Van-Hove singularities effects on the upper critical field

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We present a study of the superconducting pairing susceptibility $K_T(r)$ for a two-dimensional isotropic system with a strong power-law divergence in the density of states $N(\epsilon) \sim \epsilon^{-1+\frac{\beta}{2}}$, $b > 1$. We show that the pair propagator has the scaling form, $K_T(r) \sim r^{b-3} F(T^{1/b} r)$. An anomalous short-range behavior is found, leading straightforwardly to positive curvature in the upper critical field, for $b \leq 2$ and to a zero temperature divergence, $H_{c2} \sim T^{-2+\frac{\beta}{2}}$, for $b > 2$.

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Photoemission experiments in Copper-Oxide superconductors [1,2] have provided direct evidence for the existence of an extended saddle point in the CuO$_2$ plane bands and consequently, a strong divergence in the density of states, $N(\epsilon) \sim (\epsilon - \epsilon_{ch})^{-\alpha}$, for energies close to $\epsilon_{ch}$. Some authors have claimed that the high superconducting critical temperatures of the cuprates could be explained taking into account this divergence [3,4].

One of the most surprising properties of these materials is the upper critical field, which has been obtained in magnetoresistance experiments down to very low temperatures in the case of overdoped Tl$_2$Ba$_2$CuO$_{6+\delta}$ [5] and Bi$_2$Sr$_2$CuO$_{y}$ [6] and underdoped YBa$_2$Cu$_3$O$_{7-\delta}$ [7]. A very unusual $H_{c2}(T)$ curve is observed, with very strong positive curvature and no evidence of saturation at low temperatures. This behaviour contrasts strongly with the weak coupling BCS result [8] which predicts an approximately parabolic shape for the $H_{c2}$ curve.

Recently, Abrikosov has proposed [9] that these anomalous $H_{c2}$ curves reflect a dimensional crossover to quasi-one dimensional superconductivity due to the presence of flat regions in the energy dispersion, that is, extended saddle points. In Abrikosov’s approach, the two extended saddle points in the energy dispersion are replaced by two one-dimensional linear energy dispersions $\epsilon_1(q_x) = v_1 \cdot q_x$ and $\epsilon_2(q_y) = v_2 \cdot q_y$. This model is equivalent to a system of two transverse chains and in this case, the density of states loses completely its strong energy dependence. Furthermore, it is not surprising that he finds a dimensional crossover in $H_{c2}$. In this paper, we argue that these curves reflect not a dimensional crossover, but the strong energy dependence of the density of states which results from the presence of these extended saddle points. In the following, we present a study of the superconducting pairing susceptibility for an isotropic two-dimensional system with a strong power-law divergence in the density of states. As shown by Gorkov [4], this two-particle correlation function determines the shape of the superconducting transition $H_{c2}(T)$ of a type-II superconductor.

The superconducting transition is characterized by the vanishing of the gap function $\Delta(r,r')$, defined as

$$\Delta(r,r') = V(r-r') \langle \psi(r) \psi(r') \rangle.$$  

In the particular case of a local pairing interaction, $V(r-r') = g \delta(r - r')$, we obtain as usual the s-wave gap function, $\Delta(r,r') = \Delta(r) \delta(r - r')$. In the following, $\hbar = c = \epsilon = k_B = 1$.

In the vicinity of the superconducting transition curve, the gap parameter is small and a perturbation expansion in powers of $\Delta$ leads to the semi-classical linearized gap equation [10]

$$\Delta(r) = g \int dr' K_\beta(r-r') e^{i2A(r') \cdot (r-r')} \Delta(r').$$  

(1)

where $K_\beta(r)$ is the fermion pair propagator in real space for a given temperature $T = 1/\beta$, in the absence of the external field and the pairing interaction $g$ and is defined as

$$K_\beta(r',r) = \frac{1}{\beta} \sum_\omega G_{-\omega}(r',r) G_\omega(r',r).$$  

(2)

where the Matsubara Green’s function $G_\omega$ describes the normal state in the absence of magnetic field. Using Kramers-Kronig relations, $K_\beta(r)$ can be rewritten as

$$K_\beta(r) = \frac{2}{\pi} \int d\omega \tanh(\beta \omega/2) A(r,\omega) B(r,-\omega),$$  

