Pauli limiting of the upper critical magnetic field

M. Schossmann and J. P. Carbotte
Physics Department, McMaster University, Hamilton, Ontario, Canada L8S 4M1
(Received 12 September 1988)

We consider the effect of Pauli limiting on the upper critical magnetic field H_{c2} of a strong-coupling superconductor with arbitrary concentration of impurities. In the extreme Pauli limit, H_{c2P} is independent of the impurities but does not correspond to the highest attainable value for H_{c2} except for the dirty BCS limit. In an appropriate approximation, our equations reduce correctly to the well-known Werthamer-Helfand-Hohenberg equations with an important difference that the band-splitting term is renormalized by a factor of $(1+\lambda)^{-1}$. This greatly reduces its effect. Strong-coupling corrections that go beyond this renormalization are also considered.

I. INTRODUCTION

Following the work of Helfand and Werthamer,[1] Werthamer-Helfand-Hohenberg[2] (WHH) have given equations for the second upper critical magnetic field H_{c2} valid for a Bardeen-Cooper-Schrieffer (BCS) superconductor with Pauli paramagnetism included. These equations were generalized by Schossmann and Schachinger[3] to include strong-coupling effects. Their equations are valid for an arbitrary impurity concentration while previous equations given by Rainer *et at*[4] applied only in the dirty limit. Generalizations of the work of Schossman and Schachinger[3] to account for spin fluctuations were given by Schossmann and Carbotte[5] and functional derivatives with and without Pauli limiting studied by Marsiglio *et al.*[6] and Schossmann *et al.*,[7] respectively.

In this work, we use the equations given by Schossmann and Schachinger[3] to prove that in the extreme Pauli limiting case, H_{c2P} (Clogston limit)[8] is independent of the impurities although it still depends on the microscopic parameters describing the superconducting state namely the electron-phonon spectral density $\alpha^2F(\Omega)$ and the Coulomb pseudopotential μ^*. In order to correlate with the WHH equations, we reduce our equations to a two-square well model for the electron-phonon interaction.[9] This produces the WHH equations but with a very important $(1+\lambda)^{-1}$ renormalization of the Pauli limiting term. Here λ is the electron-phonon mass renormalization which can be quite large. This renormalization, which seems to have been recognized first by Orlando and Beasley[10] without derivation, differs significantly from the previous suggestion[11] of $(1+\lambda)^{-1/2}$ which is based on an obvious generalization of the original free-energy argument given by Clogston.[8] While free-energy arguments can give a correct order magnitude estimate for the Pauli limiting field H_{c2P}, they do not give the correct numerical factors nor the correct electron-phonon mass renormalization coming from the normal-state channel in the Eliashberg equations.

The two-square well model is used to study the effect of Pauli limiting as the slope of H_{c2} at the critical temperature (T_c) is varied. We show that a single universal curve applies for the normalized value of $H_{c2}(0)/T_c(1+\lambda)$ at zero temperature $T=0$, as a function of the normalized slope

$$\left[\frac{dH_{c2}(T)}{dT}\right]_{T_c}\frac{1}{(1+\lambda)}\equiv\dot{H}^*_{c2} \ .$$

This applies to a given normalized impurity content $t^+/T_c(1+\lambda)$ which t^+ the impurity scattering matrix which is related to the transport scattering time τ_{tr} through the equation $t^+=1/(2\pi\tau_{tr})$. In the clean limit, it is found that the extreme paramagnetic field which corresponds to the case when the orbital contribution is negligible compared to band splitting, is not the highest value of H_{c2} that can be obtained. The maximum is found instead to occur around $\dot{H}_{c2}/T_c(1+\lambda)=10$ T/K and is 1.5 T/K for $H_{c2}(0)/T_c(1+\lambda)$ to be compared with $H_{c2,P}/T_c(1+\lambda)$ of 1.32 T/K.

The two-square well results are compared with results of full strong-coupling calculations in two specific cases chosen to illustrate the possible differences that can arise. Using a δ-function model for the electron-phonon spectral density $\alpha^2F(\Omega)$, we systematically examine the effect on H_{c2} of strong coupling corrections which go beyond $1+\lambda$ corrections. In particular, we study the variation of the maximum value of H_{c2} as a function of the position of the Einstein frequency (ω_E) in the spectral density.

In Sec. II, we prove that the extreme Pauli limiting field is independent of impurity concentration. Section III considers the two-square well model and exhibits the important renormalization of the Pauli contribution by a factor of $(1+\lambda)^{-1}$ which reduces its effect very significantly. Dirty and clean limits are considered in Sec. IV and universal curves established for $H_{c2}(0)/(1+\lambda)T_c$ plotted against normalized initial slope $\dot{H}_{c2}/T_c(1+\lambda)$. A comparison with full strong-coupling results is given. Further strong coupling results for a δ-function spectral density are found in Sec. V and conclusions given in Sec. VI.

