Finally, we have pointed out the puzzling and most interesting behavior of the lettered series of lines. A more detailed study of these remains to be made.

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Hall Angle of a Normal Current Flowing through the Core of a Vortex*

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A calculation, based on the microscopic theory of superconductivity, is made of the Hall angle of a normal current flowing through the core of a single vortex. The magnetic vector potential is assumed uniform throughout the core region and the moments of the current are taken with the electric field. The ratio of these two quantities yields the tangent of the Hall angle. In agreement with a prediction of Bardeen, we find $\tan\alpha = (e\tau/mc)H_{eff}$, where τ is the relaxation time of the electrons, and the effective magnetic field H_{eff} is in part due to the depression in the order parameter at the core of the vortex and in part to the actual magnetic field in the core of the vortex. For niobium, H_{eff} is very nearly equal to H_{c2}. At 0 °K for niobium, our theory is valid for l/ξ ranging from ∞ to about 10, where l is the mean free path and ξ the coherence length.

I. INTRODUCTION

When a transport current $\vec{J}_T$ flows through a type-II superconducting sample containing a vortex, the flux line flows at a velocity $\vec{v}_L$. This occurs provided that there are no pinning forces or that the transport current is sufficiently strong to overcome pinning. In a perfectly clean sample, the vortex will flow with $\vec{J}_T$ at a Hall angle of $\frac{1}{2}\pi$, whereas in a very dirty sample, it will flow at right angles to the transport current at a Hall angle of 0.

There has been considerable theoretical and experimental interest in determining the Hall angle for situations in between these two extreme cases. In a local model of a superconductor, Bardeen and Stephen predict a Hall angle of $\tan\alpha = (e\tau/mc)H$, where τ is the relaxation time of the electrons and H is the magnetic field in the core of the vortex.[1] Using a hydrodynamic model, Nozières and Vinen obtained the same expression for $\tan\alpha$ with H replaced by H_{c2}, the upper critical field of the superconductor.[2]

There have been microscopic theories of flux flow in type-II superconductors for fields near H_{c2}.[3-5] Here a perturbation expansion in the order parameter is possible, since this quantity is small near H_{c2}. In one of these papers, Maki finds that the Hall angle α is given by $\alpha = (e\tau/mc) \times B$, where B is the magnetic induction.[4]

Experimentally, the Hall angle in flux flow was detected by Kim, Hempstead, and Strnad.[6] Improved measurements were made by Niessen and Staas on dirty samples and by Reed, Fawcett, and Kim on clean samples of niobium.[7,8] There are further examples of such measurements although we do not presume to give a comprehensive list.[9,10] For clean samples, the Hall angle increases with magnetic field. However, there is evidence that α is constant in the mixed state for clean niobium.[11] This result would agree with Nozières and Vinen and with our calculation.[2]

In Sec. II, we present our formulation of the problem which is based on the microscopic theory of superconductivity and proceed in Sec. III to evaluate the Hall angle.

II. FORMULATION

We assume that the magnetic vector potential has two components: $\hat{e}_\theta A_0(r)$ is that of a vortex at rest and is due to supercurrent flow about the vortex axis. The magnetic vector potential $\vec{A}_1(x)$ drives the transport current through the core of the vortex, and we have

$$\vec{A}(x) = \hat{e}_\theta A_0(r) + \vec{A}_1(x) \quad . \tag{1}$$

The reasonable assumption is made that $\vec{A}_1(x)$ is small compared to $A_0(r)$. The current density is then given by

$$\vec{J}(x) = \hat{e}_\theta J_0(r) - (e^2/mc)N\vec{A}_1(x) + (i/c)\langle \int_{-\infty}^{t} [\hat{J}(x), \hat{J}(x')]\rangle \cdot \vec{A}_1(x')d^4x' \ , \tag{2}$$

where $J_0(r)$ is the supercurrent flowing about the vortex axis in the absence of transport current. Based on our assumption that $\vec{A}_1(x)$ is small, we have employed linear response theory to calculate the current generated by the electric field in the core of the vortex. In Eq. (2), $\hat{J}(x)$ is the electric current operator of second quantization, and we have taken a thermal average of the current-current commutator.

