SURFACE STATES AND ADDITIONAL STRUCTURE IN THE McMILLAN-ANDERSON MODEL FOR THE TOMASCH EFFECT

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Recently McMillan and Anderson (M.A.)[1] suggested that oscillations in the tunneling characteristics observed by Tomasch[2,3] in superconducting films could be understood as a quasiparticle interference effect resulting from an energy-gap perturbation at the film surface. They calculated (first Born approximation) the change in the local quasiparticle density of states at the plane $x=0$ due to a gap perturbation $H'\delta(x-d)$ on the plane at d, and found a damped oscillatory term whose period was in excellent agreement with experiment.[2,3] In addition to a dominant series of this form, Tomasch[4] has reported the observation of extra structure in Pb, In, and Sn.

We have solved the M.A. model exactly in order to determine what additional structure is contained in the model. Some of the features of the exact solution are these: (1) Only the fundamental period occurs in the exact solution for the change in the density of states, $\delta N(\omega)$; (2) an additional oscillatory term with the fundamental period but phase shifted by $\pi/2$ from the first Born term and of comparable amplitude occurs in $\delta N(\omega)$ at energies near the gap; (3) surface eigenstates exist both below and above the energy gap. Estimates indicate that the band edge, ω_m, of these surface states extends quite far into the energy-gap region. The density of states varies as $(\omega^2-\omega_m{}^2)^{-1/2}$ near this band edge.

The exact change in the Green's function for an infinite superconductor with a gap perturbation $H'\delta(x-d)$ on the plane at $x=d$ (definition of M.A. model) is

$$\delta G(rr') = [1/(2\pi)^2]\int d^2k_\perp \exp[-ik_\perp\cdot(\rho-\rho')]g(k_\perp;x,x'),$$

$$g(k_\perp;x,x') = g^0(k_\perp;x-d)H'[I-g^0(k_\perp;0)H']^{-1}g^0(k_\perp;d-x'), \tag{1}$$

with

$$g^0(k_\perp;x-x') = S(x-x')(\omega+\varphi\tau_1)+D(x-x')\Omega\tau_3,$$

$$\left.\begin{matrix} S(x-x') \\ D(x-x') \end{matrix}\right\} = \frac{-im}{2\hbar^2\Omega}\left[\frac{\exp(ik^+|x-x'|)}{k^+} \pm \frac{\exp(-ik^-|x-x'|)}{k^-}\right],$$

$$k^\pm = (k_F{}^2-k^2 \pm 2m\Omega/\hbar^2)^{1/2} \quad \text{(imaginary part of } k^\pm \text{ is } \pm),$$

$$\Omega = (z^2\omega^2-\varphi^2)^{1/2}, \quad H'=\chi\tau_1, \quad \tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{2}$$

where k_F is the Fermi wave vector, z is the renormalization constant, and φ is the off-diagonal self-energy parameter in the Nambu theory.[5] The Born series can be generated by expanding the inverse in Eq. (1), obtaining a series in which the nth term can be interpreted as a particle propagating from x' to the perturbation surface, interacting with the potential H' n times at the surface and then propagating to x. For $x=x'=0$, all terms involve only the distance $2d$, and only the fundamental period occurs in $\delta N(\omega)$ for this model. Replacing the inverse by unity gives the M.A. result which predicts a δN which varies as Ω^{-2}. (Higher order terms depend upon higher powers of $1/\Omega$.) This nonintegrable singularity in the density of states is incorrect as $\Omega\to 0$, since perturbation theory fails in this limit.

