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Superconductivity in the dilute electron gas

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We determine the effective interaction of quasiparticles on the Fermi surface for the electron gas in a rigid positive background. The quasiparticle scattering amplitude is calculated from the two coupled Bethe-Salpeter equations for the two-particle vertex functions in the particle-hole (p-h) channels for densities from $r_s=1$ to $r_s=37$. The density and spin-density mean fields are fitted to the compressibility and spin susceptibility of Green's-function Monte Carlo calculations and the local-field factors $G(q)$ of microscopic models. We find p-wave superconductivity for $10<r_s<35$ and s-wave superconductivity for $r_s>35$.

The recent discovery[1,2] of a new class of high-T_c superconductors has triggered intensive research for unconventional mechanisms of superconductivity. On a phenomenological level, two outstanding properties of high-T_c compounds are (i) the unusual lattice structure and ensuing electronic structure and (ii) the low density of carriers. While most investigations concentrate on the nature of electronic correlations for the quasi-two-dimensional CuO_2 lattice, it may be also worthwhile to focus on the changes in electronic correlation as a function of decreasing carrier density. The simplest model, which should contain some of the relevant physics, is the electron gas moving in a rigid positive background. Does the electron gas become unstable against formation of a pair-correlated state as the density is lowered?

In a Letter as early as 1965, Kohn and Luttinger[3] addressed this problem and concluded that there should always occur a superconducting transition, into a state of nonzero angular momentum pairing. Their conclusions were based on second-order perturbation theory, the qualitative feature being an attractive interaction piece for forward or backward scattering as a consequence of the discontinuities at the Fermi surface. In real space the attraction manifests itself in the negative parts of Friedel or Ruderman-Kittel-Kasuya-Yosida (RKKY) oscillations associated with the electric potential of a test charge or spin in the Fermi liquid.

In a series of papers, Sham, Rietschel, and Grabowski have investigated the possibility of Cooper pair formation by exchange of plasmons (for a review, see Ref. 4). Solving the Eliashberg equations with a dynamically screened Coulomb potential, these authors found sizable transition temperatures even in the metallic density range. However, these high T_c's were found to be suppressed to zero (at least in the density range $r_s \sim 2$–5 considered) upon inclusion of the lowest-order vertex corrections. A similar conclusion was drawn by Shirron and Ruvalds.[5] The total effect of vertex corrections as well as the behavior at low density ($r_x>5$) remained unclear.

In this Rapid Communication we approach the problem of calculating T_c from a different direction. We concentrate on the effective interactions of quasiparticles on the Fermi surface. The Cooper pair interaction is approximately given by the scattering amplitude A for two particles in states $(\mathbf{p},-\mathbf{p})$ going into states $(\mathbf{p}',-\mathbf{p}')$.[6] For quasiparticles on the Fermi surface A is a function of spin and two angular variables, chosen as q and $\mu=\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}'$, where $\mathbf{p}_1=\mathbf{k}+\mathbf{q}/2$, $\mathbf{p}_2=\mathbf{k}'-\mathbf{q}/2$ and $\mathbf{p}_3=\mathbf{k}-\mathbf{q}/2$, $\mathbf{p}_4=\mathbf{k}'+\mathbf{q}/2$ are the momenta of the incoming and outgoing particles, respectively. The pair coupling parameters for angular momentum states l are then obtained as

$$\lambda_l=\tfrac{1}{8}\int_{-1}^{1}dz\,P_l(z)A^J(Q,\mu=-1)\,, \tag{1}$$

where $z=Q^2/2-1$, the total spin is $J=0$ or 1 for even or odd l and $P_l(z)$ are the Legendre polynomials. For negative (attractive) λ_l there is a transition into a superconducting state below a critical temperature $T_c^l=\epsilon_0\times\exp(-1/|\lambda_l|)$ where ϵ_0 is a cutoff energy of order Fermi ϵ_F describing the width of the attractive interaction regime in energy.

