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2000 J. Phys.: Condens. Matter 12 9053

(http://iopscience.iop.org/0953-8984/12/42/310)

J. Phys.: Condens. Matter **12** (2000) 9053–9060. Printed in the UK PII: S0953-8984(00)13880-9

Effects of Van Hove singularities on the upper critical field

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Received 11 May 2000, in final form 22 August 2000

Abstract. 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 $N(\epsilon) \sim \epsilon^{-1+1/b}$, $b > 1$. We show that the pair propagator has the scaling form $K_T(r) = r^{b-3}F(T^{1/b}r)$. An anomalous short-range behaviour is found, leading straightforwardly to positive curvature in the upper critical field, for $b \lesssim 2$, and to a zero-temperature divergence, $H_{c2} \sim T^{-2+4/b}$, for $b > 2$.

Photoemission experiments on copper oxide superconductors [1] 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, $N(\epsilon) \sim (\epsilon - \epsilon_{vh})^{-\alpha}$, for energies close to ϵ_{vh}. Some authors have claimed that the high superconducting critical temperatures of the cuprates could be explained by taking this divergence into account [2, 3].

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 $Tl_2Ba_2CuO_{6+\delta}$ [4] and $Bi_2Sr_2CuO_y$ [5] and underdoped $YBa_2Cu_3O_{7-\delta}$ [6]. A very unusual curve for $H_{c2}(T)$ 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 [7] which predicts an approximately parabolic shape for the H_{c2}-curve.

Recently, Abrikosov has proposed [8] 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 $\epsilon_1(q_x) = v_1 q_x$ and $\epsilon_2(q_y) = v_2 q_y$. This model is equivalent to a system of two transverse chains and, in this case, the density of states completely loses 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 [7], 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 $\Delta(\boldsymbol{r}, \boldsymbol{r}')$, defined as $\Delta(\boldsymbol{r}, \boldsymbol{r}') = V(\boldsymbol{r} - \boldsymbol{r}')\langle\psi_\downarrow(\boldsymbol{r})\psi_\uparrow(\boldsymbol{r}')\rangle$. In the particular case of a local pairing interaction, $V(\boldsymbol{r} - \boldsymbol{r}') = g\delta(\boldsymbol{r} - \boldsymbol{r}')$, we obtain as usual the s-wave gap function, $\Delta(\boldsymbol{r}, \boldsymbol{r}') = \Delta(\boldsymbol{r})\delta(\boldsymbol{r} - \boldsymbol{r}')$. In the following, $\hbar = c = e = k_B = 1$. In the vicinity of the

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superconducting transition curve, the gap parameter is small and a perturbation expansion in powers of Δ leads to the semi-classical linearized gap equation [7, 9]

$$\Delta(\boldsymbol{r}) = g \int \mathrm{d}\boldsymbol{r}' \; K_\beta(\boldsymbol{r}' - \boldsymbol{r}) \mathrm{e}^{\mathrm{i}\,2\boldsymbol{A}(\boldsymbol{r})\cdot(\boldsymbol{r}'-\boldsymbol{r})} \Delta(\boldsymbol{r}') \tag{1}$$

where $K_\beta(\boldsymbol{r})$ 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

$$K_\beta(\boldsymbol{r}', \boldsymbol{r}) = \frac{1}{\beta} \sum_\omega \mathcal{G}_{-\omega}(\boldsymbol{r}', \boldsymbol{r}) \mathcal{G}_\omega(\boldsymbol{r}', \boldsymbol{r}) \tag{2}$$

where the Matsubara Green's function $\mathcal{G}_\omega$ describes the normal state in the absence of a magnetic field. Using Kramers–Kronig relations, $K_\beta(\boldsymbol{r})$ can be rewritten as

$$K_\beta(\boldsymbol{r}) = \frac{2}{\pi} \int \mathrm{d}\omega \, \tanh(\beta\omega/2) A(\boldsymbol{r}, \omega) B(\boldsymbol{r}, -\omega) \tag{3}$$