The exact result shows that $\delta N \sim \Omega^{-1}$ as $\Omega \to 0$. The series also breaks down when the inverse is singular (a circumstance which does occur and corresponds to the existence of surface eigenstates). For these reasons it is important to work with the exact result. The change in the density of states at $x=0$ is given by

$$\delta N(\omega) = \frac{-1}{\pi}\operatorname{Im}\operatorname{Tr}\int d^2k_\perp g(k_\perp,0), \tag{3}$$

where Im indicates the imaginary part and Tr the trace. The perturbation H' gives rise to three effects in the density of states: high-frequency ($\hbar\omega \sim 2E_F$, E_F = Fermi energy) oscillations of negligible amplitude, low-frequency oscillations identified with the Tomasch effect, and, finally, terms corresponding to surface states. The exact result for the Tomasch term is

$$\delta N_T(\omega) = -\mathrm{Im}\left(\frac{m^2\omega\varphi^2 t}{\pi^2\hbar^4\Omega^2 k_F}\right)\int_0^\infty \frac{k_\perp dk_\perp \exp[i(k^+-k^-)d]}{k^+k^- \det}, \quad (4)$$

where we have introduced a dimensionless measure of the range of perturbation, t, by means of the relation $\chi = \varphi/k_F t$. Equation (4) is valid for the change in the density of states at any plane x by replacing d by $|x-d|$. The integral in Eq. (4) may be evaluated by contour integration. In order to do this, however, we must first discuss the structure of "det." This function may be written as

$$\det = \frac{(\Omega/\varphi)^2 - \alpha^4 + K^2\alpha^2 + 2iK\alpha}{(\Omega/\varphi)^2 - \alpha^4},$$

$$\alpha = \frac{(k^+-k^-)}{(4m\varphi/\hbar^2)},$$

$$K = \pm\left(\frac{m\chi^2}{\hbar^2\varphi}\right)^{1/2} = \pm\left(\frac{\varphi}{2E_F}\right)^{1/2} t$$

$$(\text{take} \pm \text{root as } \chi \gtrless 0). \quad (5)$$

As $k_\perp$ varies from 0 to ∞, α traces out the contour ζ in the complex plane as follows: along the real axis from $\alpha_T = \Omega/(2E_F\varphi)^{1/2}$ to $(\Omega/\varphi)^{1/2}$, then a 90° segment of a circle of radius $(\Omega/\varphi)^{1/2}$ arriving at the imaginary axis, then $i(\Omega/\varphi)^{1/2}$ to $+i\infty$. For $\omega^2 < \varphi^2$, Ω is replaced by $iW \equiv i(\varphi^2-\omega^2)^{1/2}$ and ζ is entirely along the imaginary axis, extending from $\eta_T = iW/(2E_F\varphi)^{1/2}$ to $+i\infty$.

New eigenstates created by the perturbation will show up as poles of g on the contour, that is, as zeros of det on the contour. Zeros off but near ζ correspond to approximate eigenstates with finite lifetimes. From Eq. (5) it is clear that the roots of det lie on the physical contour only for a gap reduction ($\chi < 0$), and only when α is pure imaginary. Writing $\alpha = i\eta$, one has

$$(K\eta-1)^2 + \eta^4 - (\omega/\varphi)^2 = 0. \quad (6)$$

There are no real roots of Eq. (6) for ω less than some minimum value ω_m. For choices of t appropriate to the Tomasch effect, $K\eta \ll 1$, so that

$$W_m/\varphi = (1-\omega_m^2/\varphi^2)^{1/2} \approx (\tfrac{3}{4})^{1/2}K = (3\varphi/8E_F)^{1/2}t. \quad (7)$$

This minimum lies within the gap region of the unperturbed states. If $|\omega| > \omega_m$, there are two real roots, η_1 and η_2, and near ω_m both roots lie on the ζ and correspond to two energy bands. As ω approaches φ, η_1 moves off ζ. η_2 persists above the gap region to a maximum energy given by $\Omega_c = 4/K^2$ above which there are no new eigenstates. These new eigenstates correspond to quasiparticle states with $k_\perp \gtrless k_F$ but decaying exponentially in the x direction away from the plane of the perturbation. It can be easily shown that the density of states varies as $(\omega^2-\omega_m^2)^{-1/2}$ near ω_m and resembles a BCS structure whose effective gap is ω_m. Since these quasiparticles are traveling parallel to the film surface, it is unlikely that they would contribute to the tunneling current in a typical tunneling experiment which measures principally electrons traveling normal to the film. On the other hand, if such states exist at a free surface of a real finite superconductor, they would give rise to effects similar to the so-called "precursor" effect seen in infrared absorption experiments.[6] Since the model is so highly schematic, this suggestion should be regarded at this stage as speculative.