II. EXTREME PAULI LIMITING

The strong-coupling equations for the upper critical magnetic field $H_{c2}(T)$ on the imaginary frequency axis derived by Schossmann and Schachinger[3] which apply for any impurity concentration are given by

$$\tilde{\Delta}_n=\pi T \sum_{m=-\infty}^{\infty} [\lambda(n-m)-\mu^*]\chi(\tilde{\omega}_m)\tilde{\Delta}_m + \pi t^+\chi(\tilde{\omega}_n)\tilde{\Delta}_n \;, \tag{1a}$$

$$\tilde{\omega}_n=\omega_n+\pi T \sum_{m=-\infty}^{\infty} \lambda(n-m)\mathrm{sgn}\omega_m+\pi t^+\mathrm{sgn}\omega_n \;, \tag{1b}$$

with μ^* the Coulomb pseudopotential, $\omega_n=\pi T(2n+1)$, $n=0,\pm1,\pm2,\ldots$, the Matsubara frequencies, $\tilde{\Delta}_n$ the complex pairing function, $\tilde{\omega}_n$ the renormalized Matsubara frequencies for the normal state and $t^+=1/(2\pi\tau_{\rm tr})$ with $\tau_{\rm tr}$ as the transport relaxation time. If $\alpha^2F(\Omega)$ denotes the electron-phonon spectral density we define

$$\lambda(n-m)=2\int_0^\infty d\Omega\frac{\Omega\alpha^2(\Omega)F(\Omega)}{\Omega^2+(\omega_n-\omega_m)^2} \;, \tag{2}$$

$$\chi(\tilde{\omega}_n)=\frac{2}{\sqrt{\alpha}}\int_0^\infty dq\, e^{-q^2}\tan^{-1}\left[\frac{q\sqrt{\alpha}}{|\tilde{\omega}_n|+i\mu_BH\,\mathrm{sgn}\tilde{\omega}_n}\right] , \tag{3}$$

where μ_B stands for Bohr's magneton and

$$\alpha=eHv_F^2/2 \tag{4}$$

with H the magnetic field at temperature T, e the electron charge, and v_F the Fermi velocity.

The functions $\chi(\tilde{\omega}_n)$ have the symmetry

$$\chi(\tilde{\omega}_n)=\chi^*(-\tilde{\omega}_n) \tag{5}$$

and a proper ansatz for $\tilde{\Delta}_n$ in (1a) is

$$\tilde{\Delta}_n=\tilde{\Delta}^*_{-n} \;. \tag{6}$$

Using the symmetries (5) and (6) formula (1a) can be rewritten

$$\begin{aligned}\tilde{\Delta}_n=\pi T &\sum_{m=0}^{\infty} [\lambda(n-m)+\lambda(n+m+1)-2\mu^*] \times \mathrm{Re}[\chi(\tilde{\omega}_m)\tilde{\Delta}_m] \\ &+ i\pi T\sum_{m=0}^{\infty}[\lambda(n-m)-\lambda(n+m+1)] \times \mathrm{Im}[\chi(\tilde{\omega}_m)\tilde{\Delta}_m]+\pi t^+\chi(\tilde{\omega}_n)\tilde{\Delta}_n \;.\end{aligned} \tag{7}$$

The usual way to solve (7) is to define

$$\bar{\Delta}_n=\tilde{\Delta}_n[1-\pi t^+\chi(\tilde{\omega}_n)] \tag{8}$$

which gives

$$\begin{aligned}\bar{\Delta}_n=\pi T &\sum_{m=0}^{\infty} [\lambda(n-m)+\lambda(n+m+1)-2\mu^*] \times \mathrm{Re}\left[\frac{\bar{\Delta}_m}{\chi^{-1}(\tilde{\omega}_m)-\pi t^+}\right] \\ &+ i\pi T\sum_{m=0}^{\infty}[\lambda(n-m)-\lambda(n+m+1)] \times \mathrm{Im}\left[\frac{\bar{\Delta}_m}{\chi^{-1}(\tilde{\omega}_m)-\pi t^+}\right] .\end{aligned} \tag{9}$$

In the sum of Eq. (1b) most of the terms cancel and we get

$$\tilde{\omega}_n=\omega_n+\left[\pi T\lambda(0)+2\pi T\sum_{m=1}^{n}\lambda(m)+\pi t^+\right]\mathrm{sgn}\omega_n \;. \tag{10}$$

