

Superconducting instabilities of the non-half-filled Hubbard model in two dimensions

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(Received 29 November 1995; revised manuscript received 20 May 1996)

The problem of weakly correlated electrons on a square lattice is formulated in terms of a one-loop renormalization group. Starting from the action for the *entire* Brillouin zone we reduce successively the cutoff Λ about the Fermi surface and follow the renormalization of the coupling U as a function of three energy-momenta. We calculate the intrinsic temperature scale T_{co} where the renormalization-group flow crosses over from the regime ($\Lambda > T_{co}$) where the electron-electron ($e-e$) and electron-hole ($e-h$) terms are equally important to the regime ($\Lambda < T_{co}$) where only the $e-e$ term plays a role. In the low-energy regime only the pairing interaction V is marginally relevant, containing contributions from all renormalization-group steps of the regime $\Lambda > T_{co}$. We identify the most attractive eigenvalue λ_{\min} of $V_{\Lambda=T_{co}}$. At low filling, λ_{\min} corresponds to the B_2 representation (d_{xy} symmetry), while near half filling the strongest attraction occurs in the B_1 representation ($d_{x^2-y^2}$ symmetry). In the direction of the van Hove singularities, the order parameter shows peaks with increasing strength as one approaches half filling. We also give a possible interpretation of angle-resolved photoemission spectroscopy experiments trying to determine the symmetry of the order parameter in the high- T_c compound $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$. [S0163-1829(96)06537-X]

I. INTRODUCTION

The problem of the interplay between a correlation-induced metal-insulator transition, antiferromagnetism, and superconductivity remains an important challenge, in particular in view of an understanding of the high- T_c cuprates. Since Anderson's original discussion of the importance of the two-dimensional Hubbard model in the vicinity of half filling,¹ enormous theoretical effort has been devoted to this problem, in particular concerning the case of strong repulsion. Nevertheless, many issues still remain controversial, largely because of the absence of general and reliable theoretical methods for handling the strong correlation problem. One might hope that the weakly correlated case provides at least some insight because the weak-coupling limit shares some general features with the strongly correlated case: in both cases the half-filled band Hubbard model is an antiferromagnetic insulator, and upon (sufficient) doping one recovers a conducting state. As the weak-coupling case at least in principle is tractable by perturbative techniques, it is clearly of interest to understand this limit further.

In the present analysis we search to know whether the Hubbard model with repulsive on-site interaction can lead to superconductivity, and if it does, to what form of the gap function. In particular, we are interested in the dependence of the results on the density of electrons. It is hoped that the results can help us to clarify the origins of the existence of a highly anisotropic BCS gap function in the cuprates where considerable experimental evidence in favor of d -wave or at least highly anisotropic superconductivity exists.

The d symmetry of the gap function is generally considered to be a sign of a pairing interaction of electronic origin, implying the absence of the standard phononic mechanism for superconductivity. The idea of a superconducting state induced by fluctuations of purely electronic origin in systems of electrons with Coulomb repulsion is originally due to Kohn and Luttinger² for the case of the three-dimensional

electron gas. Similar effects exist in a two-dimensional electron gas, and generally they depend strongly on the form of the Fermi surface. Perturbative calculations of the four-point vertex for a weakly filled band in the Hubbard model show that the model is unstable against d_{xy} superconductivity.³ Quantum Monte Carlo calculations on the same model, in the vicinity of metal-insulator transition, show that the attractive pairing interaction of $d_{x^2-y^2}$ symmetry is dominant,⁴ in agreement with the earlier arguments that antiferromagnetic fluctuations are the mediator of pairing interactions.⁵⁻¹² Direct evidence for $d_{x^2-y^2}$ superconducting ordering has however not yet been found in quantum Monte Carlo studies.

On the experimental side a large number of experiments have been performed to determine the shape of the gap function of the high- T_c superconductors.¹³ Josephson-junction experiments,^{14,15} measurements of the London penetration depth,^{16,17} and of the Cu NMR relaxation rate¹⁸ are consistent with a $d_{x^2-y^2}$ -gap. Particularly interesting are the angle-resolved photoemission spectroscopy (ARPES) data which provide rather precise information about the detailed angular dependence of the amplitude of the gap function. The experiments on the $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ compound show that the order parameter is maximal along the $(0, \pi)$ direction^{19,20} and that its amplitude in the (π, π) direction seems to attain a nonzero value at a new critical temperature below T_c .²¹

In a theoretical treatment of superconductivity in the vicinity of a correlation-driven metal-insulator transition one has to take into account that antiferromagnetic fluctuations become stronger and stronger as one approaches half filling. For weakly interacting electrons, these fluctuations are associated with a $\ln^2 T$ divergence of the electron-hole ($e-h$) loop diagram, caused by nesting of the Fermi surface and van Hove singularities of the two-dimensional problem at hand. On the other hand the pairing fluctuations, characterized by the electron-electron ($e-e$) loop, normally only linear in logarithms, cross over to a $\ln^2 T$ form in the vicinity of half filling. The perturbative treatment of an interacting system of

electrons should thus be based on the summation of all iterations of these two types of loops. The renormalization group seems to be the best way to do this. Applied to interactions between electrons placed at the van Hove points it gives an antiferromagnetic instability at half filling and superconductivity of $d_{x^2-y^2}$ symmetry if the deviation of the chemical potential μ from its value at half filling becomes of the order of critical temperature of the antiferromagnetic state.⁸ The equivalent parquet approach has been used for half filling and also finds the antiferromagnetic state.^{22,23} A direct calculation of the zero-temperature free energy²⁴ up to the second order in the bare interaction U_0 confirms that at half filling the antiferromagnetic order is stable, but finds no finite superconducting order parameter at any filling.

The renormalization-group technique for fermionic systems in two and three dimensions has recently been developed, but with some limitations. The Wilsonian mode-elimination technique was applied by Shankar²⁵ mainly to systems with an either isotropic or open, perfectly nested Fermi surface. Weinberg²⁶ has written the flow equations for a general case of an anisotropic Fermi surface, but taking into account only the electron-electron channel of the flow. Moreover, a common tendency is to do the renormalization-group procedure only for a thin ring of degrees of freedom around the Fermi surface and to linearize the spectrum in the radial direction. The starting model for such kind of approach is then called the low-energy effective action. This makes it difficult or impossible to make statements about the phase diagram of lattice models like those relevant for the description of the cuprates, due to the absence of a proper description of high-energy degrees of freedom, the elimination of which may considerably affect the low-energy effective action, in particular the interaction parameters appearing in it.

In the present paper we formulate the renormalization group starting from the Hubbard model, with the whole Brillouin zone involved in renormalization. Reducing the high-energy cutoff Λ about the Fermi surface, we follow the renormalization of two-particle interaction as a function of the energy-momenta of interacting particles. We show that for a finite μ (i.e., away from half filling) there exists a finite crossover temperature (or energy) T_{co} such that for $\Lambda > T_{co}$ both electron-electron and electron-hole contributions to the renormalization are important, while for $\Lambda < T_{co}$ only electron-electron part remains. Since T_{co} is small compared to the Fermi energy, the shell $\pm T_{co}$ around the Fermi surface can be described by a low-energy effective action $S\{T_{co}\}$ whose interaction is the result of all degrees of freedom with $\Lambda > T_{co}$. The temperature T_{co} is always inferior to $|\mu|$, which means that the available phase space is a closed smooth ring, where we can apply the tree-level (zero-order) scaling transformation and power counting argument²⁵ to the dispersion relation and coupling function appearing in $S\{T_{co}\}$. The remaining model contains then a one-particle dispersion linearized in the radial direction around the Fermi surface and a pairing interaction $V(\theta_1, \theta_2)$, where θ_1 and θ_2 are the polar angles of incoming and outgoing zero-energy Cooper pairs. The renormalization equation for $V(\theta_1, \theta_2)$ then can be easily solved in terms of the initial conditions $V_{\Lambda=T_{co}}$.

