Enhanced Superconductivity in Quasi Two-Dimensional Systems

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We show that the tendency for superconductivity of a weakly coupled 2D electron system can be significantly enhanced if the Fermi energy is close to a logarithmic Van Hove singularity in the density of states. Using results from perturbation theory, supported by quantum Monte Carlo simulations, we calculate T_c and explore the effects of the quasiparticle lifetime and higher-order interactions on this enhancement. This mechanism suggests possible new directions in the search for 2D excitonic superconductivity.

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The density of states of noninteracting electrons in a two-dimensional periodic potential always exhibits Van Hove[1] logarithmic singularities arising from saddle points in the energy-versus-k relation. One may expect an enhancement of the instabilities of the system if the Fermi energy is close to such a singularity. Rice and Scott[2] have explored the consequences of this for the charge-density-wave instability for momentum transfer connecting two saddle points at the Fermi energy. Here we explore the effect of the singularity on the superconducting instability in the presence of a weak attractive interaction between electrons. We find that the transition temperature for weak coupling can be significantly enhanced if the Fermi energy is close to a logarithmic singularity in the density of states, and we discuss the implications this has for the search for higher-temperature superconductors.

Our motivation to study superconductivity in systems of restricted dimensionality stems from the work of Little[3] and Ginzburg[4] on excitonic superconductivity. An excitonic mechanism provides a significantly larger scale for T_c than the Debye temperature. In addition, a high-frequency "instantaneous" attractive interaction is less likely to lead to charge-density-wave formation, which is favored by retardation.[5] As noted by these authors,[3,4] a one- or two-dimensional geometry offers the possibility of separately tailoring the effective interaction and the pairing electron band. The idea is that a class of materials can be developed in which the properties of the electrons which pair and those which give rise to the pairing interaction can, to a large degree, be separately manipulated. In addition, it may be that still other electrons and the ion-ion interaction stabilize the total structure providing a framework on which the pairing electrons can develop their special correlations.

The main problem associated with the separation of function between the electrons that pair and those that provide the pairing is that the coupling λ between the conducting electrons and the excitonic medium is weak, so that even with the larger energy scale, the exponential factor $\exp(-1/\lambda)$ leads to a small T_c. However, if the Fermi energy of the 2D electron band is located at a logarithmic Van Hove singularity, we find that a random-phase-approximation (RPA) summation of the ladder graphs shown in Fig. 1(a) yields an expression for T_c in which λ is replaced by $\sqrt{\lambda}$. For a weakly coupled system this can produce a significant relative enhancement of T_c.

With these considerations in mind, we have studied an attractive Hubbard model[6] on a two-dimensional square lattice:

$$H = -\sum_{ij} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}. \tag{1}$$

Here $t_{ij} = t$ for (i,j) near neighbors, $t_{ij} = t_2$ for (i,j) next-nearest neighbors, and $U < 0$. The band energy is

$$\epsilon(k) = -2t(\cos k_x + \cos k_y) - 4t_2 \cos k_x \cos k_y. \tag{2}$$

For $t > t_2/2$ the saddle points are at $(k_x, k_y) = (\pm\pi, 0)$ and $(0, \pm\pi)$ and give rise to a logarithmic singularity in the density of states,

$$N(\epsilon) \sim t^{-1} \ln(t/|\epsilon - 4t_2|), \tag{3}$$

at $\epsilon = 4t_2$. Figure 2 shows $N(\epsilon)$ for $t_2 = -0.4$ and the

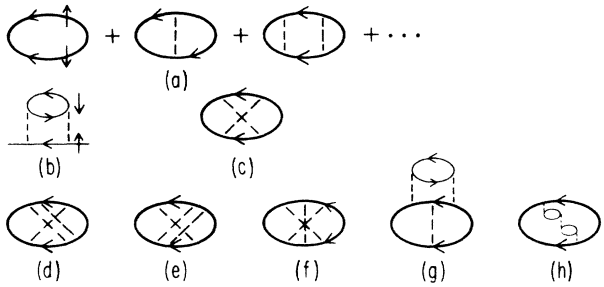

FIG. 1. Perturbation-theory diagrams associated with the pair susceptibility.