In the case of extreme Pauli limiting the orbital effects become very small which can be simulated by setting $v_F=0$. In that case the function $\chi(\tilde{\omega}_n)$ can be approximated by

$$\chi(\tilde{\omega}_n)=1/(\tilde{\omega}_n+i\mu_BH) \tag{11}$$

and the eigenvalue equation (9) becomes

$$\begin{aligned}\bar{\Delta}_n=\pi T &\sum_{m=0}^{\infty} [\lambda(n-m)+\lambda(n+m+1)-2\mu^*] \times \mathrm{Re}\left[\frac{\bar{\Delta}_m}{\tilde{\omega}_m^0+i\mu_BH}\right] \\ &+ i\pi T\sum_{m=0}^{\infty}[\lambda(n-m)-\lambda(n+m+1)] \times \mathrm{Im}\left[\frac{\bar{\Delta}_m}{\tilde{\omega}_m^0+i\mu_BH}\right]\end{aligned} \tag{12}$$

with

$$\tilde{\omega}_n^0=\omega_n+\left[\pi T\lambda(0)+2\pi T\sum_{m=1}^{n}\lambda(m)\right]\mathrm{sgn}\omega_n \;. \tag{13}$$

As all impurity factors have dropped out of Eqs. (12) and (13), we can conclude that the extreme Pauli limit field $H_{c2,P}$ is independent of impurity concentration. Of course, it still depends on the electron-phonon spectral density $\alpha^2F(\omega)$ through the $\lambda(l)$ factors in Eqs. (12) and (13) and on the Coulomb pseudopotential μ^*. This is in contrast to a BCS theory for which a single universal value of H_{c2P} applies.

III. THE TWO-SQUARE WELL MODEL

In this section, we wish to reduce our Eqs. (9) and (10) in a BCS-like model so as to compare with the WHH equation.[2,8] This is accomplished by assuming that for all important Matsubara frequencies ω_n and ω_m, the electron-phonon factor $\lambda(n-m)$ can be taken to be constant equal to its $n=m$ value $[\lambda(0)\equiv\lambda]$. We, therefore, introduce, a two-square well model with cutoff at the Debye energy ω_D. This cutoff is necessary so as to get convergence. We take[9]

$$\lambda(n-m)=\lambda(0)\Theta(\omega_D-|\omega_n|)\Theta(\omega_D-|\omega_m|) \tag{14}$$

in Eqs. (9) and (10). The imaginary part of (9) vanishes and Δ_n becomes pure real.

Within the model (14) all $\bar{\Delta}_n$ up to the cutoff N_c are constant so that the equations are reduced to $[2N_c+1)\pi T=\omega_D]$

$$1=2\pi T\sum_{m=0}^{N_c}[\lambda(0)-\mu^*]\,\mathrm{Re}\{[\chi^{-1}(\tilde{\omega}_m)-\pi t^+]^{-1}\}\ , \tag{15a}$$

$$\tilde{\omega}_n=[1+\lambda(0)\omega_n+\pi t^+\ . \tag{15b}$$

We now introduce the normalized quantities

$$H^*=H/[(1+\lambda)T_c]\ , \tag{16a}$$

$$v_F^*=v_F/\sqrt{(1+\lambda)T_c}\ , \tag{16b}$$

$$(t^+)^*=t^+/[(1+\lambda)T_c]\ , \tag{16c}$$

and find the universal relation

$$\frac{1+\lambda}{\lambda-\mu^*}=2\pi t\sum_{m=0}^{N_c}\mathrm{Re}\{\bar{\chi}^{-1}(\tilde{\omega}_m)-\pi(t^+)^*]^{-1}\} \tag{17a}$$

with

$$\bar{\chi}(\tilde{\omega}_m)=\frac{2}{(\alpha^*)^{1/2}}\int dq\, e^{-q^2}\tan^{-1}\times\left[\frac{q(\alpha^*)^{1/2}}{(2m+1)\pi t+\pi(t^+)^*+i\mu_B H^*}\right]\ , \tag{17b}$$

where $\alpha^*=eH^*v_F^{*2}/2$, $t=T/T_c$. To complete this set of equations, we need to note that in this limit the critical temperature T_c is given by

$$\frac{1+\lambda}{\lambda-\mu^*}=\ln(1.13\omega_D/T_c)\ . \tag{18}$$

Equations (17) and (18) have the same structure as the equations derived by Werthamer *et al.*[2] (WHH theory) on the basis of BCS theory. They deal, however, in the renormalized quantities $\alpha^* v_f^* H^*(t^+)^*$ rather than with the corresponding unrenormalized quantities without the $1+\lambda$ factors. We note, in particular, the factor $(1+\lambda)^{-1}$ in the band-splitting term $i\mu_B H^*$ in Eq. (17b). This is the first rigorous derivation of such a factor, although we are aware that it was anticipated without proof in the work of Orlando and Beasley.[10] Since, in many superconductors $1+\lambda$ can be of order 2 or more, the Pauli term has a much smaller effect in our theory than it has in WHH. Thus, the artificially large value of spin-orbit scattering that is often postulated in order to reduce the effect of Pauli limiting when fitting experiment is due in part to an overestimate of band-splitting effects.

We note that, in contrast to our result, Orlando *et al.*[11] conclude from free-energy arguments that the paramagnetic field term $i\mu_B H$ in (17b) should be reduced instead by a factor of $\sqrt{1+\lambda}$. This follows directly from a generalization of Clogston's original argument in which the Pauli band-splitting energy is set equal to the zero-temperature condensation energy of the superconducting state. We see for our more sophisticated approach that this simple argument, while giving the correct order of magnitude for $H_{c2,P}$, does not give the correct renormalization law. We will return to this point more explicitly in the next section.

