Superconducting Gap Anisotropy Caused by a Spin-Density Wave

A. W. Overhauser and L. L. Daemen
Department of Physics, Purdue University, West Lafayette, Indiana 47907
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The Bardeen-Cooper-Schrieffer gap equation for $\Delta(\mathbf{k})$ is solved analytically for a simple metal having a spiral or linear spin-density wave. Δ falls to zero at the spin-density-wave energy gap for the spiral case, but falls to a finite (but small) value if the spin-density wave is linearly polarized. The electronic heat capacity in the superconducting state acquires a low-temperature tail, far in excess of a BCS exponential falloff, and similar to the (hitherto enigmatic) behavior observed in pure Pb.

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Twenty-five years ago Keesom and van der Hoeven[1] discovered that the electronic heat capacity in the superconducting state of pure Pb exhibits an unexpected low-temperature tail, as shown in Fig. 1. In recent years similar behavior was found in several heavy fermion systems, and data[2] for UBe_{13} are included for comparison. Some have argued that such a dependence is indicative of exotic pairing (e.g., spin triplet, as in ^{3}He). However, Pb is a paradigm of *s*-wave, spin-singlet superconductivity. Analysis of the Pb data was interpreted[3] in terms of an extremely anisotropic energy gap ($\Delta_{max}/\Delta_{min} \sim 4$), and the disappearance[3] of the anomalous tail for Pb-$In_{0.06}$ supports this conclusion (since scattering reduces gap anisotropy). Theoretical study of the gap equation, exploiting the known phonon spectrum and Fermi surface of Pb, does not allow a gap anisotropy much larger than ten percent.[4] In this paper we propose a surprising solution to this important and long-standing puzzle.

The possibility[5] that a free-electron metal could have a spiral or linear spin-density wave (SDW) has not been pursued. (The SDW ground state[6] in the *d band* of Cr is firmly established.[7] It is well known that superconductivity and antiferromagnetism are compatible.[8] We shall assume here that the SDW is a high-temperature phenomenon, and that its energy gap, $2G$ ($G \gg \Delta$), is constant at low temperature (unlike models[9] relevant to Chevrel compounds).

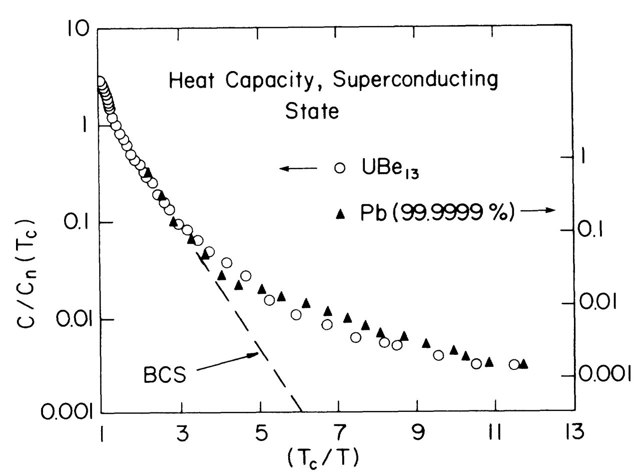

FIG. 1. Electronic heat capacity in the superconducting state for Pb and UBe_{13}. The dashed line is the behavior expected from BCS theory with small (or no) gap anisotropy.

We will demonstrate that the anisotropic gap equation for $\Delta(\mathbf{k})$, within the framework of Bardeen-Cooper-Schrieffer (BCS) theory, can be solved analytically. Consider first the spiral SDW case.[5] The one-electron Hamiltonian can be

$$H = (p^2/2m) - G(\sigma_x \cos Qz + \sigma_y \sin Qz) , \quad (1)$$

where $\{\sigma_i\}$ are the Pauli matrices and $\mathbf{Q} = 2k_F\hat{\mathbf{z}}$. The *exact* wave function for a (mostly) spin-up state is, for $k_z \geq -k_F$,

$$\phi_{\mathbf{k}\uparrow} = \cos\theta_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}\alpha + \sin\theta_{\mathbf{k}} e^{i(\mathbf{k}+\mathbf{Q})\cdot\mathbf{r}}\beta , \quad (2)$$

where α and β are Pauli spinors. The coefficients are

$$\sin\theta_{\mathbf{k}} = [(\hbar^2k^2/2m) - \epsilon_{\mathbf{k}}]/D , \quad (3)$$

$$\cos\theta_{\mathbf{k}} = G/D , \quad (4)$$

with $D \equiv [G^2 + (\epsilon_{\mathbf{k}} - \hbar^2k^2/2m)^2]^{1/2}$. The energy eigenvalue is

$$\epsilon_{\mathbf{k}} = \frac{\hbar^2}{4m}\{k^2 + |\mathbf{k}+\mathbf{Q}|^2 - [(k^2 - |\mathbf{k}+\mathbf{Q}|^2)^2 + (4mG/\hbar^2)^2]^{1/2}\} . \quad (5)$$

The "spin-up" Fermi surface is shown in Fig. 2(a) and is flattened by an energy gap, $2G$, at $k_z = -Q/2$.