corresponding Fermi surface for $\epsilon = 4t_2$. For $t_2 = 0$, the singularity occurs for the half-filled band, $\rho = 1.0$. However, there is also a complete nesting of the Fermi surface for momentum transfers $(\pi, -\pi)$ which leads to a $\log^2$ divergence for the charge- and spin-density susceptibilities.[7,8] In this case, for an attractive interaction the charge-density-wave instability will dominate as a result of umklapp and any retardation of the interaction. Thus, here we will consider the non-half-filled case (e.g., $\rho \sim 0.5$) and study the enhancement of T_c when the filling and t_2 are such that the Fermi energy is at the Van Hove singularity, but there is no nesting of the Fermi surface.[9]

From summation of the ladder graphs of Fig. 1(a), the singlet pairing RPA susceptibility is

$$P_{\mathrm{RPA}}(q) = P_0(q)/[1 + UP_0(q)], \tag{4}$$

with

$$P_0(q) = \frac{1}{N}\sum \frac{1 - f(\epsilon_{p+q}) - f(\epsilon_p)}{\epsilon_{p+q} + \epsilon_p}. \tag{5}$$

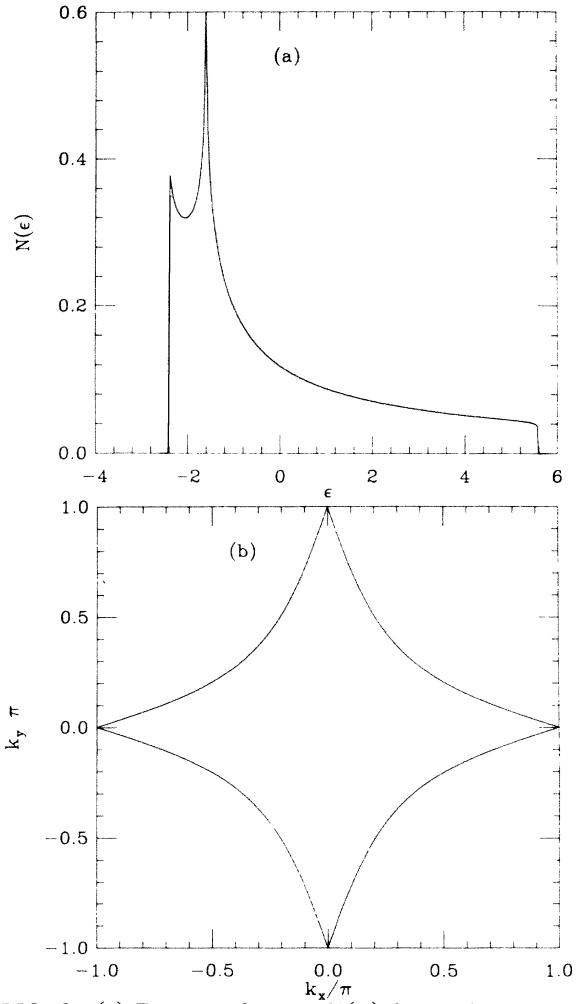

FIG. 2. (a) Density of states $N(\epsilon)$ for $t = 1$ and $t_2 = 0.4$. The singularity occurs for $\epsilon = 4t_2 = -1.6$. (b) Fermi surface for $\epsilon_F = -1.6$. The band filling for this case is $\rho = 0.58$.

When the Fermi energy is at the Van Hove singularity ($\rho = 0.58$), we have

$$P_0 = A \ln^2(t/T) + B \ln(t/T) + C, \tag{6}$$

with $A = \{4\pi^2 t[1 - (2t_2/t)^2]\}^{1/2}$. The transition temperature T_c^{RPA} obtained from the divergence of $P_{\mathrm{RPA}}(0)$ is shown as the upper dashed curve in Fig. 3. The lower dashed curve corresponds to a filling $\rho = 0.5$ for $t_2 = 0$. In this case the Van Hove singularity at $\epsilon = 0$ is well removed from the Fermi energy. To appreciate that Fig. 3 corresponds to weak coupling, we introduce an average band density of states $(8t)^{-1}$. Then $|U|/t < 1.6$ implies that $\lambda = |U|/8t < 0.2$. In this regime, the enhancement of T_c^{RPA} by the Van Hove singularity is evident, and at the upper end we will find (upper solid line) that T_c/t can be as large as 0.1.

