for small $\delta$, $A^0 \approx -1.76 - 1.65\delta$, which is negative and increases as the filling factor $\delta$ increases. The fact that $A^0$ is negative indicates the ferromagnetic tendency for low densities.

The most striking effect of the residual interaction between the quasiparticles is the Cooper instability. The scattering amplitude in Eq. (10) is sensitive to the nature of the lattice structure and we investigate in detail the simple cubic structures in two dimensions. Since the interaction $v_{\text{eff}}$ is purely repulsive, we expect unconventional $p$-like or $d$-like instability, which takes advantage of the $q$ dependence of the effective interaction. The effective interaction $v_{\text{eff}}(q)$ is plotted along two symmetry directions for different values of filling factor in Figs. 1 and 2. The coupling constants are defined by

$$c_i = \int(s/|v_k|)\sum(s'/|v_{k'}|)\times[g_i^*(k)v_{\text{eff}}(k,k')g_i(k'),$$  \hspace{1cm} (14)$$

where the integral is on the Fermi surface and the functions $g_i$ are cubic harmonics with different symmetries:

$$g_1(k) = A_1 \sin(k_x),$$

$$g_2(k) = A_2 [\cos(k_x)-\cos(k_y)],$$

$$g_3(k) = A_3 \sin(k_y) \sin(k_z)$$

with the normalization factors $A_i$ defined as $A_i = \int(s/|v_k|)g_i^*(k)g_i(k)$. In the weak-coupling

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**FIG. 1.** $v_{\text{eff}}(q_x,q_y)/t_0(1-2\delta)$ for 2D square lattice along $q_x$ direction (dot-dashed line) and along $q_x=q_y$ direction (dotted line) for $\delta=0.15$.

**FIG. 2.** $v_{\text{eff}}(q_x,q_y)/t_0(1-2\delta)$ for 2D square lattice along $q_x$ direction (dot-dashed line) and along $q_x=q_y$ direction (dotted line) for $\delta=0.45$.**
theory the coupling constants are related to the transition temperature by the approximate relation 
\[ T_c = t_0 (g_0 - \delta) \exp(-N/c_1) \]. We evaluated the integral of Eq. (14) for different values of the filling factor \( \delta \) and we find that the \( c_2 \) channel is repulsive for all filling factors \( \delta \). The coupling constants \( c_3 \) and \( c_1 \) are shown in Fig. 3 as functions of \( \delta \). We can see that at low density the \( d \)-wave coupling constant \( c_3 \) is positive, which indicates the repulsive interaction, while the \( p \)-wave coupling constant \( c_1 \) is negative and therefore attractive. When the filling factor \( \delta \) approaches zero, \( c_1, c_2, \) and \( c_3 \) approach zero, because in this limit \( v_{\text{eff}} \) is a \( q \)-independent hard-core repulsive interaction. As the filling factor \( \delta \) increases, \( c_1 \) changes to repulsive and \( c_3 \) becomes attractive.

It is interesting to notice that the above results are qualitatively consistent with the results of the RPA calculation of Scalapino, Loh, and Hirsch\(^{11}\) for \( U/t_0 \geq 8 \), where they found two different superconducting instability patterns depending on whether \( U/t_0 \) is less or greater than 8. The agreement between our calculations and those of Ref. 11 suggests that our results are not only valid when \( U/t_0 \) is strictly infinity but also are qualitatively correct for \( U/t_0 \geq 8 \). The superexchange terms which are known to introduce \( d \)-wave superconductivity with \( d_{x^2-y^2} \) symmetry, and which are totally suppressed in our model, become important when \( U/t_0 < 8 \). To treat them in the slave-boson approach, it is necessary to introduce additional auxiliary fields. This problem is left for future investigations.

In conclusion, we studied a generalized infinite-\( U \) Hubbard model using a systematic large-\( N \) expansion technique. The model under study is extremely simple compared with the spin-\( \frac{1}{2} \), finite-\( U \) Hubbard model, since the spin exchange terms are totally suppressed and the Hamiltonian contains only the kinetic energy of a highly constrained Fermi system. Nevertheless, the large-\( N \) expansion of the model exhibits many interesting features: a large mass renormalization, an additional enhancement of the magnetic susceptibility, a \( p \)-wave-like superconducting instability for low concentration, and a \( d \)-wave superconducting instability close to the half filling. It can therefore serve as a qualitative guide to the understanding of the behavior of more realistic models. Our work shows, in the framework of a systematic expansion, how superconductivity can result from a purely repulsive hard-core interaction. A physical realization of such a model is liquid \(^3\)He, which is a \( p \)-wave superfluid. An obvious limitation of the large-\( N \) expansion is the absence of ferromagnetism close to the half filling. While this work suggests that the ground state of the spin-\( \frac{1}{2} \) Hubbard model for large \( U \) and low density is a \( p \)-wave superconductor, a very different approach is needed to confirm this conjecture.

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