As a guiding principle in calculating A we assume that single particle-hole excitations are responsible for most of the momentum dependence of A, whereas multi-particle-hole excitations yield a smooth dependence, which can be modeled by a few parameters only. These parameters in turn can be adjusted to reproduce virtually exact results on the ground-state energy and the structure factor known from Green's-function Monte Carlo (GFMC) calculations.[7] The effect of simple particle-hole excitations on A is described by the two coupled Bethe-Salpeter equations for the vertex functions in the two particle-hole channels:[8]

$$A^{\lambda}_{kk'}(q)=F^{\lambda}_{kk'}(q)+\sum_{k''}F^{\lambda}_{kk''}(q)\chi_{k''}(q)A^{\lambda}_{k''k'}(q),\quad \lambda=s,a\,, \tag{2}$$

$$A^{\lambda}_{kk'}(q)=F^{\lambda}_{kk'}(q)+(\bar{F})^{\lambda}_{kk'}(q)-I^{\lambda}_{kk'}(q)\,. \tag{3}$$

Here, A is the scattering amplitude, F is the generalized Landau interaction function, and I is the so-called direct interaction (s,a refers to the spin symmetric/antisymmetric components). The overbar on F in (3) indicates the exchanged quantity, i.e., the variables are corresponding to the interchange of the two in-going (or out-going) particles. Equation (2) may be solved in good approximation by separating the energy and angle integrations in the intermediate state as described in Ref. 8, and expanding in angular momentum components,

$$A_{kk'}(q)=\sum_{l=0}^{\infty}P_l(\hat{\mathbf{k}}\cdot\hat{\mathbf{k}}')A_l(q)\ ,$$

with the result

$$A_l^\lambda(q)=\frac{F_l^\lambda(q)}{1+\chi_0(q)F_l^\lambda(q)/(2l+1)}\ ,\quad \lambda=s,a\ , \tag{4}$$

where $\chi_0(q)$ is the unscreened p-h susceptibility for electrons with effective mass m^*, which we replace by the Lindhard function. In the limit $q\to 0$, the $F_l^{s,a}(q)$ reduce to the normal Landau parameters. It is useful to split off the direct Coulomb interaction $V_c=q_{TF}^2/q^2$, where $q_{TF}=(4\pi e^2N_F)^{1/2}$ is the screening wave number in the charge response channel (i.e., $l=0,s$) as $F_0^s(q)=V_c(q)+\tilde{F}_0^s(q)$ [note that $V_c(k_F)\propto r_s$]. The quantity $\tilde{F}_0^s(q)$ determines the local-field correction factor $G(q)$,[9] usually introduced in the mean field of charge response, as $\tilde{F}_0^s(q)=-V_c(q)G(q)$. It follows from (3) that $A_0^s\to 1$ for $q\to 0$, as a consequence of the long-range Coulomb force.[10] The density of states at the Fermi surface is given by $N_F=m^*k_F/\pi^2$. The effective mass m^* is determined self-consistently from the relation $m^*/m=1+F_1^s/3$.

The important input quantity in the system of Eqs. (2) and (3) is the direct interaction I. Since I does not contain any contributions from particle-hole excitation processes (which are known to generate complex momentum dependence of the scattering amplitude) one may hope that it is a smooth function of the momenta. We approximate $I^{s,a}_{\mathbf{k},\mathbf{k}'}(q)$, (i) by the effective potential form

$$I^{s,a}_{\mathbf{k},\mathbf{k}'}(q)=V^{s,a}(q)-\tfrac{1}{2}[V^s(\mathbf{k}-\mathbf{k}')+m^{s,a}V^a(\mathbf{k}-\mathbf{k}')]\ ,$$