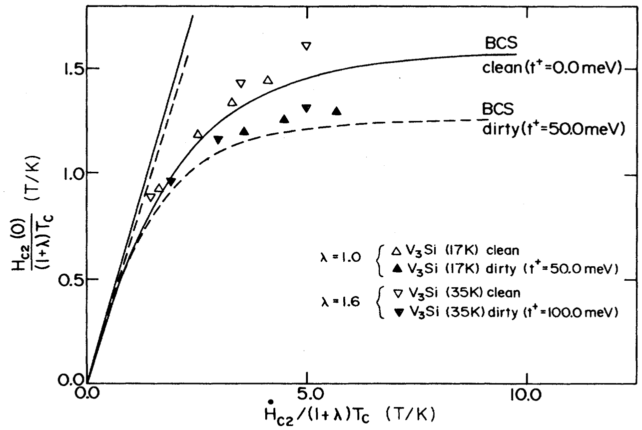

FIG. 1. The normalized zero-temperature second upper critical field $H_{c2}(0)/(1+\lambda)T_c$ as a function of the normalized initial slope at $T_c[dH_{c2}(T)/dT]_{T_c}/(1+\lambda)T_c$. The solid and dashed curves were obtained using a renormalized BCS theory including Pauli limiting and apply, respectively, to the clean and dirty ($t^+=50.0$ meV) limits. The straight lines result when Pauli limiting is neglected. The upward and downward pointing open (clean limit) and solid triangles (dirty limit) are results of full strong-coupling calculations for V_3Si with $\lambda=1.0$ and a fictitious system with $T_c=35.0$ K having the same shape $\alpha^2F(\Omega)$ as that for V_3Si but with $\lambda=1.6$.

To end this section, we point out that Eqs. (17) and (18) are universal for all superconductors provided the asterisked quantities are used. For a fix impurity concentration $(t^+)^*$, H^* is unique for a given value of v_F^*. It is, in fact, more physical to consider the slope of H_{c2}^* at T_c instead of v_F^* itself. This slope is proportional to v_F^{*2} since the universal parameter α^* is related to H_{c2}^* by $\alpha^*=eH^*v_F^{*2}/2$. Thus, when Pauli limiting is included for a given $(t^+)^*$, a universal curve results for $H_{c2}(0)/(1+\lambda)T_c$ as a function of

$$(dH_{c2}(T)/dT)_{T_c}/(1+\lambda)T_c\ .$$

In Fig. 1, we show such curves for the clean (solid curve) and dirty (dashed curve) limit. If Pauli limiting is ignored $H_{c2}(0)/(1+\lambda)T_c$ is simply proportional to the slope $[dH_{c2}(T)/dT]_{T_c}/(1+\lambda)T_c$. This corresponds to the two straight lines, solid for the clean and dashed for the dirty limit of Fig. 1 with slope of 0.73 and 0.69, respectively. In the next section, we look at these two limits in more detail.

IV. DIRTY AND CLEAN LIMITS IN TWO-SQUARE WELL MODEL

Equations (17) and (18) can be reduced analytically in the dirty and clean limits. We start with the dirty limit. In this case, the argument of the inverse tangent is small and we can write

$$\bar{\chi}^{-1}(\tilde{\omega}_m)\simeq[(2m+1)\pi t+\pi(t^+)^*+i\mu_B H^*]\times\{1+\alpha^*/3\pi^2[(t^+)^*]^2\} \tag{19}$$

and get

$$\frac{1+\lambda}{\lambda-\mu^*}=2\pi t\sum_{m=0}^{N_c}\mathrm{Re}(\{(2m+1)\pi t+i\mu_B H^*+\alpha^*/[3(t^+)^*\pi]\}^{-1}) \tag{20}$$

which gives

$$\frac{1+\lambda}{\lambda-\mu^*}=\mathrm{Re}\left[\psi\left[\frac{\omega_D}{T2\pi}+\frac{i\mu_B H^*}{2\pi t}+\frac{\alpha^*}{6\pi^2 t(t^+)^*}\right]-\psi\left[0.5+\frac{i\mu_B H^*}{2\pi t}+\frac{\alpha^*}{6\pi^2 t(t^+)^*}\right]\right], \tag{21}$$

where $\psi(x)$ denotes the digamma function. By assuming ω_D to be very large one can approximate the first digamma function in (21) by $\ln(\omega_D/T)$. Furthermore, using the T_c equation (18) we find

$$\ln(1.13\times 2\pi t)=-\mathrm{Re}\psi\left[0.5+\frac{i\mu_B H_{c2}^*}{2\pi t}+\frac{\alpha^*}{6\pi^2 t(t^+)^*}\right]. \tag{22}$$