For a given Hubbard interaction U_0 , two different regimes

exist with respect to the filling. Far from half filling, the pairing interaction $V_{\Lambda=T_{co}}$ is approximately given by the constant U_0 plus a small momentum-dependent correction of the order U_0^2 , which however is important because it gives rise to anisotropic superconductivity with a very low T_c [$T_c \sim 8t \exp(-1/U_0^2)$]. If the filling gets very close to one half, T_{co} becomes very low ($\approx |\mu|$), and the renormalization-group flow very strong even for $\Lambda > T_{co}$, which means that it cannot be treated perturbatively as it was in the first case. In this paper we give the results only for the first regime. The analysis of the second case, where the renormalization group is necessary even for $\Lambda > T_{co}$ will be published subsequently.

We must add that our renormalization group, since truncated at one loop, can provide unique information on whether the Fermi liquid is a fixed point or not. If the interaction flows to strong coupling, we can say in which direction it flows, for example in the d -type superconducting direction, but we cannot say whether another fixed point with a finite superconducting order parameter with d symmetry exists or not. This kind of problem is well known, e.g., from the renormalization group in quasi-one-dimensional compounds, where the most divergent flow in some direction is always associated with the corresponding long-range order (LRO) because already infinitesimal interchain coupling suffices for its stabilization.²⁷ Similarly, the dimensionality reason for the nonexistence of LRO in two dimensions at finite temperature can be ignored as soon as small hopping in the third direction exists. This, however, does not mean that LRO and Fermi-liquid fixed points are the only possibilities, on this question the one-loop renormalization group simply cannot give an answer.

The problem is formulated in Sec. II in terms of the functional integral for fermions. Neglecting the self-energy renormalization we derive the one-loop renormalization-group flow equation for the coupling function, starting with the full bandwidth and the exact nearest-neighbor tight-binding one-electron spectrum. In Sec. III we (a) calculate the crossover energy T_{co} to the purely electron-electron ($e-e$) part of the flow, (b) apply zero-order scaling analysis to the dispersion relation and the interaction, (c) derive the renormalization-group equation for the pairing function V , and give the formal solution in the case of the actual D_4 crystal symmetry. In Sec. IV we diagonalize the pairing interaction $V_{T_{co}}$, limiting ourselves to the case when all energies $\Lambda > T_{co}$ can be treated perturbatively. We determine the most attractive eigenfunction and the resulting critical temperature as functions of the chemical potential μ . In Sec. V we give a possible interpretation of the gap viewed by ARPES experiments. The conclusions are given in Sec VI.

II. MODEL AND FORMULATION OF THE RENORMALIZATION GROUP THEORY

The Hubbard model for a two-dimensional system of electrons on a square lattice is described by the Hamiltonian

$$H = -t \sum_{\langle i,j \rangle, \sigma} (a_{i,\sigma}^\dagger a_{j,\sigma} + a_{j,\sigma}^\dagger a_{i,\sigma}) + \frac{U_0}{2} \sum_i n_i n_i - \mu \sum_i n_i \quad (2.1)$$

where $a_{i,\sigma}(a_{i,\sigma}^\dagger)$ is an electron destruction (creation) operator at site i with spin projection σ , t is the intersite transfer integral, μ is the chemical potential, and U_0 is the onsite Coulomb repulsion. In momentum space the Hamiltonian is

$$H = \sum_{\sigma\mathbf{k}} \xi_{\mathbf{k}}^0 a_{\sigma\mathbf{k}}^\dagger a_{\sigma\mathbf{k}} + \frac{1}{2} U_0 \sum_{\sigma} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3} a_{-\sigma, \mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3}^\dagger a_{-\sigma, \mathbf{k}_2} a_{\sigma, \mathbf{k}_3}^\dagger a_{\sigma, \mathbf{k}_1}, \quad (2.2)$$

where $\xi_{\mathbf{k}}^0 = -2t(\cos k_x + \cos k_y) - \mu$ and the momenta are within the first Brillouin zone. The renormalization-group calculation is best formulated using the path-integral formalism.^{25,28} The properties of the model are then given by the partition function

$$Z = \int_{\Lambda_0} \mathcal{D}\bar{\Psi} \mathcal{D}\psi e^{S\{\Lambda_0, \xi_{\mathbf{k}}^0, U_0\}}, \quad (2.3)$$

where the functional integration is over Grassmann variables $\bar{\Psi}(\Psi)$ corresponding to the fermionic fields $a^\dagger(a)$ and the phase space is cut off at $\xi_{\mathbf{k}}^0 = \pm \Lambda_0$ around the Fermi surface. The action S is given by

$$S\{\Lambda_0, \xi_{\mathbf{k}}^0, U_0\} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \sum_{\sigma\mathbf{k}} \Theta(\Lambda_0 - |\xi_{\mathbf{k}}^0|) \bar{\Psi}_{\sigma\mathbf{k}}(i\omega - \xi_{\mathbf{k}}^0) \Psi_{\sigma\mathbf{k}} + \frac{1}{2} \sum_{\sigma\sigma'} \int_{-\infty}^{\infty} \left(\prod_{i=1}^3 \frac{d\omega_i}{2\pi} \right) \times \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3} U_0 \Theta_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4}^{(\Lambda_0)} \times \bar{\Psi}_{\sigma\mathbf{k}_3} \bar{\Psi}_{\sigma'\mathbf{k}_4} \Psi_{\sigma'\mathbf{k}_2} \Psi_{\sigma\mathbf{k}_1}. \quad (2.4)$$

The Grassmann variables are momentum and energy dependent: we write $K = (\mathbf{k}, \omega)$. $\Theta_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4}^{(\Lambda_0)} \equiv \prod_{i=1}^4 \Theta(\Lambda - |\xi_{\mathbf{k}_i}^0|)$ constrains all four momenta to lie within the energy shell $\pm \Lambda_0 = 8t$ around the Fermi surface. The energy and momentum are conserved so that $K_4(K_1, K_2, K_3) = (\omega_1 + \omega_2 - \omega_3, \mathbf{k}_1 + \mathbf{k}_2 - \mathbf{k}_3)$. Note that the size of the cutoff is equal to the bandwidth, i.e., the whole Brillouin zone is available for integration. Thus, the Θ functions have no meaning yet: they become important when the cutoff, reduced by the renormalization group, becomes lower than the distance from the Fermi level to the band boundary. Note that for a non-half-filled band the effective phase space is not particle-hole symmetric.

The renormalization-group transformation that we will use, known as the field theory approach, is defined as the mapping

$$S\{\Lambda_0, \xi_{\mathbf{k}}^0, U_0\} \rightarrow S' = S\{\Lambda_0 \rightarrow \Lambda_0 e^{-l}, \xi_{\mathbf{k}}^0 \rightarrow \xi_{\mathbf{k}}, U_0 \rightarrow U(K_1, K_2, K_3)\}, \quad (2.5)$$

where $\xi_{\mathbf{k}}$ and U depend on l in a way so that the physical properties of S' and S are the same for energies lower than $\Lambda = \Lambda_0 e^{-l}$. This requirement is fulfilled if all one-particle

irreducible vertices are invariant under reduction of the cutoff from Λ_0 to $\Lambda_0 e^{-l}$. The renormalization group can be thought of as a set of successive, infinitesimally small steps increasing l by dl . This allows us to formalize the renormalization-group requirement in a set of differential equations $\partial_l \Gamma_i = 0$, where $i=2,4,6, \dots$. Up to second order in U , it suffices to consider only Γ_2 and Γ_4 , because all higher vertices are of higher order in U . The solutions of the equations $\partial_l \Gamma_2 = 0$ and $\partial_l \Gamma_4 = 0$ give us the renormalization-group flow for $\xi_{\mathbf{k}}$ and $U(K_1, K_2, K_3)$.