Defining the retarded correlation function

$$P^R(x, x') = (i/c)\langle [\hat{J}(x), \hat{J}(x')]\rangle \,\theta(t-t') \tag{3}$$

and the response function of Abrikosov, Gor'kov, and Dzyaloshinski[12]

$$\vec{J}_1(x) = -\int Q^R(x, x')\vec{A}_1(x')d^4x' \tag{4}$$

we have

$$Q^R(x, x') = (e^2N/mc)\delta(x-x') - P^R(x, x') \quad . \tag{5}$$

In terms of the Nambu field operations

$$\Psi(x) = \begin{pmatrix} \psi_\uparrow(x) \\ \psi_\downarrow^\dagger(x) \end{pmatrix} \quad ,$$

the electric-current operator is given by

$$\hat{J}(x) = (e/2im)\{\Psi^\dagger(x)\vec{\nabla}\Psi(x) - [\vec{\nabla}\Psi^\dagger(x)]\Psi(x)\} \ , \tag{6}$$

and $J_0(r) = \langle \hat{J}(x)\rangle$.[13]

We calculate the response function in the temperature domain where

$$\mathcal{P}(x, x') = (1/c)\langle T\hat{J}(\vec{x}, \tau)\hat{J}(\vec{x}', \tau')\rangle \tag{7}$$

with τ the complex time and T the time-ordering operator. Defining a one-particle Green's function in the usual way,[14] the temperature-correlation function may be rewritten as follows with the help of Eq. (6) for the current operator:

$$P(1, 2) = -(e^2/c)[(\vec{\nabla}_1 - \vec{\nabla}_1')/2im][(\vec{\nabla}_2 - \vec{\nabla}_2')/2im] \times \mathrm{Tr}[\mathcal{G}(1, 2')\mathcal{G}(2, 1')]_{1=1', 2=2'} \quad . \tag{8}$$

Here the Green's function is a 2×2 matrix and Tr takes the trace of the product of the two Green's functions.

The Green's function may easily be expanded in terms of the eigenfunctions of the system:

$$\mathcal{G}(x, x') = T\sum_\omega e^{-i\omega(\tau-\tau')}\int_{-\infty}^{\infty}\frac{dk}{2\pi}e^{ik(z-z')} \times \sum_\mu \frac{1}{2\pi}e^{i\mu(\theta-\theta')}\sum_n \frac{\Phi_{n\mu k}(r)\Phi_{n\mu k}^\dagger(r')}{i\omega - E_{n\mu k}} \quad . \tag{9}$$

It is customary to expand $\mathcal{G}$ as the sum of two terms, one of positive-energy eigenfunctions and another for the negative-energy ones.[15] In Eq. (18), we sum over both positive and negative energies.

The Green's function appearing in Eq. (9) is that for a superconductor containing a single isolated vortex in the absence of transport current. This is the Green's function for the unperturbed system. The eigenfunctions $u(r)$ and $v(r)$, where

$$\Phi(r)=\begin{pmatrix} u(r) \\ v(r)\end{pmatrix},$$

satisfy the Bogoliubov equations with energy E for a superconductor containing a single vortex. The bound-state spectrum of this system was first investigated by Caroli and Matricon and calculations of the scattering solutions were first made by the present author.[16,17] A WKBJ technique was employed in both cases. Recently, Bardeen *et al.* have made extensive calculations of these functions for a range of κ values, where κ is the Ginzberg-Landau parameter; there have also been some recent calculations by Hansen and by Bergk and Tewordt.[18-20]

The gradient operators of Eq. (8) are confined to the x, y plane so that we can perform a Fourier expansion of $\mathcal{P}(1,2)$ in frequency and in the z component of momentum. We have

$$\mathcal{P}(\vec{r}_1, \vec{r}_2, \omega_0)=\frac{e^2}{4m^2c}\left(\frac{\partial}{\partial r_1}-\frac{\partial}{\partial r_{1'}}\right)\left(\frac{\partial}{\partial r_2}-\frac{\partial}{\partial r_{2'}}\right)\times LT\sum_\omega\int_{-\infty}^{\infty}\frac{dk}{2\pi}\times\mathrm{Tr}[\,\mathcal{G}'_{\omega}(\vec{r}_1, \vec{r}'_2, k)\,\mathcal{G}_{\omega}(\vec{r}_2, \vec{r}'_1, k]_{1=1', 2=2'}\,, \tag{10}$$

where $\omega'=\omega+\omega_0$.

The function $\mathcal{P}$ of Eq. (10) is evaluated for the zero z component of momentum, since this is the only component we shall need.