with $A(\boldsymbol{k}, \omega) = \operatorname{Im} G^R(\boldsymbol{k}, \omega)$ and $B(\boldsymbol{k}, \omega) = \operatorname{Re} G^R(\boldsymbol{k}, \omega)$ where $G^R(\boldsymbol{k}, \omega)$ is the retarded Green's function in the absence of a magnetic field and pairing potential. $A(\boldsymbol{r}, \omega)$ and $B(\boldsymbol{r}, \omega)$ are the respective Fourier transforms. A non-local $V(\boldsymbol{r} - \boldsymbol{r}')$ 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 centre 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 $\epsilon(\boldsymbol{k})$. In the case of an extended saddle point, $\epsilon(\boldsymbol{q}) \sim q_x^n - q_y^m$, where $\boldsymbol{q} = \boldsymbol{k} - \boldsymbol{k}_{vh}$, this leads to a power-law divergence in the density of states $N(\epsilon) \sim \epsilon^{-1+1/n+1/m}$. Such a form for the extended saddle point is not only indicated by the direct probing of the energy dispersion using the angle-resolved photoemission technique [1], but also by numerical work on the Hubbard model. For instance, quantum Monte Carlo work by Imada and collaboraters [10] on 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:

$$\epsilon(\boldsymbol{k}) - \epsilon_{vh} = a \operatorname{sgn}(q) |q|^b \tag{4}$$

where $q = k - k_{vh}$. The influence of anisotropy in the semi-classical upper critical field is well studied [11, 12]. Anisotropic two-dimensional systems have typically open warped Fermi surfaces or elliptical closed Fermi surfaces in the case of 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 [13]. For an open warped Fermi surface, the behaviour of the H_{c2}-curve is determined by the relation between T_{c0} and the small t_y-modulation of the Fermi surface [12, 13]. If $t_y \ll T_{c0}$, H_{c2} will diverge at a finite temperature, reflecting a reduction of the effective dimension of our system induced by the magnetic field [11, 12]. However, if $t_y \gg T_{c0}$, 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 fields 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, that the H_{c2}-divergence results from a mean-field analysis and fluctuations modify this behaviour 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 and Yamaji [12], 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 [4, 5].

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

For this simple model, we can compute the spectral function

$$A(r,\omega) = -\frac{1}{2ab}\left(\frac{|\omega|}{a}\right)^{1/b-1}\sqrt{\frac{2k_F}{\pi r}}\cos\left[r\left(\left(\frac{|\omega|}{a}\right)^{1/b}\operatorname{sgn}(\omega) + k_f\right) - \frac{\pi}{4}\right] \tag{5}$$

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

$$K_\beta(r) = r^{b-3} F\left[\left(\frac{\beta a}{2}\right)^{1/b} \Big/ r\right] \tag{6}$$

with

$$F[X] = \frac{2k_F}{\pi^2}\frac{1}{ab}\int_0^\infty \mathrm{d}\omega\, \frac{\tanh[(\omega X)^b]}{\omega^{b-1}}\left\{\frac{1}{2}\sin(2\omega) + \sum_{n=1}^{(b-1)/2} \mathrm{e}^{-\omega\sin([2\pi/b]n)} \sin\left[w\left(1+\cos\left(\frac{2\pi}{b}n\right)\right) + \frac{2\pi}{b}n\right]\right\}. \tag{7}$$

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 $K_T(r) \sim r^{-1} T^{-1+2/b}$ and, therefore, it diverges 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 cut-off was introduced in the previous integral. This procedure is valid as long as the temperature provides a smaller cut-off 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 [15].

The zero-field critical temperature is obtained from the equation

$$1/g = \frac{k_F}{\pi}\frac{1}{a^{1/b} b}\int_0^\infty \mathrm{d}\omega\, \tanh(\beta\omega/2)\omega^{1/b-2} \tag{8}$$

which leads to

$$T_{c0} \sim \left[\frac{k_F}{\pi}\frac{a^{-1/b}}{b-1} g\right]^{b/(b-1)}. \tag{9}$$