In the limit when the reduced temperature is small (22) has the solution

$$H_{c2}^*=\frac{1}{1.13}\{(ev_F^{*2}/[6\pi(t^+)^*]^2+\mu_B^2\}^{-1/2} \tag{23}$$

and the initial slope is found by differentiating (22) with respect to t:

$$\dot{H}_{c2}^*=\left.\frac{dH_{c2}^*}{dt}\right|_{t=1}=-\frac{24(t^+)^*}{ev_F^{*2}} \tag{24}$$

which can be inserted into (23) to give

$$H_{c2}^*=[(0.695\dot{H}_{c2}^*)^{-2}+(H_{c2,P}^*)^{-2}]^{-1/2}. \tag{25}$$

The extreme Pauli limit follows for infinite slop $\dot{H}_{c2}^*\to\infty$:

$$H_{c2,P}^*=\frac{1}{1.13\mu_B} \text{ or } 1.32 \text{ T/K} \tag{26}$$

which is slightly different from the Clogson[8] value obtained from free-energy considerations. In that approach, we set the band-splitting energy equal to the BCS condensation energy

$$\mu_B^2 H_{c2,P}N(0)=\tfrac{1}{2}N(0)(1+\lambda)(1.76)^2T_c^2, \tag{27}$$

where $N(0)$ is the single-spin electronic density of states at the Fermi energy. This leads to

$$\frac{H_{c2,P}}{\sqrt{1+\lambda}T_c}=\frac{1.76}{\sqrt{2}}\frac{1}{\mu_B}=\frac{1.24}{\mu_B} \tag{28}$$

as given by Orlando *et al.*[11] and Without a $1+\lambda$ correction by Decroux *et al.*[8] We see clearly that free-energy arguments cannot be used to get the correct numerical factor in such relationships or the right λ renormalization.

In the clean limit, the situation is more complicated. By setting $t^+=0$ and approximating the sum by an integral (17a) and (17b) become for low temperatures:

$$\frac{1+\lambda}{\lambda-\mu^*}=\mathrm{Re}\int_0^{\omega_D/T_c}d\omega\frac{2}{(\alpha^*)^{1/2}}\times\int_0^\infty dq\, e^{-q^2}\tan^{-1}\left[\frac{q(\alpha^*)^{1/2}}{\omega+i\mu_B H^*}\right]. \tag{29}$$

This integral can be solved in the limit of very high Debye frequencies ω_D compared to $(\alpha^*)^{1/2}$ and $\mu_B H^*$ as is shown in the Appendix, with the result:

$$\ln(1.13\mu_B H_{c2}^*)=1-\frac{e^{-\tau^2}}{2}E(\tau^2)-\tau\int_0^\infty dq\, e^{-q^2}[\ln(\tau+q)-\ln|\tau-q|], \tag{30}$$

where

$$\tau=\mu_B H_{c2}^*/(\alpha^*)^{1/2}=\mu_B(2H_{c2}^*)^{1/2}/(ev_F^{*2})^{1/2}. \tag{31}$$

It is again possible to express ev_F^* by the initial slope of H_{c2}^* which is determined by

$$\dot{H}_{c2}^*=\left.\frac{dH_{c2}^*}{dt}\right|_{t=1}=28.15/ev_F^{*2} \tag{32}$$

which gives

$$\tau=\mu_B(H_{c2}^*\dot{H}_{c2}^*)^{1/2}/\sqrt{14.075}. \tag{33}$$

The extreme Pauli limiting case is obtained for very large values of τ. It is shown in the Appendix that Eq. (30) gives in this limit

$$\ln(1.13\mu_B H_{c2,P}^*)=0 \tag{34}$$

which corresponds exactly to Eq. (26) as expected from Sec. II.

The clean limit curve (solid line) of Fig. 1 was in fact, obtained from (30) rather than from (17) and (18). In contrast to the dirty limit, H_{c2} can now be significantly greater than $H_{c2,P}$ and the upper BCS limit for $H_{c2}/T_c(1+\lambda)$ turns out to be 1.57 T/K which is reached for $H_{c2}/(1+\lambda)\cong 10$ T/K. Thus, $H_{c2,P}$ is not the maximum value of the critical magnetic field that can be reached except in the dirty limit. For very large slopes, the solid and dashed curves in Fig. 1 must, of course, meet.

V. STRONG-COUPLING CORRECTIONS BEYOND $1+\lambda$

While the factor $(1+\lambda)^{-1}$ greatly deemphasizes the effect of Pauli limiting in Eqs. (17) and (18) and reduces the need to introduce spin-orbit scattering, it is important to study strong-coupling effects beyond this factors. This is the subject of this section.