Equation (4) must be solved for self-consistency together with $\vec{\nabla}\cdot\vec{J}=0$, the equation for conservation of current. Once $\vec{A}_1$ is known and hence $\vec{E}_1$, we have for the power lost

$$P=\mathrm{Re}\int d^3x\, E_1^*\hat{e}_x\cdot\vec{J}_1 \quad. \tag{11}$$

We shall make the assumption that $\vec{A}_1$ is uniform near the core of the vortex. To the accuracy of this assumption, we may take the Hall angle as

$$\tan\alpha=-I_y/I_x\;, \tag{12}$$

$$\text{where}\quad I_x=\mathrm{Re}\int d^3x\, E_1^*\hat{e}_x\cdot\vec{J}_1 \tag{13}$$

$$\text{and}\quad I_y=\mathrm{Re}\int d^3x E_1^*\hat{e}_y\cdot\vec{J}_1\;. \tag{14}$$

In fact, I_x is equal to the power lost.

In order to determine the power P, it is necessary to determine $\vec{A}_1$ near the core, which is not equal to $\vec{A}_1$ far from the vortex. Determining the Hall angle does not necessitate this extra step as E_1 cancels out of the ratio. By avoiding the self-consistency condition, the calculation becomes tractable.

To determine the normal current from P, we consider only the contribution of the lowest branch of the bound-state spectrum. This assumption increases in validity as the temperature decreases and the more highly excited states depopulate. The approximation should be exact at $T=0$.

III. CALCULATIONS

Before proceeding with the calculation of $\mathcal{P}$, we point out how the diamagnetic term of Eq. (2) is to be treated. In a complete calculation of $\vec{J}_1$, the frequency sum in Eq. (9) must be performed prior to the momentum integration in order to obtain proper convergence. The diamagnetic term is exactly equal to $\mathcal{P}$ for a normal metal, and the difference between $\mathcal{P}$ for a superconductor and for a normal metal converges sufficiently rapidly for the momentum integration to be done prior to the frequency sum.[21] In this process $\mathcal{P}$ for the normal metal simply vanishes. In this paper, therefore, we shall neglect the diamagnetic term and do the momentum integration prior to the frequency sum.

Returning to Eq. (10), the diagonal xx component of the correlation function is given by

$$\mathcal{P}_{xx}(\vec{r}_1, \vec{r}_2, \omega_0)=\frac{e^2}{4m^2c}LT\sum_\omega\int_{-\infty}^{\infty}\frac{dk}{2\pi}\sum_{\mu,\mu'}e^{\frac{i(\mu'-\mu)(\theta_1-\theta_2)}{(2\pi)^2}}\left[\cos\theta_1\left(\frac{\partial}{\partial r_1}-\frac{\partial}{\partial r_1'}\right)-i(\mu+\mu')\frac{\sin\theta_1}{r_1}\right]$$
$$\times\left[\cos\theta_2\left(\frac{\partial}{\partial r_2}-\frac{\partial}{\partial r_2'}\right)-i(\mu+\mu')\frac{\sin\theta_2}{r_2}\right]\mathrm{Tr}[\,\mathcal{G}_{\omega'}(r_1, r_2', \mu', k)\mathrm{G}_\omega(r_2, r_1', \mu, k)]_{1=1', 2=2'}\quad. \tag{15}$$

We carry out the derivatives with respect to r in Eq. (15) and integrate $\mathcal{P}_{xx}$ over θ_1 and θ_2 to obtain

$$\int_{-\pi}^{\pi}d\theta_1\int_{-\pi}^{\pi}d\theta_2\,\mathcal{P}_{xx}(\vec{r}_1, \vec{r}_2, \omega_0)=\frac{Le^2}{16m^2c}T\sum_\omega\int_{-\infty}^{\infty}\frac{dk}{2\pi}$$
$$\times\sum_\mu\mathrm{Tr}\left\{\frac{\partial}{\partial r_1}\left[\mathcal{G}_{\omega'}(r_1, r_2, \mu-1, k)+\mathcal{G}_{\omega'}(r_1, r_2, \mu+1, k)\right]\frac{\partial}{\partial r_2}\mathcal{G}_\omega(r_2, r_1, \mu, k)\right.$$

$$-[\mathcal{G}_{\omega'}(r_1, r_2, \mu-1, k)+\mathcal{G}_{\omega'}(r_1, r_2, \mu+1, k)]\frac{\partial}{\partial r_1}\frac{\partial}{\partial r_2}\mathcal{G}_\omega(r_2, r_1, \mu, k)$$