Conservation of spin allows us to write the general K -dependent interaction part of the action as a sum of the singlet ($|\vec{\sigma} + \vec{\sigma}'| = 0$ and triplet ($|\vec{\sigma} + \vec{\sigma}'| = \sqrt{2}$) parts:

$$\bar{s}(K_4, K_3) U^S(K_1, K_2, K_3) s(K_2, K_1) + \bar{t}_\mu(K_4, K_3) U^A(K_1, K_2, K_3) t_\mu(K_2, K_1), \quad (2.6)$$

where s and t_μ are the variables of annihilation of the singlet and triplet states

$$s(K_2, K_1) \equiv \frac{1}{\sqrt{2}} \sum_{\sigma} \sigma \Psi_{\sigma K_2} \Psi_{-\sigma K_1}, \quad (2.7)$$

$$t_0(K_2, K_1) \equiv \frac{1}{\sqrt{2}} \sum_{\sigma} \Psi_{\sigma K_2} \Psi_{-\sigma K_1};$$

$$t_{\pm 1}(K_2, K_1) \equiv \Psi_{\uparrow, \downarrow K_2} \Psi_{\uparrow, \downarrow K_1}. \quad (2.8)$$

The singlet state is symmetric and the triplet antisymmetric under exchange of the momenta of two particles. Correspondingly, the coupling function $U^S(K_1, K_2, K_3)$ can be taken to be symmetric and $U^A(K_1, K_2, K_3)$ to be antisymmetric under the momentum exchange operation X , defined as

$$X\mathcal{F}(K_1, K_2, K_3) = \mathcal{F}(K_2, K_1, K_3), \quad (2.9)$$

\mathcal{F} being a function of four energy-momenta which conserves energy and momentum. If \mathcal{F} possesses time-reversal symmetry

$$\mathcal{F}(K_1, K_2, K_3) = T\mathcal{F}(K_1, K_2, K_3) \equiv \mathcal{F}(K_3, K_4(K_1, K_2, K_3), K_1), \quad (2.10)$$

which certainly is a property of the vertex, then it is equivalent whether X exchanges K_1 and K_2 or K_3 and K_4 , i.e., $\mathcal{F}(K_2, K_1, K_3) = \mathcal{F}(K_1, K_2, K_4(K_1, K_2, K_3))$. Formally, U^S and U^A are given by

$$U^A = \frac{1}{2}(1 - X)U, \quad U^S = \frac{1}{2}(1 + X)U. \quad (2.11)$$

On the other hand, the interaction can also be written as a sum of one term with equal ($\sigma = \sigma'$) and one with opposite ($\sigma = -\sigma'$) spin quantum numbers, with corresponding coupling functions named $U_{\parallel}(K_1, K_2, K_3)$ and $U_{\perp}(K_1, K_2, K_3)$, respectively. From two equal-spin electrons one can build only a triplet state, which make us conclude that

$$U_{\parallel} = U^A, \quad (2.12)$$

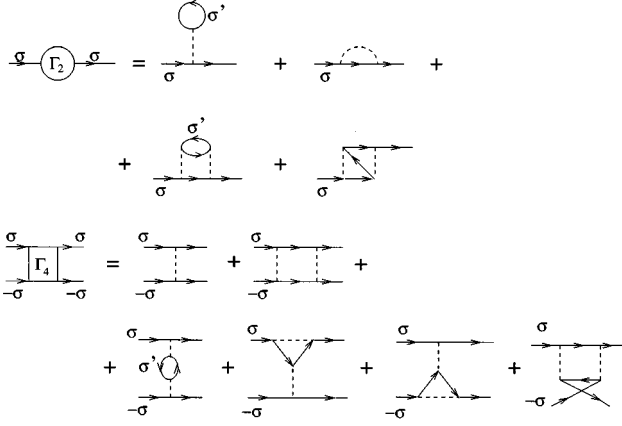


FIG. 1. The one-particle irreducible diagrams for the vertices Γ_2 and Γ_4 , generating the renormalization of the self-energy and the interaction, respectively.

while

$$U_{\perp} = U = U^A + U^S, \quad (2.13)$$

containing the singlet and the triplet interactions.

We proceed now with the derivation of renormalization-group equations. For simplicity, we will ignore the renormalization flow of $\xi_{\mathbf{k}}$, which follows from conservation of Γ_2 , renormalizing the form of the Fermi surface, the effective mass, etc. This approximation is justified in the case of the circular Fermi surface.²⁵ In the anisotropic case, the diagrams for Γ_2 have a dependence on the direction of \mathbf{k} . Moreover, even a small renormalization of the Fermi energy can give important changes of the form of the Fermi surface if one is close to half filling, because of the van Hove singularities. For filling not too close to one-half one can expect that the essential of the physics is given by just the renormalization of the coupling U using the bare dispersion relation $\xi_{\mathbf{k}}^0$ which we will call $\xi_{\mathbf{k}}$ from now on. However, it was recently argued²⁹ that if the spin-fluctuation propagator is strongly peaked at $\mathbf{q} = (\pi, \pi)$ (which certainly is the case for half or nearly half filling), the self-energy corrections kill superconductivity. As we go away from half filling, antiferromagnetic fluctuations are more and more suppressed, and the spin-fluctuation propagator becomes smoother, which lowers the importance of self-energy renormalization compared to the renormalization of the interactions.

The Feynman diagrams for Γ_2 and $\Gamma_{4\perp} = \Gamma_4$ are given in Fig. 1. The first loop in the expression for Γ_4 is of the electron-electron ($e-e$) and all others of the electron-hole ($e-h$) type. Making use of the relations (2.12), (2.13), and (2.11), we get the expression for Γ_4 in terms of U and XU . If we write the integration measure of the loop diagrams in the form

$$\int \frac{d\omega}{2\pi} \int_{-\Lambda}^{+\Lambda} d\xi \oint \frac{ds}{v(s, \xi)}, \quad (2.14)$$

s being the curves of constant energy ξ , then $d\Gamma_4$ corresponds to the integration of the two energy shells of width $|\Lambda|dl$ at $\xi = \pm\Lambda$. We obtain the following flow equation:

$$\frac{\partial U}{\partial l} = \beta_{ee}\{U, U\} + \tilde{\beta}_{eh}\{U, U\}, \quad (2.15)$$

with

$$\begin{aligned} \tilde{\beta}_{eh}\{U, U\} &= 2\beta_{eh}\{U, U\} - \beta_{eh}\{U, XU\} - \beta_{eh}\{XU, U\} \\ &\quad - XU\beta_{eh}\{XU, XU\}. \end{aligned} \quad (2.16)$$

The functionals $\beta_{ee}\{U_1, U_2\}$ and $\beta_{eh}\{U_1, U_2\}$ are the partial derivatives with respect to l of the $e-e$ and $e-h$ loops and both are bilinear forms in $U_1(K_1, K_2, K_3)$ and $U_2(K_1, K_2, K_3)$. They read

$$\beta_{ee}\{U_1, U_2\} = (\Xi\{U_1, U_2\} + \Xi\{XU_1, XU_2\}) \frac{1 + \kappa_{ee}}{2} \quad (2.17)$$

and

$$\beta_{eh}\{U_1, U_2\} = (\Pi\{U_1, U_2\} + \mathcal{T}\Pi\{U_1, U_2\}) \frac{1 + \kappa_{eh}}{2}, \quad (2.18)$$

with

$$\begin{aligned} \Xi\{U_1, U_2\} &= \frac{-\Lambda}{(2\pi)^2} \sum_{\nu=+,-} \int \frac{ds_{\nu}}{v_{\nu}} \Theta(\Lambda - |\xi_{\mathbf{k}_{\nu} - \mathbf{q}_{ee}}|) \\ &\quad \times \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{1}{i\omega - \nu\Lambda} \frac{1}{i(-\omega + \omega_{ee}) - \xi_{\mathbf{k}_{\nu} - \mathbf{q}_{ee}}} \\ &\quad \times U_1(K_1, K_2, K_{(\nu)}) U_2(K_3, K_4, K_{(\nu)}), \end{aligned} \quad (2.19)$$

$$\begin{aligned} \Pi\{U_1, U_2\} &= \frac{-\Lambda}{(2\pi)^2} \sum_{\nu=+,-} \int \frac{ds_{\nu}}{v_{\nu}} \Theta(\Lambda - |\xi_{\mathbf{k}_{\nu} + \mathbf{q}_{eh}}|) \\ &\quad \times \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{1}{i\omega - \nu\Lambda} \frac{1}{i(\omega + \omega_{eh}) - \xi_{\mathbf{k}_{\nu} + \mathbf{q}_{eh}}} \\ &\quad \times U_1(K_1, K_{(\nu)}, K_3) U_2(K_4, K_{(\nu)}, K_2). \end{aligned} \quad (2.20)$$