(3)

with $A(k,\omega) = \text{Im} G_R(k,\omega)$ and $B(k,\omega) = \text{Re} G_R(k,\omega)$ where $G_R(k,\omega)$ is the retarded Green’s function in the absence of magnetic field and pairing potential. $A(r,\omega)$ and $B(r,\omega)$ are the respective Fourier transforms. A non-local $V(r-r')$ may lead to a d-wave gap solution and a slightly modified gap equation. One can show that the upper critical field probes the behaviour of the Cooper pair center of mass and the internal symmetry of the gap function is irrelevant as long as the thermal and magnetic lengths are much larger than the interaction range.

In a bidimensional system, a van-Hove singularity (VHS) in the density of states results usually from the presence of a saddle point in the energy dispersion $\epsilon(k)$. In the case of an extended saddle point, $\epsilon(q) \sim q_x^2 - q_y^2$, where $q = k - k_{ch}$, this leads to a power-law divergence in the density of states $N(\epsilon) \sim \epsilon^{-1+\frac{\beta}{2}}$. Such form for the extended saddle point is not only indicated by the
direct probing of the energy dispersion using the angle resolved photoemission technique, but also by numerical work on the Hubbard model. For instance, Quantum Monte Carlo work by Imada and collaborators in the Hubbard model has found an extended saddle point with a quartic $q_y$ dependence at $(0, \pi)$. The effect of such a divergence on the pairing susceptibility and the superconducting phase diagram is the subject of this paper. Clearly, a system with a saddle point is not isotropic. However, in order to simplify the problem, we adopt the isotropic dispersion relation:

$$\epsilon(k) - \epsilon_{ch} = a \cdot \text{sign}(q) |q|^b$$

where $q = k - k_{ch}$. The influence of anisotropy in the semi-classical upper critical field is well studied. Anisotropic two-dimensional systems have typically open warped Fermi surfaces or elliptical closed Fermi surfaces in small particle number. For a system with an elliptical Fermi surface, in the case of a transverse magnetic field, it is simple to show that the normalized upper critical field follows the parabolic-like BCS curve. For an open warped Fermi surface, the behavior of the $H_{c2}$ curve is determined by the relation between $T_{c2}$ and the small $t_y$ modulation of the Fermi surface. If $t_y \ll T_{c2}$, $H_{c2}$ will diverge at a finite temperature, reflecting a reduction of the effective dimension of our system induced by the magnetic field. However, if $t_y \gg T_{c2}$, a BCS-like parabolic $H_{c2}$ curve is obtained. A reduction of $t_y$ enhances the zero temperature critical field, $H_{c0}$ relatively to the zero field critical temperature, $T_{c0}$, but, as long as the relation is valid, the reduced upper critical field ($H_{c2}/H_{c0}$ as a function of $T/T_{c0}$) remains unchanged. One may therefore conclude that, unless a dimensional crossover is present, the reduced upper critical field shows very little sensitivity to anisotropy. Another important point is that the contribution to superconductivity of the extended saddle-point region is much larger than the contribution of the other regions of the Fermi surface, which can therefore be neglected. These facts motivate the choice of an isotropic model for our study.

Note that, for quasi-2D systems and magnetic field applied along the planes, the dimensional crossover is from 3D to 2D. In the case of transverse fields, the crossover is from quasi-2D to quasi-1D superconductivity. One should note, however, the $H_{c2}$ divergence results from a mean-field analysis and fluctuations modify this behavior greatly in the last case. In fact, saturation should arise at low temperatures due to fluctuations, reflecting the well known impossibility of a superconducting state in one dimension. Furthermore, as recently shown by Lebed et al, saturation should also be observed due to Pauli pair breaking. Therefore, it seems unlikely that a dimensional crossover could explain results obtained by Mackenzie and others.

We assume that the VHS is pinned at the Fermi level, that is, $k_F = k_{ch}$. We will comment on the pinning assumption at the end of the paper. The density of states for the above model is $N(\epsilon) \sim a^{-1/b}b^{-1}(\epsilon - \epsilon_{ch})^{1/b-1}$. Let us assume for now that $b$ is an odd integer.