$$-\frac{\partial}{\partial r_1}\frac{\partial}{\partial r_2}[\mathcal{G}_{\omega'}(r_1, r_2, \mu-1, k)+\mathcal{G}_{\omega'}(r_1, r_2, \mu+1, k)]\mathcal{G}_\omega(r_2, r_1, \mu, k)$$

$$+\frac{\partial}{\partial r_2}[\mathcal{G}_{\omega'}(r_1, r_2, \mu-1, k)+\mathcal{G}_{\omega'}(r_1, r_2, \mu+1, k)]\frac{\partial}{\partial r_1}\mathcal{G}_\omega(r_2, r_1, \mu, k)$$

$$-\frac{1}{r_1}[(2\mu-1)\mathcal{G}_{\omega'}(r_1, r_2, \mu-1, k)-(2\mu+1)\mathcal{G}_{\omega'}(r_1, r_2, \mu+1, k)]\frac{\partial}{\partial r_2}\mathcal{G}_\omega(r_2, r_1, \mu, k)$$

$$+\frac{\partial}{\partial r_2}\frac{1}{r_1}[(2\mu-1)\mathcal{G}_{\omega'}(r_1, r_2, \mu-1, k)-(2\mu+1)\mathcal{G}_{\omega'}(r_1, r_2, \mu+1, k)]\mathcal{G}_\omega(r_2, r_1, \mu, k)$$

$$+\frac{\partial}{\partial r_1}\frac{1}{r_2}[(2\mu-1)\mathcal{G}_{\omega'}(r_1, r_2, \mu-1, k)-(2\mu+1)\mathcal{G}_{\omega'}(r_1, r_2, \mu+1, k)]\mathcal{G}_\omega(r_2, r_1, \mu, k)$$

$$-\frac{1}{r_2}[(2\mu-1)\mathcal{G}_{\omega'}(r_1, r_2, \mu-1, k)-(2\mu+1)\mathcal{G}_{\omega'}(r_1, r_2, \mu+1, k)]\frac{\partial}{\partial r_1}\mathcal{G}_\omega(r_2, r_1, \mu, k)$$

$$-\frac{1}{r_1 r_2}[(2\mu-1)^2\mathcal{G}_{\omega'}(r_1, r_2, \mu-1, k)+(2\mu+1)^2\mathcal{G}_{\omega'}(r_1, r_2, \mu+1, k)]\mathcal{G}_\omega(r_2, r_1, \mu, k)\bigg\} . \qquad (16)$$

In order to simplify our calculation, we shall assume that $p_F\xi$ is very large and that $\mu/p_F\xi$ is small. These approximations ensure that we are in the linear part of the bound-state spectrum and that the wave functions are given by

$$\Phi_\mu(r)=\frac{A}{(p_F r\sin\alpha)^{1/2}}\begin{pmatrix}\cos[p_F r\sin\alpha-\frac{1}{2}\mu\pi-\frac{1}{4}\pi+\frac{1}{2}\eta_\mu]\\ \cos[p_F r\sin\alpha-\frac{1}{2}\mu\pi-\frac{1}{4}\pi-\frac{1}{2}\eta_\mu]\end{pmatrix}e^{i\xi_\mu} , \qquad (17)$$

except for a very small region about $p_F r\sin\alpha=\mu$. A is a normalization constant. At $r=0$, the wave functions vanish. The functions η_μ and ξ_μ are those Bardeen *et al.*[18] $i\xi_\mu$ is real and negative. In what follows, we keep in mind that $(\partial/\partial\mu)\eta_\mu\sim 1/p_F\xi$.[18]

With the wave function given by Eq. (17), we may easily see that the derivative terms $\partial/\partial r$ in Eq. (16) are of order $(p_F\xi)^2$ larger than the $1/r$ terms. In the calculation, we encounter the matrix elements $\int\Phi_{\mu+1}\times(r)(\partial/\partial r)\Phi_\mu(r)r\,dr$ which are of order p_F because of the phase factor $\frac{1}{2}\pi\mu$ which appears in the wave function. On the other hand, $\int\Phi_{\mu+1}(r)\Phi_\mu(r)\,dr\sim(1/p_F\xi^2)$, since the wave functions are almost orthorgonal. Again, this is due to the $\frac{1}{2}\pi\mu$ factor in the wave function. The last five terms in Eq. (16) may be immediately discarded as they are at least of order $\mu(p_F\xi)^{-2}$ smaller than the terms which we keep.