The index $\nu = +, -$ symbolizes two energy shells at $+\Lambda$ and $-\Lambda$; v_{ν} stands for $v(s_{\nu}, \xi = \nu\Lambda)$; $\omega_{ee} \equiv \omega_1 + \omega_2$; $\omega_{eh} \equiv \omega_1 - \omega_3$; $\mathbf{q}_{ee} \equiv \mathbf{k}_1 + \mathbf{k}_2$; $\mathbf{q}_{eh} \equiv \mathbf{k}_1 - \mathbf{k}_3$; $K_{\nu} \equiv (\mathbf{k}_{\nu}, \omega)$, where \mathbf{k}_{ν} is the momentum running along the path s_{ν} . κ_{ee} and κ_{eh} are nonanalytic functions of the momenta, given by

$$\kappa_{ee} = \begin{cases} 0 & \text{for } \mathbf{q}_{ee} = 0 \\ 1 & \text{otherwise;} \end{cases}$$

$$\kappa_{eh} = \begin{cases} 0 & \text{for } \mathbf{q}_{eh} = (\pm\pi, \pm\pi); \mu = 0 \\ 1 & \text{otherwise.} \end{cases}$$

Their origin is in the derivatives over Λ of the products like

$$\Theta(\Lambda - |\xi_{\mathbf{k} + \mathbf{q}}|) \Theta(\Lambda - |\xi_{\mathbf{k}}|)$$

when $\xi_{\mathbf{k}} = \xi_{\mathbf{k} + \mathbf{q}}$.

III. CROSSOVER TEMPERATURE AND RENORMALIZATION GROUP FOR THE LOW-ENERGY EFFECTIVE ACTION

A. The crossover temperature T_{co}

A particularity of the renormalization-group approach treating e - e and e - h fluctuations in more than one dimension is the absence of self-similarity of the problem. In fact, there is an intrinsic energy scale which is a function of the band filling. It is associated with charge and spin fluctuations coming from the e - h term. We will proceed by estimating the characteristic energy scales which appear in β_{ee} and β_{eh} , when all four particles are at the Fermi surface, with zero energy. If we are exactly at half filling, it is known that in the limit $\omega \rightarrow 0$ both e - e and e - h loops scale like l^2 , which corresponds to the square-logarithmic divergence in both channels. This gives an explicit $\sim l$ dependence in the β functionals. Let us suppose now that the filling is slightly lower than one-half, i.e., that μ is small and negative. We expect two regimes. One is for $l \lesssim l_x \sim \ln|8t/\mu|$, where the flow is still unaffected by the small changes of the Fermi surface due to nonzero μ and remains proportional to l . In the second regime, where $l \gtrsim l_x$, the e - e flow is just a constant (i.e., only a \ln divergence), while the e - h flow decays exponentially due to disappearance of nesting. Even far from half filling it is possible to define a crossover l_x , beyond which the flow in the e - h channel disappears exponentially. We can summarize saying that for any filling, l_x is a crossover from a regime where both e - e and e - h loops contribute to a regime where β_{eh} starts to behave like $\beta_{eh} \sim \Lambda^{\eta(\mathbf{q})}$. Here $\eta(\mathbf{q})$ is positive for all values of the momentum transfer $\mathbf{q} = \mathbf{q}_{eh}$.

To estimate the dependence of l_x on the filling $\langle n \rangle$, we consider the static limit of the partially integrated e - h loop

$$P_{eh}(l, \mathbf{q}, \omega=0) = \frac{1}{U_0^2} \int_0^l dl \beta_{eh}\{U_0, U_0\} \quad (3.1)$$

with the momentum transfer \mathbf{q} equal to $2\mathbf{k}_F$ in the direction (π, π) . Note that the energy integration is performed over $8t < \xi < 8t \exp(-l)$. The derivative of $P_{eh}(l, \mathbf{q}, \omega=0)$ with respect to l gives the explicit l dependence in the β_{ee} functional. Figure 2 shows $P_{eh}(l)$ and $\partial_l P_{eh}(l)$ for two different values of μ . It is reasonable to define l_x as the point where $\partial_l P_{eh}(l)$ starts to decrease. In the exponential regime the function $\partial_l P_{eh}(l)$ decays like $\exp(-l/2)$ [i.e., $\eta(2\mathbf{k}_F) = 1/2$, valid for any orientation of \mathbf{k}_F], while the regime $l < l_x$ remembers the \ln^2 divergence of P_{eh} at half filling.³⁰ The dependence $l_x(\langle n \rangle)$ is shown in Fig. 3. Near $\langle n \rangle = 1$ there is a divergence of the form $l_x(\langle n \rangle) \approx \ln|8t/\mu(\langle n \rangle)|$ because of nesting, while the increasing l_x as the filling goes to zero mirrors the fact that, for low density, the Fermi energy appears as the new scale instead of the bandwidth being used. The inset shows the function $\langle n \rangle(\mu)$.

Once in the exponential regime, β_{eh} can be neglected after it becomes smaller than e^{-1} of its value at $l = l_x$. Putting $\eta = 1/2$, this defines the crossover

$$l_{co}(\mu) = l_x(\mu) + 2, \quad (3.2)$$

corresponding to the crossover temperature $T_{co} = 8t \exp(-l_{co})$. Suppose that we now integrate the flow equation (2.15) from $l=0$ to $l=l_{co}$. Once l has reached l_{co} , only

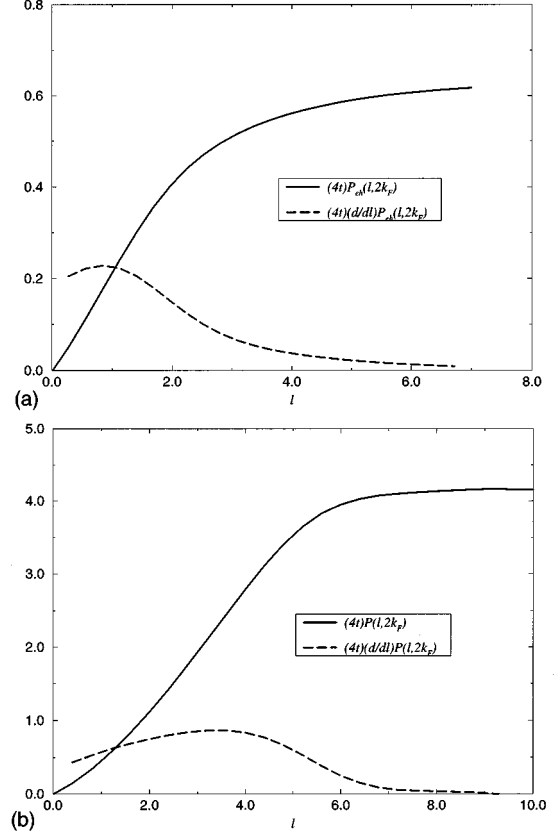


FIG. 2. The e - h bubble (solid line) and its derivative over l (dashed line) for $\mu/4t = -0.25$ (a) and $\mu/4t = -0.02$ (b), for momentum transfer $\mathbf{q}_{eh} = 2\mathbf{k}_F \parallel (\pi, \pi)$.

the term $\beta_{ee}\{U\}$ remains in the flow equations, and one has a partially renormalized $U(l=l_{co})$ as initial condition.