For this simple model, we can compute the spectral function

$$A(r, \omega) = -\frac{1}{2ab} \left\{ \frac{|\omega|}{a} \right\}^{1/b-1} \cdot \sqrt{\frac{2k_F}{\pi r}} \cos \left[ r \left( \frac{|\omega|}{a} \right)^{1/b} \text{sign}(\omega) + k_f \right] - \frac{\pi}{4}$$

and the retarded Greens function $G^R(r, \omega)$, since $G^R(q, \omega)$ is a meromorphic function in the complex $q$-plane. Note that $A(r, \omega) = \Im G^R(r, \omega)$ and $B(r, \omega) = \Re G^R(r, \omega)$. After some lengthy but straightforward algebra, one obtains the following expression for the pair propagator,

$$K_{\beta}(r) = r^{b-3} F \left[ \left( \frac{\beta a}{2} \right)^{b-1}/r \right]$$

with

$$F[X] = \frac{2k_F}{\pi^2} \frac{1}{ab} \int_0^\infty d\omega \frac{\tanh(\omega X)}{\omega^{b-1}} \left\{ \frac{1}{2} \sin(2\omega) + \sum_{n=1}^{b-1} e^{-\omega \sin(\frac{2\pi}{b} n)} \sin \left[ w(1 + \cos(\frac{2\pi}{b} n)) + \frac{2\pi}{b} n \right] \right\}.$$  

When $X \gg 1$, $F[X] \sim X^{b-2}$ and for $X \ll 1$, the function is exponentially small. Note that the thermal length is given by $\xi_T \sim (a/T)^{1/b}$. The pair propagator for distances smaller that the thermal length is approximately given by $K_T(r) \sim r^{-1}T^{1-1/b}$ and therefore, as the temperature goes to zero.  We will show that this will lead to a zero temperature divergence in the upper critical field. Note that no Debye-like frequency cutoff was introduced in the previous integral. This procedure is valid as long as the temperature provides a smaller cutoff in the integrand, that is, $T^{1/b} \ll \omega_c$. This reflects the well known reduction of the isotope effect in the van-Hove scenario.

The zero field critical temperature is obtained from the equation

$$1/g = \frac{k_F}{\pi} \frac{1}{a^{1/b}} \int_0^\infty d\omega \tanh(\beta \omega/2)\omega^{1-2}$$

which leads to

$$T_{c0} \sim \frac{k_F}{\pi} \frac{a^{1/b}}{b - 1} \left[ \frac{1}{g} \right]^{b/(b-1)}$$

This result and the role of the frequency cutoff can be qualitatively understood using the usual BCS relation for the critical temperature $T_{c0} \sim \omega_c e^{-1/(\pi\epsilon_{c0}^2)}$, but also by numerical work on the Hubbard model.
where \( N(\epsilon)T_c \) is the thermal averaged density of states \( N(\epsilon)T \sim \int d\epsilon (\partial f/\partial \epsilon)N(\epsilon) \) and \( f \) is the Fermi distribution function. In this case, \( (N(\epsilon))T_c \sim a^{-1}b^{-1}T_c^{\beta-1} \) and therefore ln(\( \omega_c/T_c \))\( T_c^{\beta-1} \sim 1/g \). In the weak coupling limit, one can neglect the logarithmic correction and thus, the above dependence for the critical temperature is reproduced. In the usual case of an extended saddle point, this broadening argument leads correctly to a transition temperature \[ T_{co} \propto g^2. \] The enhancement of the critical temperature is clearly bounded by the equivalent of the Debye Temperature in this problem, that is, \( T_{lim} \sim \omega_D \), where \( \omega_D \) is our cutoff in frequency. The energy dispersion as given by Eq. (4) may also be limited to an energy range \( \omega_c < \omega_D \) and in that case \( T_{lim} \sim \omega_D e^{-1/(N(\epsilon))}\sim g \). This dependence on the extent of the anomalous energy dispersion could offer an explanation for the low critical temperatures of, for example, Bi2201 and Sr2RuO4. \[ \] Photoemission experiments in these materials have found a VHS near the Fermi level, but also a smaller extent of the flat regions in the energy dispersion. A similar thermal broadening argument can be applied to the zero temperature slope of the \( H_{c2} \) curve.