Consider from the first two terms in the curly brackets of Eq. (16)

$$\mathrm{Tr}\left\{\frac{\partial}{\partial r_1}[\mathcal{G}_{\omega'}(r_1, r_2, \mu-1, k)]\frac{\partial}{\partial r_2}\mathcal{G}_\omega(r_2, r_1, \mu, k)-\mathcal{G}_{\omega'}(r_1, r_2, \mu-1, k)\frac{\partial}{\partial r_1}\frac{\partial}{\partial r_2}\mathcal{G}_\omega(r_2, r_1, \mu, k)\right\}$$

$$=\Phi^\dagger_{\mu-1}(r_2)\frac{\partial}{\partial r_2}\Phi_\mu(r_2)\Big/(i\tilde{\omega}'-E_{\mu-1,k})(i\tilde{\omega}-E_{\mu,k})\left\{\Phi^\dagger_\mu(r_1)\frac{\partial}{\partial r_1}\Phi_{\mu-1}(r_1)-\frac{\partial}{\partial r_1}[\Phi^\dagger_\mu(r_1)]\Phi_{\mu-1}(r_1)\right\} .$$

Here we have introduced a renormalized frequency in the usual way $\tilde{\omega}=\omega+(1/2\tau)\,\mathrm{sgn}(\omega)$ to take care of scattering.

From the third and fourth term in the curly brackets of Eq. (16) we get

$$-\frac{\partial}{\partial r_2}[\Phi^\dagger_{\mu-1}(r_2)]\Phi_\mu(r_2)\left\{\Phi^\dagger_\mu(r_1)\frac{\partial}{\partial r_1}\Phi_{\mu-1}(r_1)-\frac{\partial}{\partial r_1}[\Phi^\dagger_\mu(r_1)\Phi_{\mu-1}(r_1)\right\}\Big/(i\tilde{\omega}'-E_{\mu-1,k})(i\tilde{\omega}-E_{\mu,k})$$

for the $\mu-1$ terms.

When the integration over r_1 and r_2 is performed, we may carry out an integration by parts:

$$\int_0^\infty r\,dr\frac{\partial}{\partial r}[\Phi^\dagger_\mu(r)]\Phi_{\mu-1}(r)=r\Phi^\dagger_\mu(r)\Phi_{\mu-1}(r)\Big|_0^\infty-\int_0^\infty r\,dr\,\Phi^\dagger_\mu(r)\frac{\partial}{\partial r}\Phi_{\mu-1}(r)-\int_0^\infty dr\,\Phi^\dagger_\mu(r)\Phi_{\mu-1}(r) . \qquad (18)$$

The wave functions vanish at 0 and ∞ and the last integral is of order $(p_F\xi)^{-2}$ relative to the first. Therefore, the four terms we have considered may be approximated by

$$-4\frac{\partial}{\partial r_2}[\Phi^\dagger_{\mu-1}(r_2)]\Phi_\mu(r_2)\Phi^\dagger_\mu(r_1)\frac{\partial}{\partial r_1}\Phi_{\mu-1}(r_1)\Big/(i\tilde{\omega}'-E_{\mu-1,k})(i\tilde{\omega}-E_{\mu,k}) .$$

Similarly, the terms in $\mu+1$ give

$$-4\Phi^{\dagger}_{\mu+1}(r_2)\frac{\partial}{\partial r_2}\Phi_\mu(r_2)\frac{\partial}{\partial r_1}\left[\Phi^{\dagger}_{\mu}(r_1)\right]\Phi_{\mu+1}(r_1)\Big/(i\tilde{\omega}'-E_{\mu+1,k})(i\tilde{\omega}-E_{\mu,k}) \quad .$$

We have, therefore, for the integral of the correlation function

$$\int d\vec{r}_1 d\vec{r}_2\, \mathcal{P}_{xx}(\vec{r}_1,\vec{r}_2,\omega_0)=-\frac{Le^2}{4m^2c}T\sum_{w}\int_{-\infty}^{\infty}\frac{dk}{2\pi}\sum_{\mu}\left[\int r\,dr\,\Phi^{\dagger}_{\mu}(r)\frac{\partial}{\partial r}\Phi^{\dagger}_{\mu\pm1}(r)\right]^2$$

$$\times\{[1/(i\tilde{\omega}'-E_{\mu-1})][1/(i\tilde{\omega}-E_{\mu})]+[1/(i\tilde{\omega}'-E_{\mu+1})][1/(i\tilde{\omega}-E_{\mu})]\}\,. \tag{19}$$

Here we have employed the fact that the wave functions are real.