B. Tree-level (zero-order) scaling for $\Lambda = T_{co}$

We will now use the fact that $T_{co}/8t$ is a small parameter, i.e., the inequality $|\xi_{\mathbf{k}}| < T_{co}$ determines a thin ring of degrees of freedom, containing no van Hove points, as one can conclude looking at Fig. 3. This allows us to rescale the

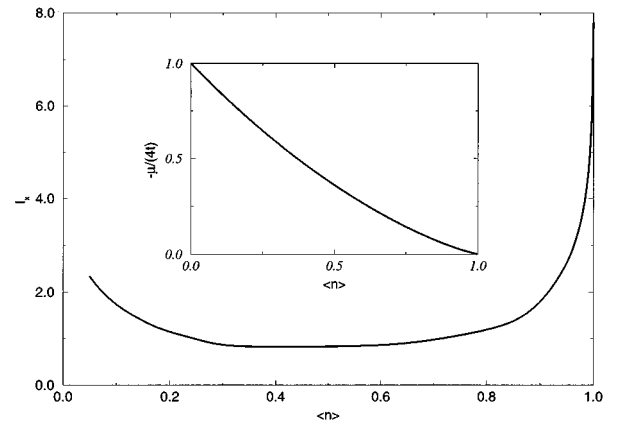


FIG. 3. The scale l_x as a function of filling $\langle n \rangle$. For $l > l_x$ the e - h flow decays exponentially. The inset shows the relation between μ and $\langle n \rangle$.

momenta $k_{\perp} = \hat{\mathbf{n}}(\mathbf{k} - \mathbf{k}_F)$, where $\hat{\mathbf{n}}$ is the unit vector normal to Fermi surface, dependent on the direction of \mathbf{k} . To clarify the reason for which a tree-level scaling is not allowed for energies higher than the deviation of the Fermi level from van Hove singularity, let us write the phase-space integration measure in terms of energy (ξ) and polar angle (θ) variables

$$\frac{1}{2\pi} \int d\mathbf{k} = \frac{1}{2\pi} \int d\xi d\theta J(\xi, \theta) \quad (3.3)$$

with $J(\xi, \theta) = k(\xi, \theta)/v(\xi, \theta)$, k being the radial wave number and v is the group velocity. Tree-level scaling²⁵ tells us via a power counting argument to consider $J(\xi, \theta)$ as function of θ , neglecting any ξ dependence about $\xi=0$, which is possible if $J(\xi, \theta)$ is an analytic function of ξ at the whole shell $\pm\Lambda$ which, consequently, should contain no singularity.

We can also rescale the frequencies if $U(l_{co})$ is an analytic function of ω in the interval $\pm T_{co}$ about the Fermi surface, which we assume to be the case.³¹ In the scope of the tree-level scaling, the slope of the electronic dispersion around the Fermi surface is irrelevant and the two marginal interactions correspond to two different constraints on the four-momenta in U . Since any k_{\perp} and ω dependence in U is irrelevant, both marginal interactions depend only on coordinates of the zero-frequency particles placed at the Fermi surface. For the first, ‘‘Fermi liquid’’ or forward interaction, the momenta satisfy the equation $\mathbf{k}_1 = \mathbf{k}_3$, where the meaning of momenta can be seen from the Eq. (2.4). This interaction is slightly ($\sim U_0^2$) renormalized by the high-energy-modes ($l < l_{co}$), and is not involved in further renormalization. The second interaction is the pairing potential V , where the momenta satisfy the condition $\mathbf{k}_1 = -\mathbf{k}_2$. The pairing V depends only on angular coordinates of annihilated and created pairs. Keeping in mind the above remarks, we can write the action for the electrons in the ring $\pm T_{co}$ around the Fermi surface as

$$\begin{aligned} S = \int_0^{\infty} d\tau \left\{ \sum_{\sigma} \int_{\epsilon < T_{co}} \frac{d\epsilon}{2\pi} \oint \frac{ds}{2\pi v(\theta)} \bar{\Psi}_{\sigma}(\epsilon, \theta) \right. \\ \times (\partial_{\tau} - \epsilon) \Psi_{\sigma}(\epsilon, \theta) + \frac{1}{2} \sum_{\sigma\sigma'} \int \frac{d\mathbf{q}_{ee}}{(2\pi)^2} \oint \frac{ds}{2\pi v(\theta)} \\ \times \oint \frac{ds'}{2\pi v(\theta')} \bar{\Delta}_{\sigma'\sigma, \mathbf{q}_{ee}}(\theta') V_{l=l_{co}}(\theta, \theta') \\ \left. \times \hat{\Delta}_{\sigma'\sigma, \mathbf{q}_{ee}}(\theta) + \text{FL} \right\}, \quad (3.4) \end{aligned}$$

where $\epsilon = k_{\perp} v(\theta)$, closed-loop integrations are over the the Fermi surface, and FL stands for the effective Fermi-liquid interaction. $\hat{\Delta}_{\sigma'\sigma, \mathbf{q}_{ee}}(\theta)$ is the energy-integrated number of pairs defined as

$$\begin{aligned} \hat{\Delta}_{\sigma_1, \sigma_2, \mathbf{q}_{ee}}(\theta) \equiv \int_{\epsilon < T_{co}} \frac{d\epsilon}{2\pi} \Psi_{\sigma_1}(\mathbf{k}) \Psi_{\sigma_2}(-\mathbf{k} + \mathbf{q}_{ee}) \\ \times \Theta(T_{co} - |(\mathbf{k}_F(\theta) - \mathbf{k} + \mathbf{q}_{ee}) \cdot \hat{\mathbf{n}}v(\theta)|). \quad (3.5) \end{aligned}$$

Note that the integration measure over small momentum \mathbf{q}_{ee} goes to zero as $l \rightarrow \infty$. A form similar to Eq. (3.4) has been used by Weinberg,²⁶ but taking $V_{l=l_{co}}(\theta, \theta')$ phenom-

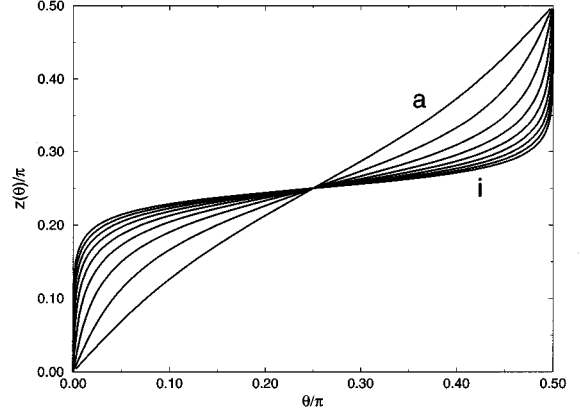


FIG. 4. The relation between the angular variable z and the observable polar angle θ for $-\mu/4t = 2 \times 10^{-n}$; $n = 1(a), 2, \dots, 9(i)$.

enologically and not as the partially renormalized pairing interaction which we get from $U_{l=l_{co}}(\theta_1, \theta_2, \theta_3)$ putting incoming particles 1 and 2 to θ and $\theta + \pi$ and outgoing 3 and 4 to θ' and $\theta' + \pi$. Note that the loop integration over s can be understood as the scalar product over ‘‘vector components’’ of a ‘‘spin,’’ where the number of components N corresponds to $8t/T_{co}$.^{25,32}

C. The renormalization of the pairing potential V

The integrations in Eq. (3.4) have the weight factor $1/v(\theta)$, $v(\theta)$ being the anisotropic Fermi velocity, what suggests to introduce a new angular coordinate

$$z(\theta) = \frac{\int^s [ds/v(\theta)]}{2\pi N_F}, \quad (3.6)$$

where N_F is the density of states at the Fermi level. The function $z(\theta)$ is shown in Fig. 4 for few different values of μ . Starting from the new action Eq. (3.4) we can calculate now the function $\beta_{ee}\{V\}$ in z space and obtain the flow equation

$$\partial_l V(z, z') = -\frac{N_F}{2\pi} \oint dz'' V(z, z'') V(z'', z'), \quad (3.7)$$

where the coordinate z appears instead of $\theta(z)$. For initial condition we take $V_{l=l_{co}}[\theta(z), \theta(z')]$.

To make the differential equation (3.7) solvable one has to diagonalize the pairing potential $V(z, z')$.^{25,26} Since it is invariant under all symmetry elements of the D_4 point group, its most general form in z space can be written as

$$V(z, z') = \sum_{\gamma} \sum_{m,n} V_{m,n}^{\gamma} f_{m,n}^{\gamma}(z, z'), \quad (3.8)$$

where $V_{mn}^{\gamma} \equiv \langle m\gamma | V | n\gamma \rangle$ and $f_{m,n}^{\gamma}(z, z') \equiv \langle m\gamma | z \rangle \langle n\gamma | z' \rangle$. The function $\langle m\gamma | z \rangle$ is the m th basis state of the γ representation of the point group D_4 . It is proportional to the function $\cos 4mz$, $\sin 4mz$, $\cos(4m+2)z$, $\sin(4m+2)z$, and $[\cos(2m+1)z \pm \sin(2m+1)z]$, for $\gamma = A_1, A_2, B_1, B_2$, and E respectively. Using Eq. (3.8), the flow equation (3.7) becomes

$$\partial_l V_{m,n}^\gamma = -\frac{N_F}{2\pi} \sum_v V_{m,v}^\gamma V_{v,n}^\gamma \quad (3.9)$$

with the initial condition

$$V_{m,n}^\gamma(l=l_{co}) = \int dz dz' f_{m,n}^\gamma(z, z') V_{l_{co}}(z, z'). \quad (3.10)$$

To solve exactly Eq. (3.9) one has to diagonalize five infinite dimensional matrices $V_{m,n}^\gamma(l=l_{co})$, thus decoupling completely the flow Eq. (3.9) into a set of differential equations whose solution is

$$V_\lambda^\gamma(l) = \frac{V_\lambda^\gamma(l_{co})}{1 + [N_F V_\lambda^\gamma(l_{co}) / 2\pi](l - l_{co})}. \quad (3.11)$$

Here λ labels the eigenvalues within the representation γ . If $V_\lambda^\gamma(l_{co})$ is negative, the denominator has a zero at $l = l_c(\gamma, \lambda)$ and an instability occurs.