The analytical determination of the upper critical curve for the complete temperature range is a difficult task. So, we obtain the \( H_{c2} \) curves by numerical solution of the gap equation and study its behavior analytically only at low temperatures or close to \( T_c \). For numerical purposes, it is more convenient to work with the gap function in a mixed representation. If one chooses the Landau gauge \( A = (0,Hx,0) \) and makes use of the degeneracy of the gap function, one can rewrite Eq. (9) as

\[ \Delta(x) = g \int dx' \bar{K}_\beta(x') - x, -H(x + x')|\Delta(x'), \]  

where \( \Delta(x) \) is the \( y \) integrated gap function and \( \bar{K}_\beta(x,y) \) is the Fourier transform of \( K_\beta(x,y) \). At zero temperature, the gap equation simplifies to

\[ \Delta(r) \sim g \int dr' r^{1 - \frac{4}{b}} e^{i\phi(\sqrt{x^2 + y^2})} \Delta(r'). \]  

where \( \phi \) is the magnetic phase acquired by the Cooper pair, which is independent of the magnetic field if \( r \) is written in magnetic length units. Note that this form for the gap equation is independent of our gauge choice. The numerical gap solutions show a perfect scaling \( \Delta(x) = F(x/\sqrt{H}) \), that is, all gap solutions fall into an universal Gaussian curve (see Fig. 2), if the x-axis unit is the magnetic length and therefore, with the variable change \( x = x/\sqrt{H} \) in the previous equation, the gap function becomes independent of \( H \) and we obtain the low temperature scaling of the upper critical field, \( H_{c2}(T) \sim T^{-2\beta/3} \).

In Fig. 3 \( H_{c2} \) curves for several values of \( b \), obtained numerically from Eq. (10) are displayed. These curves are characterized by a strong divergence of the upper critical field as \( T \to 0 \) and linear behavior close to \( T_{co} \). In the inset, the low temperature scaling is clearly observed in a log-log scale. This behavior is clearly distinct from a dimensional crossover in \( H_{c2} \) which would lead to a divergence even in a log-log scale.

While Eq. (10) for the pair propagator was derived for odd integer \( b \), we believe this equation is qualitatively correct for any value of \( b \geq 1 \). Clearly, Eq. (10) for the spectral function is valid for any \( b \) and one can show that the pair propagator for \( b > 1 \) will have the same qualitative short and long range behavior as that given by Eq. (11). For \( b = 1 \), with the introduction of a cutoff, we recover the usual BCS results and, in particular, \( H_{co} \sim T_{co}^{1/2} \). For \( 1 \leq b < 2 \), \( F[X] \sim \text{const} \) if \( X \ll 1 \) and therefore, the pair propagator shows a different short range dependence, \( K_T(r) \sim r^{-b-3} \). The pair propagator does not diverge as we decrease the temperature, and with a scaling argument, we can show that now the zero temperature critical field is finite, \( 1/g \sim H_{co}^{(1-b)/2} \) and thus, \( H_{co} \sim T_{co}^{2/b} \).

The low temperature dependence of \( H_{c2} \) can be obtained expanding the pair propagator in powers of \( T \),

\[ [K_T(r) - K_0(r)]/r^{b-3} \sim -rT^{1/b} \]

and following Gorkov, one obtains \( H_{c2}(T) - H_{c2}(0) \sim -T^{2c/b} \). Curiously, a power-law low temperature dependence of \( H_{c2} \) has also been suggested by Kotliar and Varma as a consequence of a zero temperature critical point. This dependence, in our picture, results from the scaling form of the pair propagator as given by Eq. (11), but the value of \( c \) depends on the specific form of the integrand of Eq. (11). One knows that when \( b \to 1 \), the usual expression for the pair propagator should be recovered, which is the one given by Eqs. (9) and (10) only with the...
sine function in the integrand. For $b > 2$, the exponential term in Eq. 7 dominates and the sine contribution becomes irrelevant. Therefore, when $b \to 1$, the low temperature behavior should be determined by the sine term and as $b$ goes away from 1, the exponential term should take over. With this assumption, $c$ can be determined and the result is $c = (2 - b)/2$, when $b \sim 2$ and $c = (3 - b)/2$, when $b \to 1$.