To a very good approximation

$$\left[\int r\,dr\Phi^{\dagger}_{\mu}(r)\frac{\partial}{\partial r}\Phi_{\mu\pm1}(r)\right]^2=p_F^2\sin^2\alpha \quad . \tag{20}$$

This is in part due to the fact that $(d/d\mu)\eta_\mu\sim1/p_F\xi$.[18]

The sum over ω and μ may easily be performed:

$$T\sum_{\omega}\sum_{\mu}[1/(i\tilde{\omega}'-E_{\mu-1})][1/(i\tilde{\omega}-E_{\mu})]+[1/(i\tilde{\omega}'-E_{\mu+1})][1/(i\tilde{\omega}-E_{\mu})]=(4\omega_0/\epsilon)\{1/[1+(\tau\epsilon)^2]\}\,.$$

We take $E=\mu\epsilon$, where ϵ is independent of μ. The sum over μ is converted to an integral and the limits of integration can be extended to $\pm\infty$, since the integral is convergent.

For ϵ we approximate

$$\epsilon\simeq(\Delta_\infty/p_F\xi\sin\alpha) \tag{21}$$

from Caroli and Matricon, and also $\epsilon\simeq(eH_{\text{eff}}/mc)=\omega_c$ from Bardeen *et al.*[16,18]

Performing the analytic continuation $\omega_0=-i\omega_1$, we have for the spatial integrals of the retarded correlation function

$$\int d\vec{r}_1\int d\vec{r}_2\,P^R_{xx}(\vec{r}_1,\vec{r}_2,\omega_1)=i\omega_1 L\frac{\sigma_n}{1+\langle(\omega_c\tau)^2\rangle}\,\xi^2\,\frac{9\pi^3}{16}\ , \tag{22}$$

which has the correct sign for positive resistance.

If we estimate $\int d\vec{r}_2\simeq\pi(a\xi)^2$ where $a\simeq2.4$, we find that the cores have a conductivity $\sigma_n/[1+\langle(\omega_c\tau)^2\rangle]$ equal to that of the normal metal in a magnetic field $\langle H_{\text{eff}}\rangle$. This is an interesting result often employed by theorists and experimentalists alike. Equation (22) demonstrates that our result for the diagonal component of the conductivity tensor is quite reasonable.

The off-diagonal component of $\mathcal{P}$ is given by

$$\mathcal{P}_{yx}(\vec{r}_1,\vec{r}_2,\omega_0)=\frac{e^2}{4m^2c}LT\sum_{\omega}\int_{-\infty}^{\infty}dk\sum_{\mu,\mu'}\frac{1}{(2\pi)^2}\left[\sin\theta_1\left(\frac{\partial}{\partial r_1}-\frac{\partial}{\partial r_1'}\right)+\frac{i}{r_1}\cos\theta_1(\mu+\mu')\right]$$

$$\times\left[\cos\theta_2\left(\frac{\partial}{\partial r_2}-\frac{\partial}{\partial r_2'}\right)-\frac{i}{r_2}\sin\theta_2(\mu+\mu')\right]e^{i(\mu'-\mu)(\theta_1-\theta_2)}\,\mathrm{Tr}\,[\mathcal{G}'_\omega(r_1,r_2',\mu',k)\,\mathcal{G}_\omega(r_2,r_1',\mu,k)]_{1=1',2=2'}\,. \tag{23}$$

Integrating over θ_1 and θ_2, we have

$$\int_{-\pi}^{\pi}d\theta_1\int_{-\pi}^{\pi}d\theta_2\mathcal{P}_{yx}(\vec{r}_1,\vec{r}_2,\omega_0)=-(Le^2/16m^2c)T\sum_{\omega}\int_{-\infty}^{\infty}(dk/2\pi)$$

$$\times\mathrm{Tr}\Big\{+i\frac{\partial}{\partial r_1}[\mathcal{G}_{\omega'}(r_1,r_2,\mu-1,k)-\mathcal{G}_{\omega'}(r_1,r_2,\mu+1,k)]\frac{\partial}{\partial r_2}\mathcal{G}_\omega(r_2,r_1,\mu,k)$$

$$-i[\mathcal{G}_{\omega'}(r_1,r_2,\mu-1,k)-\mathcal{G}_{\omega'}(r_1,r_2,\mu+1,k)]\frac{\partial}{\partial r_1}\frac{\partial}{\partial r_2}\mathcal{G}_\omega(r_2,r_1,\mu,k)$$