IV. PERTURBATIVE CALCULATION OF $V(l_{co})$

One can expand $V(l_{co})$ in a perturbative series in U_0

$$V(l_{co}) = U_0(1 + I_1 U_0 + I_2 U_0^2 + \dots). \quad (4.1)$$

We can stop at the term $I_1 U_0$ if

$$I_1 U_0 < 1. \quad (4.2)$$

All other terms will then converge rapidly since $I_n \sim I_1^n$.⁸ It is easy to calculate I_1 from first iteration of the renormalization equation (2.15): it corresponds to a sum of partially integrated electron-electron and electron-hole loops

$$I_1 = P_{ee}(l_{co}) + P_{eh}(l_{co}) \approx P_{ee}(l_{co}) + P_{eh}(\infty), \quad (4.3)$$

where $P_{ee}(l)$ is an integral of β_{ee} , in a same way as $P_{eh}(l)$ in Eq. (3.1). In P_{eh} the argument l_{co} can be replaced by ∞ in Eq. (4.3) simply by the definition of l_{co} : for $l_{co} < l < \infty$ the e-h flow can be neglected. The line $I_1(\mu)U_0 \sim 1$ is shown in Fig. 5; below the line the perturbative calculation of $V(l_{co})$ is justified.

$P_{ee}(l_{co})$ has no dependence on z and z' , since it depends on external momenta only through $\mathbf{k}_1 + \mathbf{k}_2$, which we put to zero. Consequently, its only nonzero component is $\langle 0A_1 | P_{ee} | 0A_1 \rangle$. Thus, for the calculation of all other components of $V(l_{co})$ we use just the bubble $P_{eh}(\infty)$ with the momentum transfer $\mathbf{q} = \mathbf{k}_F(z) - \mathbf{k}_F(z' + \pi)$. Figure 6(a) shows $P_{eh}(l \rightarrow \infty)$ as a function of z and z' for chemical potential $\mu/4t = -0.2$.

The minimal eigenvalues of $V(l_{co})$ in all five channels, named λ_{\min}^γ are shown in Fig. 6(b) as functions of μ . These curves indicate which kind of superconducting symmetry becomes critical at some given μ . The eigenvalues for each channel are calculated taking only the first four harmonics for A_1 , A_2 , B_1 and B_2 , and the first six harmonics for the E representation. The corresponding eigenvectors determine the Fourier spectrum of the gap function. A very important result is that the relevant harmonic of the superconducting fluctuations in the B_1 channel occurs very close to just $\cos(2z)$, being thus determined only by the structure of the Fermi surface and not by the interaction. Figure 7(a) show

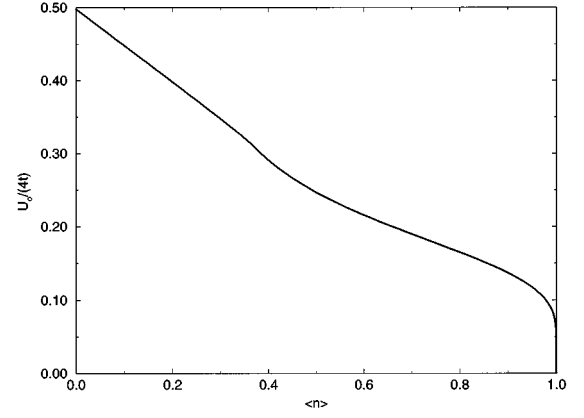


FIG. 5. The curve $U_0 P_{eh}(l \rightarrow \infty) = 1$. Below the curve, the e - h contribution to the renormalization can be treated perturbatively. This is the region considered in the present paper.

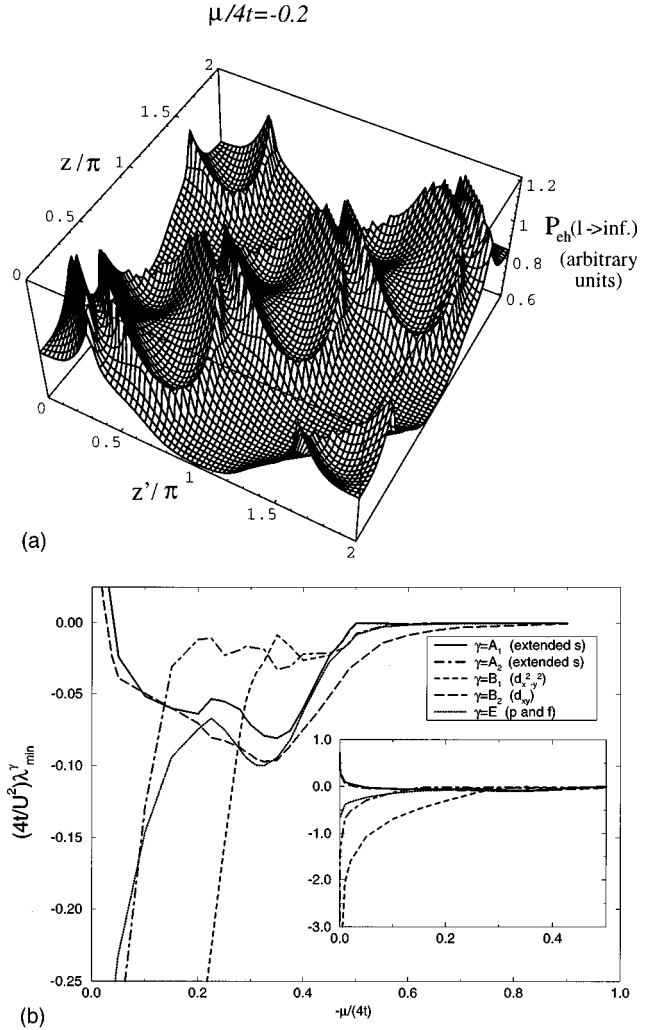


FIG. 6. (a) The shape of the function $P_{eh}(l \rightarrow \infty)$ in (z, z') space at $-\mu/4t = 0.2$. The nesting at half filling occurs for $z = z' = \pi/4$. The split singular lines show the best incommensurate nesting vector. (b) The minimal eigenvalue of the pairing $V(z, z')$ in each of the five irreducible representations of the D_4 point group.

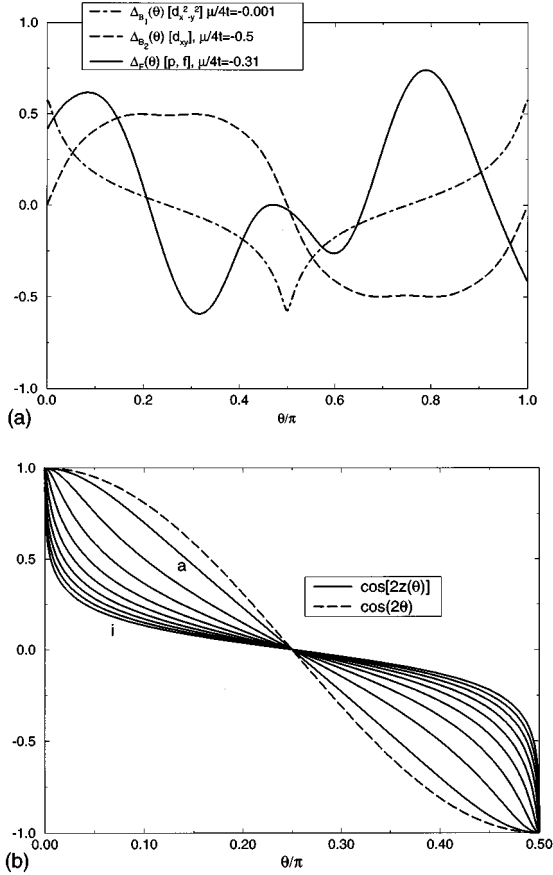


FIG. 7. (a) The shape of three possible gap functions: $\Delta_{B_1}(\theta)$ for $\mu/4t = -0.001$ (dot-dashed), $\Delta_{B_2}(\theta)$ for $\mu/4t = -0.5$ (dashed), and $\Delta_E(\theta)$ for $\mu/4t = -0.31$ (solid line). (b) A very good approximation for $\Delta_{B_1}(\theta)$ is just $\cos 2z(\theta)$, shown here for the same choice of μ as in Fig. 4. The dashed line shows $\cos \theta$ to comparison.