The state $\phi_{\mathbf{k}\uparrow}$, Eq. (2), will be paired with its *degenerate* partner

$$\phi_{-\mathbf{k}\downarrow} = \cos\theta_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}}\beta + \sin\theta_{\mathbf{k}} e^{-i(\mathbf{k}+\mathbf{Q})\cdot\mathbf{r}}\alpha , \quad (6)$$

which is, however, *not* the time reverse of (2). The "spin-down" Fermi surface, not shown in Fig. 2(a), is flattened by an energy gap $k_z = Q/2$.[5] For every point, $\mathbf{r}$, (2) and (6) have opposite $\hat{z}$ components of spin, but have parallel $\hat{x}$ and $\hat{y}$ components.

In the BCS approximation the matrix element $V_{\mathbf{k}\mathbf{k}'}$, of the phonon-mediated interaction between plane-wave

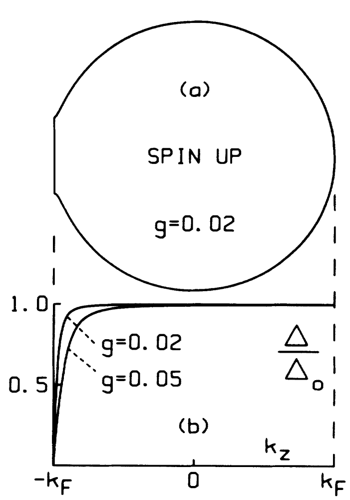

FIG. 2. (a) Fermi surface for the spin-up electrons of a metal having a spiral SDW. (b) Anisotropy of the superconducting gap parameter, $\Delta(k_z)$, for a spiral SDW. g is the (dimensionless) SDW-gap parameter, Eq. (9).

pairs $(\mathbf{k}\uparrow, -\mathbf{k}\downarrow)$ and $(\mathbf{k}'\uparrow, -\mathbf{k}'\downarrow)$ is taken as a constant, V. We adopt this simplification for "plane-wave" *contributions*. However, the matrix element of the pairing Hamiltonian for the SDW pairs, (2) and (6), is

$$V_{\mathbf{k}\mathbf{k}'} = V\cos(2\theta_{\mathbf{k}})\cos(2\theta_{\mathbf{k}}) . \tag{7}$$

Obtaining Eq. (7) is straightforward provided one observes that the virtual-scattering element now has an exchange term (as well as a direct one) on account of the spin admixtures in (2) and (6). The remarkable fact that $V_{\mathbf{k}\mathbf{k}'}$ appears in factorized form means that the gap equation can be solved analytically.[10] The result is immediate:

$$\Delta(\mathbf{k},T) = \Delta_0(T)\cos(2\theta_{\mathbf{k}}) . \tag{8}$$

Since $\theta_{\mathbf{k}} = 45°$ at the SDW energy gap, which can be seen from Eq. (4), Δ vanishes at the SDW gap. The Fermi-surface neck, shown in Fig. 2(a), has (in general) a finite circumference; so a spiral SDW produces a line of nodes on the Fermi surface. Such a feature automatically leads to a low-temperature, power-law tail in the heat capacity.

To illustrate the influence of the gap anisotropy, Eq. (8), on thermodynamic properties we define a dimensionless SDW-gap parameter:

$$g \equiv 2mG/\hbar^2Q^2 \approx G/4E_F . \tag{9}$$

Δ/Δ_0 is shown in Fig. 2(b) for several values of g. (Δ_0 varies with T in a way similar to the isotropic Δ of BCS theory.) Although the anisotropy of Δ is enormous, it is confined to a small fraction of the Fermi surface near the SDW gap. In the weak coupling limit the equation for T_c can be solved exactly. One finds a BCS-type result:

$$k_BT_c = 1.14\hbar\omega_D \exp(-1/\lambda_{\text{eff}}) , \tag{10}$$

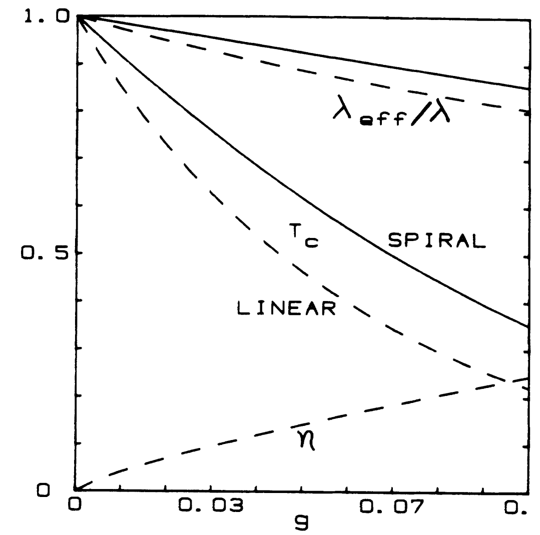

FIG. 3. g dependence of λ_{eff} and T_c (from McMillan's equation with $\lambda = 0.4$, $u^* = 0.1$). $\eta\Delta_0$ is the superconducting gap parameter at the (linear) SDW gap. ($\eta \equiv 0$ for the spiral case.)

the only difference being that λ is replaced by

$$\lambda_{\text{eff}} \equiv \lambda[1 - g\arctan(1/g)] . \tag{11}$$

It is interesting to substitute λ_{eff} for λ in McMillan's formula[11] for T_c. Figure 3 shows λ_{eff} and T_c vs g. Superconductivity is quenched by a large SDW gap. This effect has been envisioned[12] for Li, which is not superconducting, but which should (otherwise) have $T_c \sim 2$ K.

The electronic heat capacity $C_{es}(T)$ can be obtained by numerical evaluation of[13]

$$C_{es} = \frac{2}{k_BT^2}\sum_{\mathbf{k}} f_{\mathbf{k}}(1-f_{\mathbf{k}})\left[(\epsilon_{\mathbf{k}} - E_F)^2 + \Delta^2 - T\Delta\frac{\partial\Delta}{\partial T}\right] . \tag{12}$$

$f_{\mathbf{k}}$ is, of course, the Fermi-Dirac function. $C_{es}(T)$ is shown in Fig. 4 for three values of g. The asymptotic behavior of each tail is $\sim T^2$.

The theory for a linear SDW is more complicated, so we shall quote the results from a detailed study.[14] The one-electron Hamiltonian can now be

$$H = (p^2/2m) - 2G\sigma_z\cos Qz . \tag{13}$$

For small G the solutions may be approximated as a linear combination of two plane waves.[15] For $-\frac{1}{2}Q < k_z < 0$,

$$\phi_{\mathbf{k}\uparrow} \cong (\cos\theta_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}} + \sin\theta_{\mathbf{k}}e^{i(\mathbf{k}+\mathbf{Q})\cdot\mathbf{r}})\alpha , \tag{14}$$

$$\phi_{\mathbf{k}} \cong (\sin\theta_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}} - \cos\theta_{\mathbf{k}}e^{i(\mathbf{k}+\mathbf{Q})\cdot\mathbf{r}})\beta , \tag{15}$$

where $\sin\theta_{\mathbf{k}}$ and $\cos\theta_{\mathbf{k}}$ are the same as in Eqs. (3) and (4). The solutions for $0 < k_z < \frac{1}{2}Q$ mix $|k\rangle$ and

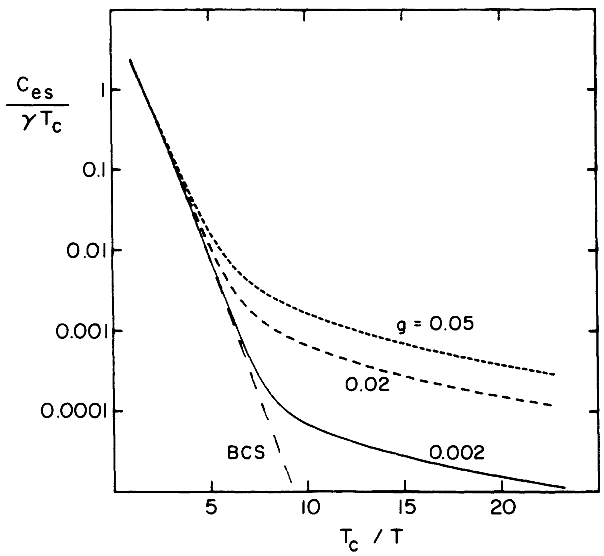

FIG. 4. Electronic heat capacity in the superconducting state vs T_c/T for a spiral SDW.