$$-i\frac{\partial}{\partial r_1}\frac{\partial}{\partial r_2}[\mathcal{G}_{\omega'}(r_1,r_2,\mu-1,k)-\mathcal{G}_{\omega'}(r_1,r_2,\mu+1,k)]\,\mathcal{G}_\omega(r_2,r_1,\mu,k)$$

$$+i\frac{\partial}{\partial r_2}[\mathcal{G}_{\omega'}(r_1,r_2,\mu-1,k)-\mathcal{G}_{\omega'}(r_1,r_2,\mu+1,k)]\frac{\partial}{\partial r_1}\mathcal{G}_\omega(r_2,r_1,\mu,k)$$

$$+i\frac{\partial}{\partial r_1}\frac{1}{r_2}\left[(2\mu-1)\mathcal{G}_{\omega'}(r_1,r_2,\mu-1,k)+(2\mu+1)\mathcal{G}_{\omega'}(r_1,r_2,\mu+1,k)\,\mathcal{G}_{\omega'}(r_2,r_1,\mu,k)\right]$$

$$-\frac{i}{r_2}\left[(2\mu-1)\mathcal{G}_{\omega'}(r_1,r_2,\mu-1,k)+(2\mu+1)\mathcal{G}_{\omega'}(r_1,r_2,\mu+1,k)\right]\frac{\partial}{\partial r_1}\mathcal{G}_{\omega}(r_2,r_1,\mu,k)$$

$$-\frac{i}{r_1}\left[(2\mu-1)\mathcal{G}_{\omega'}(r_1,r_2,\mu-1,k)+(2\mu+1)\mathcal{G}_{\omega'}(r_1,r_2,\mu+1,k)\right]\frac{\partial}{\partial r_2}\mathcal{G}_{\omega}(r_2,r_1,\mu,k)$$

$$+\frac{i}{r_1}\frac{\partial}{\partial r_2}\left[(2\mu-1)\mathcal{G}_{\omega'}(r_1,r_2,\mu-1,k)+(2\mu+1)\mathcal{G}_{\omega'}(r_1,r_2,\mu+1,k)\right]\mathcal{G}_{\omega}(r_2,r_1,\mu,k)$$

$$-\frac{i}{r_1r_2}\left[(2\mu-1)^2\mathcal{G}_{\omega'}(r_1,r_2,\mu-1,k)-(2\mu+1)^2\mathcal{G}_{\omega'}(r_1,r_2,\mu+1,k)\right]\mathcal{G}_{\omega}(r_2,r_1,\mu,k)\Big\}. \tag{24}$$

As in the case of the diagonal components of $\mathcal{P}$, we need only evaluate the first four terms in the curly brackets of Eq. (24). Here, however, the neglected terms are only of order $\mu^2(p_F\xi)^{-2}$ smaller than those kept. This is due to the fact that the terms in $\mu-1$ and $\mu+1$ subtract instead of add.

We have for the correlation function

$$\int d\vec{r}_1\int d\vec{r}_2\,\mathcal{P}_{yx}(\vec{r}_1,\vec{r}_2,\omega_0)=\Big(Le^2iT\sum\nolimits_\omega/4m^2c\Big)\int_{-\infty}^{\infty}\frac{dk}{2\pi}\sum\nolimits_\mu\left[\int r\,dr\,\Phi_\mu^\dagger(r)\frac{\partial}{\partial r}\Phi_{\mu\pm1}(r)\right]^2$$

$$\times\{[(i\tilde{\omega}'-E_{\mu-1})(i\tilde{\omega}-E_\mu)]^{-1}-[(i\tilde{\omega}'-E_{\mu+1})(i\tilde{\omega}-E_\mu)]^{-1}\}\quad . \tag{25}$$

Performing the sum over ω and μ, we have

$$T\sum\nolimits_\omega\sum\nolimits_\mu\{[(E_{\mu-1}-i\tilde{\omega}')(E_\mu-i\tilde{\omega})]^{-1}-[(E_{\mu+1}-i\tilde{\omega}')(E_\mu-i\tilde{\omega})]^{-1}\}=-i4\omega_0\tau^2/(1+\epsilon^2\tau^2). \tag{26}$$

The Hall angle is therefore given by

$$\tan\alpha=\int_0^\pi[1+\epsilon^2\tau^2]^{-1}\sin^3\alpha d\,\alpha\tau\Big/\int_0^\pi[\epsilon(1+\epsilon^2\tau^2)]^{-1}\sin^3\alpha d\alpha\ , \tag{27}$$

which is positive and of the correct sign for negative carriers.