with $m^s=3$ and $m^a=-1$, and (ii) by choosing $V^{s,a}(q)$ such as to reproduce the data for the compressibility and the spin susceptibility. In order to further pin down V^s and V^a we require that the resulting local-field corrections factor $G(q)$ is given by a monotonically increasing function of q leveling off at high q at values between $\frac{1}{2}$ and 1.[11] Such a behavior was obtained for the choices $V^s(q)=q_{TF}^2/(q^2+\tilde{q}^2)$ and $V^a(q)=V_1^a q^2$, with the parameters $\tilde{q}$ and V_1^a fitted to charge and spin susceptibility extracted from GFMC calculations. While the values for the charge susceptibility were taken from Ref. 12, in order to determine the spin susceptibility we used the interpolation formula

$$\chi_0/\chi=1-\alpha r_s/\pi+\tfrac{3}{2}\alpha^2r_s^2f''(0;y)(\epsilon_c^F-\epsilon_c^P)\ ,$$

similar to expressions proposed in Ref. 13, with the energy difference of the ferro- and paramagnetic states $(\epsilon_c^F-\epsilon_c^P)$ in Ry taken from Ref. 7, and the polarization function

$$f(z;y)=[(1+z)^{1+y/3}+(1-z)^{1+y/3}-2]/[2(2^{y/3}-1)]$$

appropriate for a correlation energy of density dependence $\epsilon_c\propto r_s^{-y}$. Here f'' is the second derivative of f with respect to the relative polarization z and exponent is determined from the tables given in Ref. 13 by $y(r_s)=-d\ln\epsilon_c^P/d\ln r_s$. χ_0 is the susceptibility of the noninteracting system and the constant $\alpha=(4/9\pi)^{1/3}$. Note that $\chi_0/\chi=(1+F_0^a)(m/m^*)$, such that F_0^a is not completely determined by χ_0/χ, but has to be calculated self-consistently with the effective mass ratio m^*/m.

The system of Eqs. (2) and (3) for given I is solved for A and F by expanding all quantities in terms of the polynomial eigenfunctions of the exchange operator on the Fermi surface $X_{lk}(\mu,Q)$, where $\mu=\mathbf{k}\cdot\mathbf{k}'$ and $Q=q/k_F$ (see Refs. 8 and 14 for details). Polynomials up to order 5 in μ and Q^2 were found to be sufficient to insure convergence. The system of nonlinear equations for the expansion coefficients was solved iteratively.

The results for the Landau parameters $\tilde{F}_0^s$ and F_0^a, the effective-mass ratio m^*/m, the components of the scattering amplitude A_1^a, A_2^s, and the pair coupling constants λ_0 and λ_1 for r_s values from 1 to $\sim$40 are shown in Table I. The input parameter $\tilde{F}_0^s$ is seen to grow large and negative, approximately as $\tilde{F}_0^s\approx -0.2r_s\ (m^*/m)$, whereas F_0^a is slowly approaching the ferromagnetic instability point where $F_0^a=-1$. In the region considered, both A_0^a and A_1^a increase approximately linearly with r_s to large negative values, whereas A_1^s increases to positive values as does the effective-mass ratio $m^*/m=1/(1-\frac{1}{3}A_1^s)$. For still larger values of r_s, A_1^s is expected to slowly approach the limit $A_1^s=3$, where $m^*\to\infty$. Whether or not this point coincides with the ferromagnetic transition or the transition to the Wigner lattice, found[7] to occur at $r_s\simeq 80$ and $r_s\simeq 120$, respectively, cannot be decided on the basis of our results. We observe, however, a tendency towards a charge-density wave instability at $q=2k_F$, where the denominator in Eq. (4) for $l=0$, $\lambda=s$ vanishes. On the other hand, the exchange interaction parameter $F_0^a(q)$ is found to decrease in magnitude with q for $r_s>5$, rendering a spin-density wave instability unlikely. In the limit of high density ($r_s>5$), $|F_0^a(q)|$ increases with q such that at $r_s=1$ $F_0^a(2k_F)\simeq -0.9$, and the system is close to a

TABLE I. Landau parameters $\tilde{F}_0^s$ and F_0^a, effective-mass ratio m^*/m, components of the scattering amplitude $A_l^{s,a}$, and pair-interaction constants λ_l for various densities.