The results obtained up to now can be collected into a equation similar to the usual one, \[ 1/g = \int dr K_B(r)e^{-r^2H} \] with a qualitative pair susceptibility given by

\[ K_T(r) = \frac{1}{r^{3-b}} \frac{(rT^{1/b})^c}{\sinh (rT^{1/b})^d} \]  

with $c = 0$ and $d = b - 2$, if $b > 2$. If $1 \leq b < 2$, $c = d$ with $c$ having the behavior described above in order to reproduce the low temperature dependence of the upper critical field. In particular, $c = 1$, if $b = 1$ and the usual BCS equation is recovered. If $b \to 2$, $c \to 0$. In Fig. 2, $H_{c2}$ curves obtained with this qualitative kernel are displayed. A drastic transformation from conventional parabolic-like curves (obtained with $c = (3 - b)/2$) to curves with strong positive curvature (obtained with $c = (2 - b)/2$) is observed as the low temperature exponent $2c/b$ goes from 2 to 0.

In Fig. 2, the experimental $H_{c2}$ points obtained by Mackenzie et al for $\text{Tl}_2\text{Ba}_2\text{CuO}_6+\delta$ are also displayed and fitted with our qualitative $H_{c2}$ curves. Note that this is a one-parameter fit ($c = (2 - b)/2$), since the normalized curves do not depend on the coupling constant $g$. An impressive agreement is observed for $2c/b = .45$, which according to the picture presented in this paper, implies that the density of states diverges as $N(\epsilon) \sim \epsilon^{-28}$. Most photoemission experiments have found saddle points with quadratic dispersion along one direction and much flatter (higher power dependence) behavior along the other (transversal) direction, indicating therefore a divergence exponent $\alpha$ smaller than $1/2$. In the case of saddle point obtained in [17], a good fit is obtained with a quartic dependence, leading to $\alpha \approx 0.25$ which agrees reasonably with the value extracted from the experimental $H_{c2}$ curve. We emphasize that for a given exponent $\alpha$, the normalized $H_{c2}$ curve is as universal as the usual BCS curve ($\alpha = 0$). A suggestion of some sort of universality is indeed observed in Fig. 4 of Ref. [6], where $H_{c2}$ curves of two different materials, $\text{YBa}_2(\text{Cu}_{0.97}\text{Zn}_{0.03})_3\text{O}_7 - \delta$ and $\text{Tl}_2\text{Ba}_2\text{CuO}_{6+\delta}$, apparently fall onto the same curve in a plot of reduced $H_{c2}(T)$ versus reduced temperature. Such universal $H_{c2}$ behavior is not observed in the case of a simple saddle point which leads to a weak logarithmic divergence in the density of states. In this case, $H_{c2}$ depends on the coupling constant $g$ and shows upward curvature which becomes stronger as $g$ is decreased. Note that $H_{co}$ and $T_{co}$ have a weaker enhancement in this case, with log squared relations to the inverse of the coupling constant $g$, while for the extended singularity power-law relations have been obtained.

It has been assumed throughout the paper that the VHS was pinned at the Fermi level. It has been shown in Ref. [14] that a deviation from the Fermi level of the VHS leads to $H_{c2}$ saturation at low temperature, the temperature range of this region being proportional to the energy difference, $k_B T_{cross} \sim E_F - E_{vh}$. However, this has not been observed in the experimental $H_{c2}$ curves, even though the respective samples are in the overdoped or underdoped regime. According to the van-Hove scenario, one should expect a certain deviation of the VHS from the
Fermi level in these regimes in order to account for the decrease of the zero field critical temperature. However, it is possible that, (at least, in some interval of doping range) the reduction of critical temperature results not from the deviation of the VHS from the Fermi level, but, instead, from the weakening of the VHS due to a reduction of the extent of the saddle point as suggested by King et al. [18]. Photoemission experiments on YBa$_2$Cu$_3$O$_{6.9}$, YBa$_2$Cu$_3$O$_{6.5}$, and YBa$_2$Cu$_3$O$_{6.3}$ support this picture, since they report a clear doping independence of the pinning of the Fermi level at the VHS. Moreover, this doping independence of the pinning is predicted by many numerical studies, from slave-boson calculations [24,25] to renormalization group calculations [26].