For ϵ, we employ the result of Hansen as given by Bergk and Tewordt:[19,20]

$$\epsilon=(e/2mc)[(H_{c2}/\sin\alpha)+h(0)]\ , \tag{28}$$

where H_{c2} is the upper critical field and $h(0)$ is the field in the core of the vortex.

Our result for the tangent of the Hall angle can be expressed as

$$\tan\alpha=(e\,H_{\rm eff}/mc)\tau\ ,$$

where $H_{\rm eff}$ is a function of κ, the Ginzberg-Landau parameter, and of τ, the relaxation time. The dependence on τ, however, is very weak. As predicted by Bardeen *et al.*, $H_{\rm eff}$ is due in part to the actual field in the core of the vortex, $h(0)$, and due in part to the depression of the order parameter which gives an effective field of order H_{c2}.

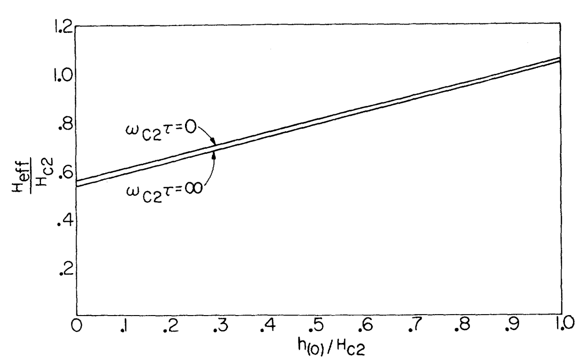

FIG. 1. $H_{\rm eff}/H_{c2}$ versus $h(0)/H_{c2}$ for $\omega_{c2}\tau=0$ and ∞. The tangent of the Hall angle is given by $\tan\alpha=(eH_{\rm eff}/mc)\tau$ and $\omega_{c2}=(eH_{c2}/mc)$. H_{c2} is the upper critical field and $h(0)$ the field in the core of the vortex. $h(0)/H_{c2}$ is inversely proportional to κ, the Ginzburg-Landau parameter.

In the ultra-clean limit, $l\to\infty$, we may neglect the 1 factor in Eq. (27) as compared to $(\epsilon\tau)^2$. For niobium at 0 °K, $p_F\xi\simeq 100$ and if we take $\mu=30$ as an upper bound for μ, we obtain a ratio $l/\xi\simeq 10$. For this value of μ, the terms neglected in $\mathcal{P}_{xx}$ are of order 0.003 and those for $\mathcal{P}_{yx}$ of order 0.1. Our theory is therefore valid for l/ξ ranging from ∞ to about 10.

For $l/\xi\sim 10$, $\tau\simeq 1/30$ so that $1+(\tau\epsilon)^2\simeq 1$. In Fig. 1, we plot H_{eff}/H_{c2} versus $h(0)/H_{c2}$ for $\omega_{c2}\tau=0$ and ∞, where $\omega_{c2}=eH_{c2}/mc$. For niobium $h(0)/H_{c2}\simeq 0.75$ and we have nearly $\tan\alpha=\omega_{c2}\tau$, which agrees with the experiment of Maxfield.[11]

Our calculation is performed in a frame at rest with the vortex. In this frame, the impurity scatters are moving at a velocity v_L. Our neglect of this fact probably introduces errors of order v_L/v_F which are clearly negligible.

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Orthogonalized-Plane-Wave Convergence of Some Tetrahedral Semiconductors

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The orthogonalized-plane-wave (OPW) series convergence up to 900 OPW's is illustrated for equal-core-size compounds C, Si, ZnSe, and CdTe, for large-cation-small-anion compounds ZnO, AIN, and Zns, and for large-anion-small-cation compounds BAs, BeTe, and ZnTe. Herman's overlapping-free-atom-potential model is used primarily, although self-consistent OPW convergence results are given for BAs. It is found that the first row of the Periodic Table is exceedingly difficult to handle with the OPW formalism. The primary factors involved in OPW convergence are found to be the presence or absence of core functions in the OPW's (which was realized long ago) and the relative core sizes of anion and cation. Criteria are given for estimating the OPW convergence behavior of compounds.

I. INTRODUCTION

A number of different techniques have been developed to calculate the energy-band structure of crystals. The best-known techniques are the augmented-plane-wave[1] (APW), Korringa-Kohn-Rostoker[2] (KKR), and the orthogonalized-plane-