In order to estimate strong-coupling corrections beyond the $1+\lambda$ rescaling that appears in the modified BCS results, we calculated the reduced upper critical magnetic field $H_{c2}^* = H_{c2}/[(1+\lambda)T_c]$ as a function of the reduced initial slope $\dot{H}_{c2}^* = \dot{H}_{c2}/(1+\lambda)$ for several cases. As was shown in the previous section, there is only one such curve in BCS given a fixed reduced impurity concentration $t^+/[(1+\lambda)T_c]$. This is no longer the case when realistic values for $\alpha^2F(\omega)$ are taken into account. In Fig. 1, we show some of our results based on the full strong-coupling equations (1a) and (1b). In one calculation (triangular symbols pointing up), we have used the electron-phonon spectral density $\alpha^2F(\omega)$ determined by Kihlstrom[12] for V_3Si from tunneling data. The value of λ is 1.0 and we chose μ^* to give a $T_c = 17.0$ K for this value of λ. This corresponds fairly closely to a sample studied by Orlando *et al.*[11] with a fairly low residual resistivity of 5.2 $\mu\Omega$ cm at 20 K and an estimated mean free path of 95 Å and an electromagnetic coherence length of 56 Å. In Fig. 1, two cases are considered. The first is the clean limit results with $t^+ = 0.0$ meV open triangles which are seen to fall above the BCS clean limit curve but not by very much. In this case, strong-coupling corrections beyond the very essential factor of $1+\lambda$ are not very pronounced. The same remarks apply to the solid triangles describing the dirty limit. To get larger corrections, we have arbitrarily increased the area under the spectral density $\alpha^2F(\omega)$ of V_3Si by multiplication by a constant amount to increase the corresponding λ from 1.0 to 1.6 and, at the same time, raise T_c to 35 K which is not very different from the critical temperature found recently in $La_{1.85}Sr_{0.15}CuO_4$ (Ref. (13) a high T_c oxide superconductor. The clean limit results are the open triangles pointing downward in Fig. 1. We see that, in this case, the deviations from BCS are much more significant than for V_3Si itself. This shows clearly that, in some cases at least, it is necessary to perform a full strong-coupling calculation based on Eqs. (1a) and (1b) in order to get an accurate value for $H_{c2}(0)/[1+\lambda(0)]T_c$. Additional results for dirty samples (solid downward triangles) are also given in Fig. 1 and compared to the BCS $t^+ = 50.0$ meV curve. Again, significant corrections can arise and this should be kept in mind in the analyses of data.

Finally, we return to the solid and dashed lines in Fig. 1, giving the slope of $H_{c2}(0)/[1+\lambda]T_c$ as a function of the initial slope at T_c, $\dot{H}_{c2}(T_c)/(1+\lambda)$. These straight lines apply, respectively, to the clean and dirty limits in BCS when Pauli limiting (band splitting) is ignored. The bending over of solid and dashed curves away from these straight lines gives the effect of band splitting. In the work of Orlando *et al.*,[11] they quote for $\dot{H}_{c2}(T_c)$ in V_3Si a value of 2.0 T/K. If we divide by $1+\lambda$, we get for the horizontal variable a value $H_{c2}(T_c)/(1+\lambda) \cong 1.0$ T/K which indicates that Pauli limiting is not a large effect in V_3Si. This conclusion was also reached by Schossmann and Schachinger[3] on the basis of detailed numerical consideration. In our case, we need only realize that in this region the solid and dashed curves do not differ very much from the corresponding straight lines.

To investigate further the effect of phonon dynamics on the normalized quantity $H_{c2}(0)/(1+\lambda)T_c$ as a function of normalized initial slope $\dot{H}_{c2}(T_c)/(1+\lambda)$, in Fig. 2 we present further results obtained for a δ function spectral density of the form

$$\alpha^2F(\omega) = A\,\delta(\omega-\omega_E)\ , \qquad (35)$$

where ω_E is some Einstein frequency which we will vary and A is the area under the δ function. In all calculations, we have taken $\mu^* = 0.1$ and adjusted A to get a $T_c = 1.0$ meV so that the only remaining parameter is the choice of ω_E. Different ω_E's will give different curves. For very large ω_E we expect to recover BCS. Both clean

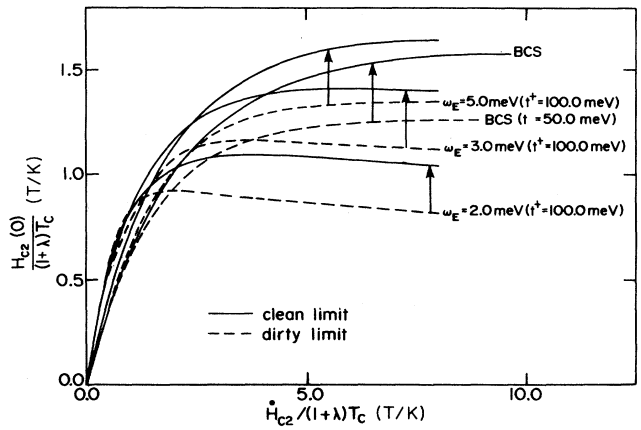

FIG. 2. The normalized zero-temperature second upper critical magnetic field $H_{c2}(0)/(1+\lambda)T_c$ as a function of the normalized initial slope at $T_c[dH_{c2}(T)/dT]_{T_c}/(1+\lambda)T_c$. These curves were all calculated using the full strong-coupling equations (1a) and (1b) and come in pairs. The solid applies to the clean limit, the dashed to the dirty limit with impurity content as labeled. The lower pair applies for an Einstein frequency $\omega_E = 2.0$ meV, the next set for 3.0 meV and the fourth set for 5.0 meV. The third set represents the BCS results and is included for comparison.