the unstable order parameters Δ_{B_2} for $\mu = -0.5$, Δ_E for $\mu = -0.31$, and Δ_{B_1} for $\mu = -0.001$ as a function of the Fermi-surface angle θ . The evolution of the function $\cos 2z(\theta)$ (i.e., the first harmonic of B_1) with $\log(-\mu)$, given only by the dependence of z on θ , is shown in Fig. 7(b). The strength of the peaks near the van Hove points increases and the magnitude in the area between the peaks decreases as one approaches half filling.

The critical temperature is given by a cutoff for which the most attractive diagonal component of V diverges, i.e.,

$$T_c = 8t \exp[-l_c(\gamma, \lambda_{\min})], \quad (4.4)$$

where $\lambda_{\min} = \min\{\lambda_{\min}^{\gamma}\}$. Figure 8 shows l_c as a function of $\ln(\mu)$. The critical temperature decreases extremely fast as we go away from the half filling. An increase of U_0 could save the situation, but in that case our perturbative method ceases to be sufficient (see Fig. 5). Since the cuprates are superconductors for fillings quite far from one electron per site ($\langle n \rangle \sim 1 - 0.17$), this result means that the small- U Hubbard model cannot describe these systems quantitatively. However, the model gives very precious informations about the form of the gap function in the B_1 -instable regime, which will not change considerably with increasing U_0 , as long as $\cos(2z(\theta))$ is the dominant attractive harmonic in $V(l_{co})$.

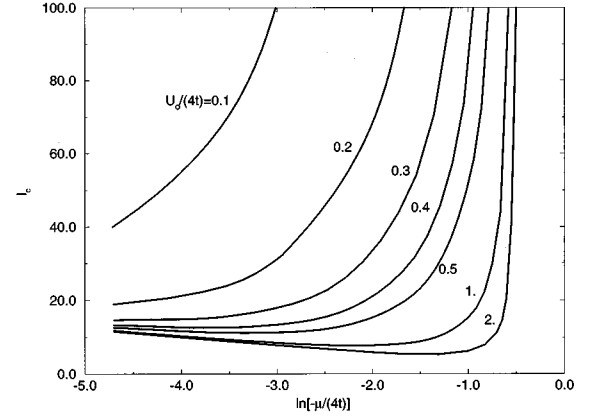


FIG. 8. The scale $l_c = -\ln T_c / 8t$ as a function of the logarithm of the chemical potential, for a few values of coupling U_0 . For very small μ and for $U_0/4t > 0.5$ the curves are out of the range of validity (see Fig. 5).

V. MIXED-SYMMETRY SUPERCONDUCTIVITY

Once the renormalization flow has been integrated for $l < l_{co}$, assuming that the interaction did not diverge earlier in the antiferromagnetic channel, the detailed angular dependence of the superconducting gap function can be easily found. In general, a superconducting state with the symmetry corresponding to the lowest of the eigenvalues λ_{\min}^{γ} will be formed. However, when two of the λ_{\min}^{γ} are close to each other, a more complicated situation can occur: for definiteness, consider the region $0.206 < |\mu/4t| < 0.276$ in Fig. 6(b), where the B_2 eigenvalue is the most attractive after the B_1 . Let us suppose that the B_1 order of the simplest form $\Delta_{B_1} \sim \cos 2z$ has formed and that the temperature is close to T_c . Among the remaining symmetry channels, B_2 is the only one which can give a large gap function in the node points of Δ_{B_1} and zero in the points where Δ_{B_1} is maximal. Consequently, we expect that the flow of the type Eq. (3.11) with $\gamma = B_2$ will not be strongly affected by the existing B_1 order. Considering to a first approximation the two flow equations ($\gamma = B_1$ and $\gamma = B_2$) as independent, and taking only the first harmonics of the B_1 and B_2 representations, we can construct the relevant part of the pairing interaction which gives two phase transitions, one with B_1 and the other with B_2 symmetry:

$$V_{l_{co}}(\theta_1, \theta_2) = V^{(B_1)} \frac{1}{\pi} \cos 2z(\theta_1) \cos 2z(\theta_2) + V^{(B_2)} \frac{1}{\pi} \sin 2z(\theta_1) \sin 2z(\theta_2), \quad (5.1)$$

where all details of the Fermi surface are contained in the dependence of z on θ . From Eq. (3.11) one finds that the ratio between two critical temperatures is given by $T'_c/T_c = \exp[-2\pi(1/V^{(B_1)} - 1/V^{(B_2)})/N_F]$. From Fig. 6(b) note that the ratio T'_c/T_c is very sensitive to the variation of the chemical potential. The gap function resulting from Eq. (5.1) has the form

$$\Delta(\theta) = \Delta_{B_1} e^{i\phi_1} \cos 2z(\theta) + \Delta_{B_2} e^{i\phi_2} \sin 2z(\theta), \quad (5.2)$$

where Δ_{B_1} , Δ_{B_2} , ϕ_1 , and ϕ_2 are real. These parameters can be determined minimizing the mean-field expression for the free energy per site³³

$$F = -\frac{2T}{N} \sum_{\mathbf{k}} \Theta(T_{co} - |\xi_{\mathbf{k}}|) \text{Incosh} \frac{E_{\mathbf{k}}}{2T} + |\Delta_1|^2/V^{(B_1)} + |\Delta_2|^2/V^{(B_2)}, \quad (5.3)$$

where $E_{\mathbf{k}} \equiv \sqrt{\xi_{\mathbf{k}}^2 + |\Delta(\theta)|^2}$ and the θ function constrains the momentum summation to run only over the states within the energy shell $\pm T_{co}$ about the Fermi surface. The minimization of F with respect to $\cos(\phi_1 - \phi_2)$ gives

$$\phi = \phi_1 - \phi_2 = \pm \frac{\pi}{2}, \quad (5.4)$$

i.e., the resulting gap function is of the type $B_1 \pm iB_2$. It is interesting to remark that the same kind of gap function has been obtained by Laughlin using the anion picture.³⁴ The particularity of this gap function (and of any gap consisting of two different symmetry terms with a phase difference of $\pm \pi/2$) is that it breaks time-reversal symmetry.

We can now try to understand recent ARPES measurements by Ma and co-workers²¹ on the $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8$ compound. From their experiment it appears that two superconducting instabilities occur; the first one is at $T = T_c$ and has probably the B_1 symmetry. The second instability occurs at $T'_c = 0.81T_c$; it introduces a nonzero gap at the points $\theta = (2n+1)\pi/4$, i.e., halfway between the corners of the half-filled Fermi surface. The function measured by ARPES is $|\Delta(\theta)|$ and in the picture discussed above has no zeros and minima on the diagonals of the Brillouin zone if both Δ_{B_1} and Δ_{B_2} are finite, $|\Delta_{B_1}| > |\Delta_{B_2}|$ and $\phi = \pm \pi/2$. This is in agreement with the experiments because the gap in the diagonal direction is just equal to Δ_{B_2} , introduced at $T = T'_c$. The minimum of $|\Delta(\theta)|$ on the diagonals is in agreement with other ARPES experiments^{19,20} as well. One should of course notice that in our model closeness of two different λ 's only occurs in very narrow parts of the parameter space and therefore to a certain degree is accidental.