In conclusion, we have studied the effect of a power-law divergence of the density of states at the Fermi level $N(\epsilon) \sim \epsilon^{-\alpha}$ on the upper critical field of a clean isotropic weak-coupling superconductor. We have shown that for a weak divergence ($\alpha$ less than 1/2), the zero temperature critical field is finite, but strong positive curvature appears in $H_{c2}$ as $\alpha$ approaches 1/2. For a stronger divergence ($\alpha$ larger than 1/2), $H_{c2}(T)$ has a power-law divergence at $T = 0$. A very good one-parameter fit was obtained to the experimental results by Mackenzie et al [4]. According to the picture described in this paper, the anomalous $H_{c2}$ behavior reflects the short-range enhancement of the pair propagator and the unusual temperature dependence of the thermal length which result from the existence of a strong divergence of the density of states at the Fermi level.

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[1] K. Gofron, J. C. Campuzano, A. A. Abrikosov, M. Lindroos, A. Bansil, H. Ding, D. Koelling, and D. Dabrowski, Phys. Rev. Lett. 73, 3302 (1994).
[2] J. Labbe and J. Bok, Europhys. Lett. 3,1225 (1987).
[3] J. Friedel, J. Phys. Condens. Matter 1, 7757 (1989).
[4] A. P. Mackenzie et al, Phys. Rev. Lett. 71, 1238 (1993).
[5] M. S. Osofsky et al, Phys. Rev. Lett. 71, 2315, (1993).
[6] D. J. C. Walker et al, Phys. Rev. B 51, 9375 (1993).
[7] L. P. Gorkov, JETP 10, 503 (1960).
[8] A. A. Abrikosov, Phys. Rev. B 56, 5112 (1997)
[9] A. A. Abrikosov, L. P. Gorkov, and I. E. Dzyaloshinskii, Methods of Quantum Field Theory in Statistical Physics, p.323, Dover (1963).
[10] M. Imada, Rev. Mod. Phys. 40, 1039 (1998).
[11] R. A. Klemm, M. R. Beasley, and A. Luther, J. Low Temp. Phys. 16, 607 (1974); R. A. Klemm, A. Luther and M. R. Beasley, Phys. Rev. B 12, 877 (1975).
[12] A. G. Lebed and K. Yamaji, Phys. Rev. Lett. 80, 2697 (1998).
[13] R. G. Dias, Ph. D. Thesis, University of Cambridge, UK (1996).
[14] R. G. Dias and J. W. Wheatley, Solid State Comm. 98, 859 (1996).
[15] C. C. Tsuei, D. M. Newns, C. C. Chi, and P. C. Pattnaik, Phys. Rev. Lett. 65, 2724, (1990).
[16] J. Labbe, S. Barisic, and J. Friedel, Phys. Rev. Lett. 19, 1039 (1967).
[17] A. A. Abrikosov, J. C. Campuzano, and K. Gofron, Physica C 214, 73 (1993).
[18] D. M. King, Z.-X. Shen, D. S. Dessau, D. S. Marshall, C.-H. Park, W. E. Spicer, J. L. Peng, Z. Y. Li, and R. L. Greene, Phys. Rev. Lett. 73, 3298 (1994).
[19] D. H. Lu, M. Schmidt, T. R. Cummins, and S. Schupperl, Phys. Rev. Lett. 76, 4845 (1996).
[20] G. Kotliar and C. M. Varma, Phys. Rev. Lett. 77, 2296 (1996).
[21] R. G. Dias and J. W. Wheatley, Phys. Rev. B 50, 13887 (1994).
[22] J. C. Campuzano, K. Gofron, H. Ding, R. Liu, B. Dabrowski, and B. J. W. Veal, J. Low T. Physics 95, 245 (1994).
[23] R. Liu, B. W. Veal, C. Gu, A. P. Paulikas, P. Kostic, and C. G. Olson, Phys. Rev. B 52, 553 (1995).
[24] R. S. Markiewicz, J. Phys. Cond Matt. 2, 665 (1990).
[25] D. M. Newns, P. C. Pattnaik, and C. C. Tsuei, Phys. Rev. B 43, 3075 (1991).
[26] J. González, F. Guinea, and M. A. H. Vozmediano, Europhys. Letts. 34, 711 (1996).