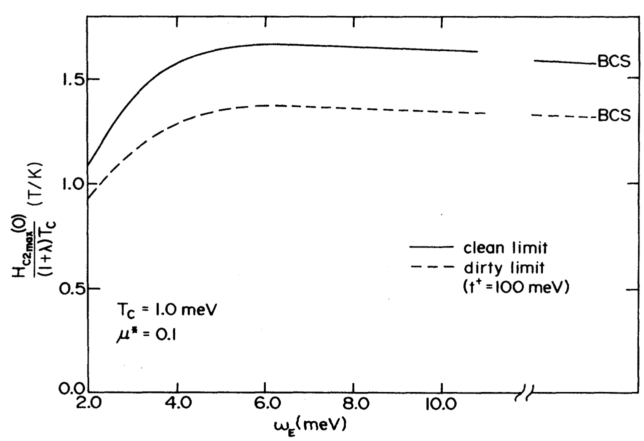

FIG. 3. The maximum value of the normalized second upper critical magnetic field $H_{c2}(0)_{max}/(1+\lambda)T_c$ as a function of Einstein frequency ω_E for the clean (solid line) and dirty (dashed line) limits, respectively. By dirty we mean $t^+ = 100.0$ meV.

and dirty limits are considered as labeled in the figure. Shown for comparison are BCS results. We first note that for $\omega_E = 2.0$ meV, the differences with BCS are striking and full strong-coupling calculations are definitely necessary. For $\omega_E = 3.0$ and 5.0 meV, the differences are reduced but are still quite significant. To characterize these results with a single parameter, we have chosen to consider the value of $H_{c2}(0)/(1+\lambda)T_c$ at maximum which is 1.32 T/K in the dirty BCS limit and 1.57 T/K in the corresponding clean limit. As can be seen in Fig. 3 where the maximum $H_{c2}(0)$ is plotted against the Einstein frequency ω_E the maxima can be quite different for δ-function electron-phonon spectral densities. In particular, when ω_E is small the maxima can be less in BCS theory while at intermediate values of ω_E they can be larger but it would appear not by very much.

VI. CONCLUSIONS

We have established that the extreme Pauli limiting field is independent of impurity content but varies with electron-phonon spectral density $\alpha^2F(\Omega)$ and Coulomb pseudopotential μ^*. Using a two-square well model in the full strong-coupling equations leads to the well-known BCS equations of WHH with some very significant renormalization by a factor of $l+\lambda$, where λ is the electron-phonon mass renormalization. In particular, the effect of Pauli limiting is greatly reduced by this renormalization. This means that it is not necessary to introduce such large spin-orbit scattering corrections as has been needed in the past in order to reduce Pauli limiting effects. We have also given analytic results for the extreme Pauli limiting field in dirty and clean limits. In addition, results are given of full strong-coupling calculations for V_3Si, for a spectrum of the V_3Si type but with a $T_c = 35.0$ K and $\lambda = 1.6$ and for a series of δ-function spectra. In all cases, the results are presented for the normalized zero-temperature critical magnetic field $H_c(0)/(1+\lambda)T_c$ as a function of the normalized slope at T_c namely

$$\left[\frac{dH_{c2}(T_c)}{dT}\right]_{T_c} /(1+\lambda)T_c$$

which we believe to be particularly useful in analyses of experiments. On such a plot, a straight line would result if Pauli limiting is ignored and it is, therefore, deviations from this straight line that measure the effect of Pauli limiting.

ACKNOWLEDGMENTS

This research was supported in part by the Natural Sciences and Engineering Research Council of Canada. One of us (J.P.C.) received additional support from The Canadian Institute for Advanced Research.