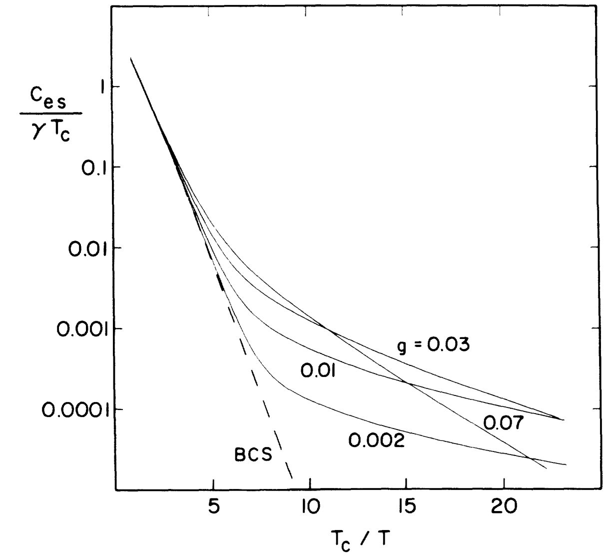

FIG. 5. Electronic heat capacity in the superconducting state vs T_c/T for a linear SDW.

$|\mathbf{k}-\mathbf{Q}\rangle$. The virtual-scattering matrix element, taking a pair from $(\phi_{\mathbf{k}\uparrow},\phi_{-\mathbf{k}\downarrow})$ to $(\phi_{\mathbf{k}'\uparrow},\phi_{-\mathbf{k}'\downarrow})$ is now more complicated than Eq. (7), even though there is no longer an exchange term:

$$V_{\mathbf{k}\mathbf{k}'} = V[\cos(2\theta_{\mathbf{k}})\cos(2\theta_{\mathbf{k}'}) + \tfrac{1}{2}\sin(2\theta_{\mathbf{k}})\sin(2\theta_{\mathbf{k}'})]\,. \quad (16)$$

We have again embraced the BCS constant-V approximation for plane-wave contributions. The origin of the complexity in (16) is the fact that each coupling can occur through virtual emission of phonons $\mathbf{q}$, $\mathbf{q}+\mathbf{Q}$, and $\mathbf{q}-\mathbf{Q}$.

The Markowitz-Kadanoff theory[10] can no longer be used because $V_{\mathbf{k}\mathbf{k}'}$ does not have a factorized form. However, the BCS gap equation with (16) for the kernel can still be solved exactly. After considerable work, we found

$$\Delta(\mathbf{k},T) = \Delta_0(T)[\cos(2\theta_{\mathbf{k}}) + \eta\sin(2\theta_{\mathbf{k}})]\,, \quad (17)$$

where η is independent of T:

$$\eta = u/2[(\lambda_{\text{eff}}/\lambda) - v]\,, \quad (18)$$

where $u \equiv g\ln[1+(1/4g^2)]$, $v \equiv g\arctan(1/2g)$, g is still defined by Eq. (9), and

$$\lambda_{\text{eff}}/\lambda = \tfrac{1}{2}\{1 - v + [(1-3v)^2 + 2u^2]^{1/2}\}\,. \quad (19)$$

The variations of λ_{eff}, T_c, and η (with g) for the linear SDW case are shown by the dashed curves in Fig. 3.

Finally, we have calculated C_{es} from Eq. (12), and the results are displayed in Fig. 5. The second term of Eq. (17) prevents Δ from falling to zero at $k_z = \pm\frac{1}{2}Q$, the linear SDW gaps, but Δ does fall to a small value, $\eta\Delta_0$, shown in Fig. 3. In the low-T limit, C_{es} reverts to an exponential falloff, but to one having a much smaller slope than ideal BCS behavior.

The foregoing theory shows that a heat-capacity tail similar to that observed in Pb can be caused by the presence of SDW's. Since an alternative explanation has not been forthcoming despite the challenge lasting one-quarter of a century, we propose that Pb may have a cubic family of small-amplitude, linear SDW's: e.g., $\mathbf{Q}$'s along twelve {211} axes. The only sure test of such a suggestion would be observation of magnetic satellite reflections by neutron diffraction. Failure to have noticed small gaps in tunneling studies[16] of Pb might be attributed to the fact that normal tunneling directions are [111] or [100]. The discrepancy[17] between λ determined from T_c and λ determined from tunneling, transport, or heat capacity, may be the SDW effect given by Eq. (19).

It is possible to estimate the SDW transition temperature T_{SDW} from the data in Fig. 1. We suppose that Pb has twelve linear SDW's. The heat-capacity tail (near $T_c/T=11$) caused by each SDW would be about $\frac{1}{12}$ of the value shown in Fig. 1, i.e., slightly above the curve for $g=0.002$ in Fig. 5. It follows from Eq. (9) that each SDW energy gap is $2G \sim 0.2$ eV. Since $2G \sim 3.5kT_{\text{SDW}}$,[18] we find $T_{\text{SDW}} \sim 660$ K, which is above the melting point. Accordingly we would not anticipate transport anomalies caused by a SDW phase transition in the normal state of (crystalline) Pb.

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