r_s	$\tilde{F}_0^s$	F_0^a	m^*/m	A_1^a	A_2^s	λ_0	λ_1
2	−0.41	−0.30	0.91	−0.03	−0.06	0.51	0.05
5	−0.95	−0.43	1.02	−0.25	−0.04	0.59	0.03
10	−2.1	−0.48	1.08	−0.30	−0.02	0.68	0.01
15	−3.51	−0.53	1.17	−0.40	0.05	0.68	−0.01
20	−6.2	−0.61	1.53	−0.79	0.33	0.46	−0.04
30	−15	−0.71	2.44	−1.30	0.76	0.11	−0.06
35	−23	−0.72	3.05	−1.46	0.88	−0.03	−0.06
37	−26	−0.74	3.29	−1.52	0.94	−0.09	−0.06

SDW state. The values of the components $A_l^{s,a}$ for $l>2(s)$ and $l>1(a)$ have been found to be small.

As seen from Table I, the p-wave coupling constant λ_1 goes negative at $r_s \simeq 10$, but stays at a small negative value -0.06 as r_s is increased. This implies p-wave superconductivity below a critical temperature of order $T_c \simeq 10^{-5}$ K. The s-wave coupling constant, on the other hand, decreases rapidly from a large positive value at small r_s and becomes negative for $r_s \gtrsim 30$. At $r_s \simeq 37$, the largest r_s value at which we were able to calculate, we found $\lambda_0 \simeq -0.09$. The corresponding value of the transition temperature is hard to determine without further information on the cutoff energy ϵ_0 in the T_c formula. An upper bound of $T_c < 10^{-1}$ K is obtained by taking $\epsilon_0 \simeq \epsilon_F$.

This is still a rather low transition temperature, but in contrast with λ_1, the interaction parameter λ_0 decreases rapidly with increasing r_s, the slope at $r_s = 37$ being as large as $d\lambda_0/dr_s \cong -0.03$. If this trend were to continue up to $r_s \sim 50-60$, the coupling would be of order -1. The transition temperature would be increased by as much as a factor of e^{10} compared to the value at $r_s \simeq 37$, but the cutoff energy ϵ_0 would be smaller, partially offsetting the gain.

It is instructive to analyze the different contributions to λ_1 in the subspace of s- and p-wave components, when $\lambda_0 = \frac{1}{4}(A_0^s - 3A_0^a - A_1^s + 3A_1^a)$ and $\lambda_1 = -\frac{1}{6}(A_1^s + A_1^a)$. We find that (i) A_1^s and A_1^a nearly compensate each other, rendering λ_1 small [note that A_2^s is non-negligible and hence $A_1^s + A_1^a$ is not equal to $-(A_0^s + A_0^a)$], and (ii) the spin-density fluctuation contribution $-3A_0^a$ to λ_0 is nearly compensated by the spin-current-density fluctuation contribution $+3A_1^a$, leaving as the major attractive term $-A_1^s$. Note that the parity of a fluctuation vertex—odd parity for current-density fluctuations versus even parity for density fluctuations—determines the sign of the respective pair interaction contributions $\langle \mathbf{k}, -\mathbf{k} | V | \mathbf{k}', -\mathbf{k}' \rangle$, since the total particle-hole momentum of the fluctuation changes from $\mathbf{k}+\mathbf{k}'$ to $-(\mathbf{k}+\mathbf{k}')$ in the exchange process.

As one approaches the ferromagnetic transition more closely, i.e., for values of F_0^a lower than about -0.74, the assumption of a smooth momentum dependence of the direct interaction breaks down. Preliminary investigation indicates that the singular behavior of I necessary to drive a ferromagnetic transition is generated in the particle-particle channel and that multi-particle-hole excitations start to generate pronounced momentum dependence.

In conclusion, we have shown that the low-density electron gas is unstable against Cooper pairing. The attractive interaction necessary to bind the pairs is provided for the main part by exchange of transverse current fluctuations and to a lesser extent by exchange of spin-density fluctuations, leading to s-wave and p-wave pairing, respectively.

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