APPENDIX

In Eq. (19) we have to deal with a function of the structure:

$$f(z) = \mathrm{Re}\int_0^z dx\, 2\int_0^\infty dq\, e^{-q^2}\tan^{-1}\left[\frac{q}{x+i\tau}\right] \quad \text{(A1)}$$

with $z = \omega_D/[T_c(\alpha^*)^{1/2}]$ and $\tau = \mu_B H^*/(\alpha^*)^{1/2}$. The transformation $x = x - i\tau$ can be used to rewrite Eq. (A1)

$$f(z) = \mathrm{Re}2\int_0^{z+i\tau} dx \int_0^\infty dq\, e^{-q^2}\tan^{-1}(q/x) - \mathrm{Re}\int_0^\tau dx \int_0^\infty dq\, e^{-q^2}\ln[(x+q)/(x-q)]\ . \quad \text{(A2)}$$

The first integral in (A2) can be performed by making the transformation $q/x \to q$ and carrying out the integration over x:

$$2\int_0^{z+i\tau} dx \int_0^\infty dq\, e^{-q^2}\tan^{-1}(q/x) = \lim_{\epsilon\to 0}\left[\int_\epsilon^\infty \frac{dq}{q^2}\tan^{-1}q - \int_\epsilon^\infty \frac{dq}{q^2} e^{-q^2(z+i\tau)^2}\tan^{-1}q\right]$$

$$\simeq \lim_{\epsilon\to 0}\left[1 - \ln\epsilon - \int_\epsilon^\infty \frac{dq}{q} e^{-q^2(z+i\tau)^2}\right] = 1+\gamma/2 + l\ln(z+i\tau)\ . \quad \text{(A3)}$$

In (A3) we assumed the z is large enough so that $e^{-q^2(z+i\tau)^2}$ is going towards zero very fast and, therefore, that $\tan^{-1}q \sim q$. Furthermore, we used the approximate behavior of the integral $(z\to 0)$

$$\int_z^\infty \frac{dx}{x} e^{-x} \simeq -\gamma - \ln z \quad \text{(A4)}$$

with γ Euler's constant. In the second term of (A2) we can do the x integral to get

$$\int_0^\tau dx \int_0^\infty dq\, e^{-q^2}[\ln(x+q) - \ln|x-q|] = \tau\int_0^\infty dq\, e^{-q^2}[\ln(\tau+q) - \ln|\tau-q|] + \int_0^\infty dq\, e^{-q^2} q[\ln(\tau+q) + \ln|\tau-q|] - 2\int_0^\infty dq\, q e^{-q^2}\ln q\ . \quad \text{(A5)}$$

The first integral in (A5) equals

$$\ln\tau + \frac{e^{-\tau^2}}{2}\int_{-\tau^2}^{\infty} dx \frac{e^{-x}}{x} \equiv \ln\tau + \frac{e^{-\tau^2}}{2} E(\tau^2) \qquad \text{(A6)}$$

and the last is minus Euler's constant. Thus we arrive at the final form:

$$f(z) = \ln(z/\tau) + 1 - \frac{e^{-\tau^2}}{2} E(\tau^2) - \tau \int_0^{\infty} dq\, e^{-q^2}[\ln(\tau+q) - \ln|\tau - q|] , \qquad \text{(A7)}$$

where we assumed $(z^2+\tau^2)^{1/2} \sim z$.

For the extreme Pauli limiting case we have to investigate (A7) in the limit $\tau \gg 1$. The logarithm of the integral in Eq. (A7) can be approximated by

$$\ln(\tau+q) - \ln|\tau-q| \sim 2q/\tau + 0[(q/\tau)^3] \qquad \text{(A8)}$$

so that

$$\lim_{\tau \gg 1} f(z) \simeq \ln(z/\tau) \qquad \text{(A9)}$$

because z is still supposed to be very large compared to τ.

[1]E. Helfand and N. R. Werthamer, Phys. Rev. **147**, 288 (1966).

[2]N. R. Werthamer, E. Helfand, and P. C. Hohenberg, Phys. Rev. **147**, 295 (1966).

[3]M. Schossmann and E. Schachinger, Phys. Rev. B **33**, 6123 (1986).

[4]D. Rainer, G. Bergmann, and V. Eckhart, Phys. Rev. B **8**, 5324 (1973).

[5]M. Schossmann and J. P. Carbotte, Phys. Rev. B **34**, 1550 (1986).

[6]F. Marsiglio, M. Schossmann, E. Schachinger, and J. P. Carbotte, Phys. Rev B **35**, 3226 (1987).

[7]M. Schossmann, E. Schachinger, and J. P. Carbotte, Phys. Rev. B **36**, 8360 (1987).

[8]M. Decroux and O. Fischer, in *Superconductivity in Ternary Compounds* (Springer-Verlag, New York, 1982), Vol. II.

[9]P. B. Allen and B. Mitrovic, in *Solid State Physics,* edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic, New York, 1982), Vol. 37, p. 1.

[10]T. P. Orlando and M. R. Beasley, Phys. Rev. Lett. **46**, 1598 (1981).

[11]T. P. Orlando, E. J. McNiff, Jr. S. Foner, and M. R. Beasley, Phys. Rev. B **19**, 4545 (1979).

[12]K. E. Kihlstrom, Phys. Rev. B **32**, 2891 (1985).

[13]J. P. Carbotte, in *CAP-NSERC Summer Institute in Theoretical Physics,* edited by G. Kunstatter, H. C. Lee, F. C. Khanna, and H. Umezawa (World Publisher, Singapore, 1988), p. 28.