Now, clearly a logarithmic singularity can be weakened by a variety of effects. For example, if $T_c = 0.1t$, any 3D coupling between layers must be less than $kT_c \sim 0.1t$ and the lattice perfection must be such that the impurity mean free path $l > \hbar v_F/kT_c \sim t/T_c \sim 10$ lattice units. Furthermore, if $N(0)$ is singular, then one must examine other higher-order contributions since $N(0)|U|$ is not really a "small parameter." However, we find that $\lambda = |U|/8t$ is still a useful parameter, and that while the leading self-energy and interaction corrections [Figs. 1(b) and 1(c)] diverge as $\lambda^2 \ln(t/T)$, these terms are of order $\lambda^{3/2}$ when the ladder graphs diverge at $\lambda \ln^2(t/T_c) = 1$. Thus, for weak coupling we expect that perturbation theory should be reliable.

Formally, it is useful to express the pair susceptibility in terms of dressed single-particle propagators and a two-particle irreducible interaction. Including the self-energy, Fig. 1(b), in the electron propagators alters P_0 in Eq. (4), introducing lifetime effects which dynami-

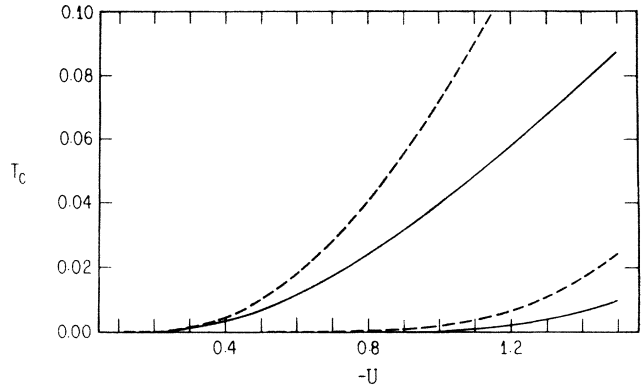

FIG. 3. T_c vs U in units where $t = 1$. The upper dashed curve is the RPA result when $t_2 = -0.4$ and $\rho = 0.58$, and the lower dashed curve is for $t_2 = 0.0$ and $\rho = 0.5$. The solid curves show the effect of the higher-order corrections (Fig. 1).

cally smear the logarithmic singularity and reduce the predicted T_c.[10] The leading correction to the interaction, Fig. 1(c), represents the beginning of a "paramagnon" contribution which is repulsive and also reduces T_c. Higher-order U^3 contributions to the irreducible interaction are shown in Figs. 1(d)–1(h). Carrying out both momentum sums and some of the Matsubara frequency sums numerically we have evaluated the pair propagator[11] P, taking into account the contributions to the self-energy and the irreducible interaction shown in Fig. 1.

To test the perturbation-theory results, we have compared them with Monte Carlo simulations. The Monte Carlo method we use has been discussed in detail in Refs. 7, 8, and 12. Figure 4 shows results for $P(q=0,T)$ obtained on 4×4 and 6×6 lattices with $U=-2$ for both $t_2=0$, $\rho=0.5$ and $t_2=-0.4$, $\rho=0.58$. The dashed line is P_{RPA}, the solid line in each figure is the result of perturbation theory, and the points are data from the Monte Carlo simulations. Note the large increase in pairing correlations when $t_2\neq0$, and the close agreement of the perturbative results with the Monte Carlo results over the whole temperature range studied. Figure 5 shows P vs U for a 4×4 lattice with $\beta=3$. For the weak-coupling regime $|U|\lesssim2$, the perturbation-theory calculation shown as the solid curves is in excellent agreement with the simulations. In fact, for $t_2=0.0$ and $\rho=0.5$, where the electron density of states $N(\epsilon)$ is slowly varying (and finite) near the Fermi energy, perturbation theory agrees well with the simulations for $|U|\lesssim3$. Note also that while the RPA expression, shown as the dashed line in Fig. 5, overestimates P, perturbation theory underestimates it.