This result and the role of the frequency cut-off can be qualitatively understood using the usual BCS relation for the critical temperature $T_{c0} \sim \omega_c \mathrm{e}^{-1/\langle N(\epsilon)\rangle_{T_{c0}} g}$, where $\langle N(\epsilon)\rangle_{T_{c0}}$ is the thermally averaged density of states

$$\langle N(\epsilon)\rangle_T \sim \int \mathrm{d}\epsilon\ (\partial f/\partial\epsilon) N(\epsilon)$$

and f is the Fermi distribution function. In this case, $\langle N(\epsilon)\rangle_{T_{c0}} \sim a^{-1/b} b^{-1} T_{c0}^{1/b-1}$ and therefore $\ln(\omega_c/T_{c0}) T_{c0}^{1/b-1} \sim 1/g$. 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 [16, 17] $T_{c0} \propto g^2$. The enhancement of the critical temperature is clearly bounded by the equivalent of the Debye temperature in this problem—that is, $T_{\mathrm{lim}} \sim \omega_D$, where ω_D is our cut-off in frequency. The energy dispersion as given by equation (4) may also be limited to an energy range $\omega_c < \omega_D$ and in that case $T_{\mathrm{lim}} \sim \omega_D \mathrm{e}^{-1/\langle N(\epsilon)\rangle_{\omega_c} g}$. This dependence on the extent of the anomalous energy dispersion could offer an explanation for the low critical temperatures of, for example, Bi2201 [18] and Sr_2RuO_4 [19]. Photoemission experiments on these materials [18, 19] 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 behaviour 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 $\boldsymbol{A} = (0, Hx, 0)$ and makes use of the degeneracy of the gap function, one can rewrite equation (1) as

$$\widetilde{\Delta}(x) = g \int \mathrm{d}x'\ \widetilde{K}_\beta[x' - x, -H(x + x')]\widetilde{\Delta}(x') \tag{10}$$

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

$$\Delta(\boldsymbol{r}) \sim g \int \mathrm{d}\boldsymbol{r}'\ \frac{T^{1-2/b}}{|r' - r|} \mathrm{e}^{\mathrm{i}\phi(r'/\sqrt{H}, r/\sqrt{H})} \Delta(\boldsymbol{r}') \tag{11}$$

where ϕ 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 $\widetilde{\Delta}(x) = F(x/\sqrt{H})$—that is, all gap solutions fall onto a universal Gaussian curve (see figure 2), if the x-axis unit is the magnetic length and, therefore, with the variable change $\widetilde{x} = x/\sqrt{H}$ in the previous equation, the gap function becomes independent of H and we obtain the low-temperature scaling of the upper critical field, $H_{c2}(T) \sim T^{-2+4/b}$.

In figure 1, H_{c2}-curves for several values of b, obtained numerically from equation (10), are displayed. These curves are characterized by a strong divergence of the upper critical field as $T \to 0$ and linear behaviour close to T_{c0}. In the inset, the low-temperature scaling is clearly observed on a log–log scale. This behaviour is clearly distinct from a dimensional crossover in H_{c2} which would lead to a divergence even on a log–log scale.

While equation (6) for the pair propagator was derived for odd integer b, we believe that this equation is qualitatively correct for any value of $b \geqslant 1$. Clearly, equation (5) 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 behaviour as that given by equation (6). For $b = 1$, with the introduction of a cut-off, we recover the usual BCS results and, in particular, $H_{c0} \sim T_{c0}^2$. For $1 \leqslant b < 2$, $F[X] \sim$ constant if $X \ll 1$ and, therefore, the pair propagator shows a different short-range dependence, $K_T(r) \sim r^{b-3}$.