VI. CONCLUSIONS

We have investigated the problem of electrons on a square lattice interacting via a weak repulsion, as described by the Hubbard model. The problem of coexisting fluctuations in the electron-electron and electron-hole channels has been approached using a one-loop renormalization-group approach. Considering only the renormalization of the interaction function and ignoring the self-energy corrections, which is certainly justified if we are far enough from half filling, we have in particular demonstrated the existence and type of superconducting instabilities which we generally found to be of the d -wave type.

We have in particular considered the case of band filling different from one-half (the half-filled case almost certainly has an antiferromagnetic ground state) and have taken into account contributions to the interactions from the whole Brillouin zone (i.e., initially the energy cutoff Λ equals the full bandwidth $8t$). We have shown that there is an important energy (temperature) scale, T_{co} , separating a high-energy regime where both electron-electron and electron-hole-type diagrams contribute from a low-energy regime where only the electron-electron-type diagrams are important, however with effective interactions containing renormalizations from the high-energy regime. Correspondingly, the renormalization-group flow for $l = \ln(8t/\Lambda)$ inferior to some crossover $l_{co} \equiv \ln(8t/T_{co})$ contains contributions from both the electron-electron and electron-hole diagrams. On the other hand, for $l < l_{co}$ only the electron-electron diagram contributes, while the electron-hole contribution decays exponentially as $\exp(-l/2)$. Here l_{co} depends on band filling, but is independent on the strength of the interaction. The degrees of freedom with energy inferior to T_{co} lie then in a thin and smooth ring around the Fermi surface. They can be described by a low-energy effective action containing a dispersion relation linearized in the direction perpendicular to the Fermi surface with angle-dependent Fermi velocity. The only marginally relevant interaction remains the BCS pairing interaction $V(\theta_1, \theta_2)$, a function only of the angular positions of incoming (θ_1) and outgoing (θ_2) Cooper pairs. We decompose the pairing interaction into its Fourier components in the five irreducible representations of the D_4 point group, defined at the Fermi surface. Diagonalizing $V(l_{co})$ in each representation, we get five sets of decoupled BCS flow equations. The minimal (i.e., the most negative) eigenvalue of $V(l_{co})$ determines the critical temperature and the eigenvector gives the form of the gap function. Unlike the usual approach,³⁵ the characteristic of the procedure presented here to obtain the symmetry of the gap function is that only the angular coordinates at the Fermi surface is relevant, while the radial dependence is ‘‘scaled out.’’ Moreover, the renormalization-group treatment of the whole Brillouin zone, and not only of the narrow belt about the Fermi surface has allowed us to show that the origin of the attractive part of the pairing interaction in the Hubbard model is in electron-hole fluctuations on rather high energy scales, up to the bandwidth.

Two regimes exist in interaction-chemical potential space: In the first regime $U_0 P_{eh}(2k_F) < 1$ (essentially weak coupling and far from half filling) the pairing $V(l_{co})$ is a result of a simple perturbative integration of all degrees of freedom at $0 < l < l_{co}$. The second regime is the one with still weak U_0 , but $U_0 P_{eh}(2k_F) > 1$ due to the enhanced nesting so that we have to do a full renormalization group even for $0 < l < l_{co}$. In this paper, we give results only for the first case: the diagonalization of $V(l_{co})$ in terms of angular harmonics gave us the type of superconducting instability: for weak filling, the instability occurs in the B_2 (d_{xy}) singlet channel, while for filling close to one-half, the B_1 ($d_{x^2-y^2}$) singlet instability strongly overwhelms all others, in agreement with previous work.^{3,9,10} Particularly interesting is the fact that the order parameter $\Delta_{B_1}(\theta)$ can be very well approximated by the function $\cos 2z(\theta)$, where the function

$z(\theta)$ depends only on the anisotropic Fermi velocity and on the geometry of the Fermi surface. This gives for $\Delta_{B_1}(\theta)$ a function that has peaks in the directions of the van Hove singularities. The slope of the peaks increases as we approach half filling. This can be a justification to consider the interaction only between electrons in the close vicinity of the van Hove points as relevant if we are very close to half filling.⁸ We believe that the form of $\Delta_{B_1}(\theta)$ does not depend considerably on the strength of interaction, and recent T -matrix calculations³⁶ for realistic values of the interaction U_0 give a gap function in agreement with this.

We find a superconducting instability at any electron concentration away from half filling. The underlying physical mechanism, namely exchange of spin- or charge-density fluctuations, is the same as in previous approaches.⁵⁻¹² We do however feel that our present results are on a more solid footing than the previous work because the present one-loop renormalization-group scheme does not make any *a priori* assumptions about important or unimportant diagrams and provides a more systematic way of handling the dynamics of the fluctuations being exchanged. The only restrictions come from (i) the limitation to one-loop order (equivalently, lowest nontrivial order in perturbation theory), necessitating weak coupling, and (ii) the requirement that the e - h diagram are a perturbation with respect to the e - e diagrams, implying that we cannot be too close to half filling. The region of validity of the approach is shown in Fig. 5. Further, self-energy diagrams have been neglected, however, these are expected to produce important effects only at two-loop order, and therefore are expected to be negligible in weak coupling.

In our weak-coupling model the superconducting critical temperature is very small (but it exists, for any filling) if we are not in the immediate vicinity of half filling, which means that the Hubbard model with small U_0 and small (perturbative) antiferromagnetic fluctuations does not suffice to describe the high critical temperature ($\sim 0.02t$) of the cuprates. There exist two possible ways (related to two restrictions of our calculations) to increase the critical temperature. The first is to simply increase U_0 and to remain far from the half filling, keeping the e - h channel nonsingular. To treat this case, an approach perturbative in U_0 is only of limited use. Ideally, renormalization should be done exactly, and not using a simple one-loop (or n -loop) scheme (which is actually just an “intelligent” version of the perturbative summation). We can speculate and suppose that even in the case of strong coupling there exists the crossover \tilde{l}_{co} , above which the flow is of the BCS type. It is to be expected that \tilde{l}_{co} is not very different from the l_{co} that we have calculated. This means

that the cutoff \tilde{T}_{co} for the effective BCS theory is $\Lambda_0 \exp(-l_{co})$ [see Fig. 3. and Eq. (3.2)], where Λ_0 is the initial cutoff of the theory, equal to $8t$. The second possibility to increase T_c is to approach half filling very closely, making Fermi-surface nesting important but remaining in a weak-coupling regime. For that case, a simplified one-loop renormalization-group calculation⁸ has shown that superconductivity wins over antiferromagnetism only if the e - h contribution to the flow decays before the divergence in the antiferromagnetic channel takes place. Thus, we can say that here too, the effective theory is of the BCS type. The difference with the first scenario is that the effective cutoff is very small (Fig. 3), and that the coupling constant is very strong, due to the strong flow in both e - e and e - h channels at all scales $l < l_{co}$. A very important feature of the nested case with a small U_0 is that it can be treated in terms of the one-loop renormalization group, renormalizing U as a function only of three angular variables. This is allowed because all important physics (i.e., the majority of the e - e and e - h flow) is contained in the vicinity of the Fermi surface, making the effective phase space to be a rather narrow square region $\pm \Lambda_i$; ($8t \gg \Lambda_i \gg \Lambda_{co}$) where the marginally relevant interaction is a function only of the angular position of the particles on the square. This is one of the key ideas of the renormalization-group analysis treating nesting and pairing divergence on the same footing which will be published subsequently.

Finally, we have discussed the possibility of a superconducting state with a mixed symmetry in a narrow region in parameter space. In the presence of B_1 order, the flow in the B_2 channel (which is the second most attractive one for $0.206 < \mu < 0.276$) will be only weakly affected by a nonzero order parameter of B_1 symmetry. This gives rise to two superconducting instabilities, with the critical temperatures T_c for the B_1 and T'_c for the B_2 channel, and $T'_c < T_c$. We have given the form of the pairing function for the effective BCS theory. At $T < T'_c$ the relative phase of two order parameters is $\phi = \pm \pi/2$. The resulting form of the energy gap $|\Delta(\theta)|$ has no zeros and minima are in diagonal directions, providing a possible qualitative explanation of ARPES experiments by Shen¹⁹ and the decrease of the anisotropy with decreasing T .²¹

ACKNOWLEDGMENTS

We are indebted to N. Dupuis and L. Guerin for a number of helpful discussions. This work was supported by EC Contract No. ERBCHRXCT 940438.

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