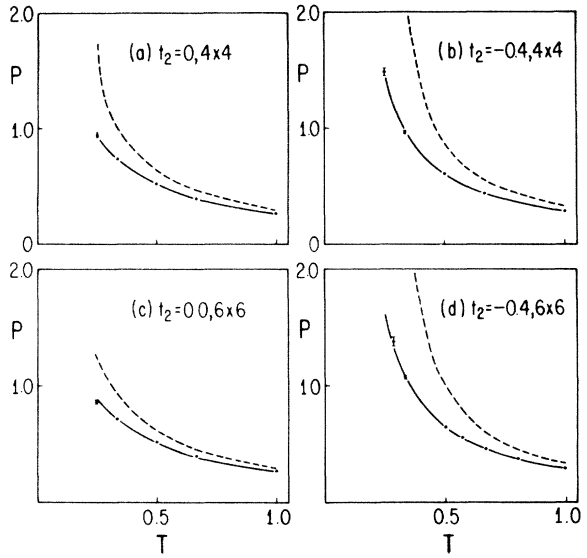

FIG. 4. Singlet pair susceptibility P vs temperature T on 4×4 and 6×6 lattices with $U=-2.0$. (a) $t_2=0$, $\rho=0.5$; (b) $t_2=-0.4$, $\rho=0.58$. The dashed line is the RPA prediction, Eq. (4), and the full line the perturbation-theory calculation including the corrections shown in Fig. 1. The points are obtained from Monte Carlo simulations.

In order to go to low temperatures, large lattices ($L\sim v_F/kT$) are required which cannot be simulated by use of present Monte Carlo algorithms. However, encouraged by the close agreement of the perturbation theory results with the Monte Carlo runs on small lattices and the fact that the corrections should be of order $\lambda^3/2$, we have used it to determine the temperature at which P^{-1} vanishes. The resulting values for T_c vs U are plotted as the upper and lower solid lines in Fig. 3 for $t_2=-0.4$, $\rho=0.58$, and $t_2=0.0$, $\rho=0.5$, respectively. For a strictly 2D system, the superconducting transition is altered by the formation of vortex-antivortex pairs.[13] However, because of the large intrinsic pair size, the characteristic temperature at which the system exhibits superconducting properties is set by the temperature at which P^{-1} vanishes. Note in Fig. 3 that the solid lines show the suppression of T_c from the RPA results. Nevertheless, in the weak-coupling regime the occurrence of a Van Hove singularity at the Fermi energy clearly enhances T_c over its value when the singularity is displaced.

Thus, our analysis suggests that two-dimensional metallic structures with logarithmic Van Hove singularities near the Fermi energy represent interesting materials to explore in the search for excitonic mediated superconductivity. Signatures of the fact that the Fermi energy is close to such a singularity can be seen in the temperature dependence of various thermodynamic properties. In particular, the specific-heat coefficient γ should have a logarithmic temperature dependence,

$$\gamma\sim\tfrac{1}{3}[1-(2t_2/t)^2]^{-1/2}\ln(t/T)+\text{const},$$

and there is a similar logarithmic dependence in the

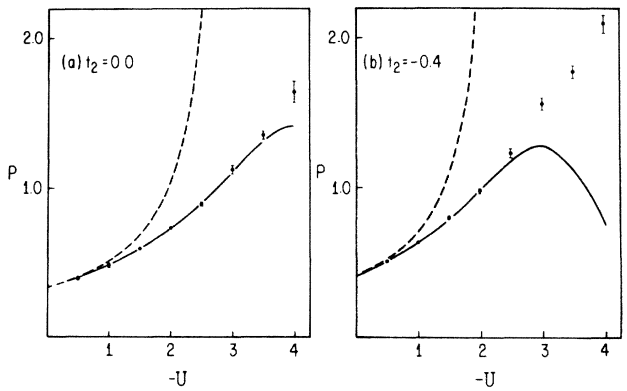

FIG. 5. P vs U on a 4×4 lattice with $T^{-1}=3$. (a) $t_2=0$, $\rho=0.5$; (b) $t_2=-0.4$, $\rho=0.58$. The dashed line shows P_{RPA} and the solid line shows the perturbation-theory result for P. The points are results from Monte Carlo simulations.

susceptibility.[2]

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