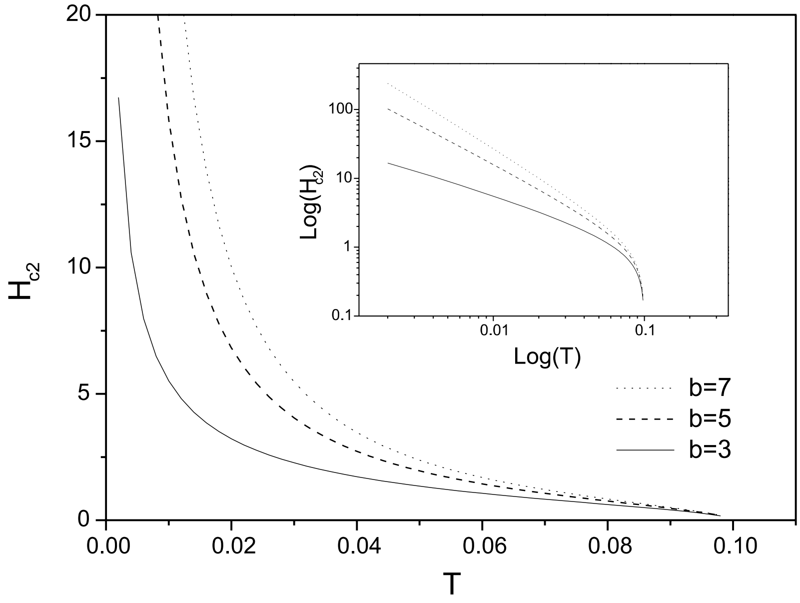

Figure 1. H_{c2}-curves for $b = 3$, 5 and 7, obtained numerically from equation (10). Inset: the same curves on a logarithmic scale, showing clearly the low-temperature power-law behaviour.

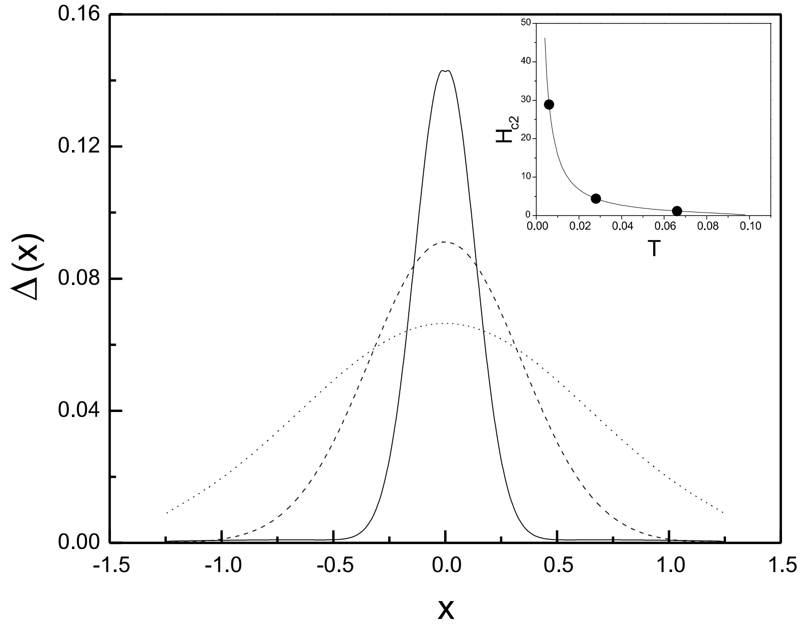

Figure 2. The numerically obtained gap solution at different points of the transition curve shown in the inset ($b = 5$). All solutions are Gaussian.

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, $1/g \sim H_{c0}^{(1-b)/2}$ and, thus, $H_{c0} \sim T_{c0}^{2/b}$.

The low-temperature dependence of H_{c2} can be obtained by expanding the pair propagator in powers of T:

$$[K_T(r) - K_0(r)]/r^{b-3} \sim -(rT^{1/b})^c \tag{12}$$

and, following Gorkov [7], 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 [20], 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 equation (6), but the value of c depends on the specific form of the integrand of equation (7). One knows that when $b \to 1$, the usual expression for the pair propagator should be recovered, which is the one given by equations (6) and (7) but with the sine function in the integrand [9, 21]. For $b > 2$, the exponential term in equation (7) dominates and the sine contribution becomes irrelevant. Therefore, when $b \to 1$, the low-temperature behaviour 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 [21]:

$$1/g = \int \mathrm{d}r\ K_\beta(r)\mathrm{e}^{-r^2 H}$$

with a qualitative pair susceptibility given by

$$K_T(r) = \frac{1}{r^{3-b}} \frac{(rT^{1/b})^c}{\sinh[(rT^{1/b})^d]} \tag{13}$$

with $c = 0$ and $d = b - 2$, if $b > 2$. If $1 \leqslant b < 2$, $c = d$ with c having the behaviour 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 [9, 21]. If $b \to 2$, $c \to 0$. In figure 3, 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 figure 3, the experimental H_{c2}-points obtained by Mackenzie *et al* for $Tl_2Ba_2CuO_{6+\delta}$ [4] 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 $2c/b = 0.45$, which, according to the picture presented in this paper, implies that the density of states diverges as $N(\epsilon) \sim \epsilon^{-0.28}$. Most photoemission experiments have found saddle points with quadratic dispersion along one direction and much flatter (higher-power dependence) behaviour along the other (transverse) direction, indicating therefore a divergence exponent α smaller than 1/2. In the case of the saddle point obtained in [17], a good fit is obtained with a quartic dependence, leading to $\alpha \approx 0.25$ which agrees reasonably well with the value extracted from the experimental H_{c2}-curve. We emphasize that for a given exponent α, the normalized H_{c2}-curve is as universal as the usual BCS curve [7] ($\alpha = 0$). A suggestion of some sort of universality is indeed observed in figure 4 of reference [6], where H_{c2}-curves for two different materials, $YBa_2(Cu_{0.97}Zn_{0.03})_3O_{7-\delta}$ and $Tl_2Ba_2CuO_{6+\delta}$, apparently fall onto the same curve in a plot of reduced $H_{c2}(T)$ versus reduced temperature. Such universal H_{c2}-behaviour is not observed in the case of a simple saddle point which leads to a weak logarithmic divergence in the density of states [14]. 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_{c0} and T_{c0} have a weaker enhancement in this case [14], with log-squared relations to the inverse of the coupling constant g, while, for the extended singularity, power-law relations have been obtained.

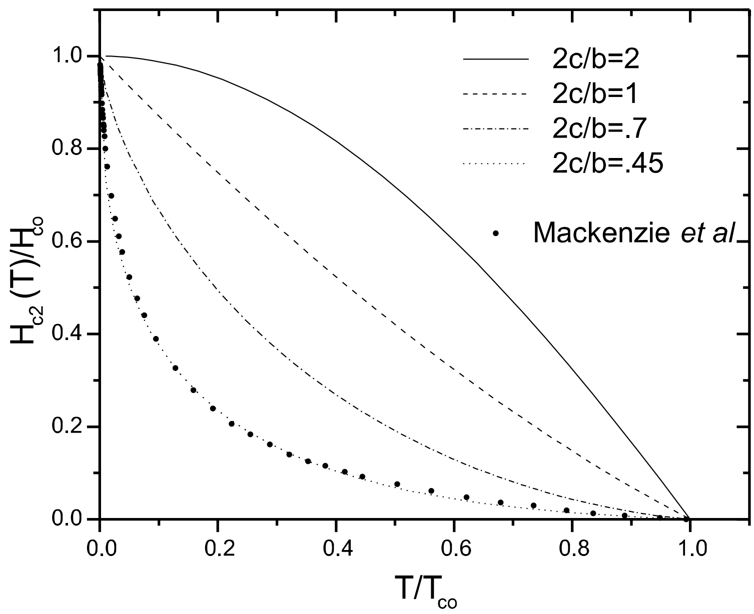

Figure 3. The qualitative normalized H_{c2}-curves for $1 < b < 2$. As the dispersion relation changes from linear to quadratic, the upper critical curve changes from the usual BCS curve to a curve with strong positive curvature.

It has been assumed throughout the paper that the VHS was pinned at the Fermi level. It has been shown in reference [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 [4, 6], 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 the doping range) the reduction of the 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 $YBa_2Cu_3O_{6.9}$ [22], $YBa_2Cu_3O_{6.5}$ and $YBa_2Cu_3O_{6.3}$ [23] 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 (α less than 1/2), the zero-temperature critical field is finite, but strong positive curvature appears in H_{c2} as α approaches 1/2. For a stronger divergence (α 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 given by Mackenzie *et al* [4]. According to the picture described in this paper, the anomalous H_{c2}-behaviour 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.

Acknowledgment

This research was funded by the Portuguese MCT PRAXIS XXI programme under Grant No 2/2.1/Fis/302/94.

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