For a positive gap perturbation there are no surface eigenstates, although there are poles close to the physical contour corresponding to long-lived states which will produce scattering resonances.

Returning to the $\delta N_T(\omega)$ of Eq. (4), we note that the integral may be written as an integral with the complex variable α over the contour ζ. After some manipulation one obtains by contour integration

$$\mathrm{Si}\left(\frac{2\Omega d}{hv_F}\right) + \mathrm{Im}K\int_0^{\alpha_T} d\alpha \frac{\exp[2i(m\varphi/\hbar^2)^{1/2}\alpha d](K\alpha+2i)}{(\Omega/\varphi)^2-\alpha^4+K^2\alpha^2+2iK\alpha}$$

$$+\pi\sum_i [R_r(i) - R_l(i)]. \quad (8)$$

The first term corresponds exactly to the M.A. result for the first Born approximation, where

$$\mathrm{Si}(x) = \int_x^\infty \frac{\sin y}{y} dy. \quad (9)$$

The second term gives additional structure resulting from all higher order terms in a Born series. The last term is the contribution due to surface states. In this expression $R_r(i)$ is the residue of the integrand in Eq. (4) at the ith pole which occurs in the upper half complex plane to the right of the contour ζ, while $R_l(i)$ is the residue to the left of ζ in the upper half plane. (Poles on the contour are treated by letting $\Omega \to \Omega + i0^+$.) The ratio of the change in the density of states due to the first Born term to the unperturbed BCS density of states, $N(\omega)$, is

$$\frac{\delta N_{\mathrm{T}}^{(1)}(\omega)}{N(\omega)} = \frac{\varphi^2 t}{2\Omega E_{\mathrm{F}}} \mathrm{Si}\left(\frac{2\Omega}{\hbar v_f} d\right), \quad \frac{\Omega}{\varphi} \gg \left(\frac{\varphi}{E_{\mathrm{F}}}\right) t,$$

$$N(\omega) = \frac{\omega}{\Omega} \frac{m k_{\mathrm{F}}}{\pi^2 \hbar^2}. \tag{10}$$

We may estimate t by requiring this ratio to be of the order of 10^{-2} at $(2\Omega/\hbar v_{\mathrm{F}})d = \pi$ (~1% Tomasch effect in dV/dI). Taking $(\varphi/E_{\mathrm{F}}) \sim 3 \times 10^{-4}$ and $k_{\mathrm{F}} d \sim 10^5$, one obtains $t \sim 40$. For this value of t, the second term in Eq. (8) contributes

$$\frac{\delta N_{\mathrm{T}}^{(2)}(\omega)}{N(\omega)} \approx \left(\frac{\varphi^2 t}{2\Omega E_{\mathrm{F}}}\right)\left[\frac{t}{k_{\mathrm{F}} d}\left(\frac{\varphi}{\Omega}\right)^2\right] \sin\left(\frac{2\Omega d}{\hbar v_{\mathrm{F}}}\right),$$

$$\frac{\Omega}{\varphi} \gg \left(\frac{\varphi}{E_{\mathrm{F}}}\right) t. \tag{11}$$

This term is also of the order of 1% at its first maximum and thus comparable to the first Born term and shifted in phase by $\pi/2$. One observes the total δN, and it may not be possible to decompose this into the two terms. A careful study of the amplitude of δN with Ω should, however, reveal the presence of $\delta N_{\mathrm{T}}^{(2)}$ since it varies as Ω^{-4}. One would expect δN to vary initially as Ω^{-4} and change to Ω^{-3} as the energy increases.

It is also interesting to note for $t = 40$ that the surface-states band edge occurs according to Eq. (7) at $\omega_m \approx 0.8\varphi$ so that such a system has a double gap. If these surface states exist in real films, it may be possible to observe their effects in a tunneling experiment in which the edges of two films are separated by an insulating barrier.

In conclusion we would like to make a simple observation concerning the effect of an ordinary potential perturbation. If one considers a perturbation $V\tau_3\delta(x-d)$ at the film surface, it is readily seen that this induces a localized gap perturbation at the surface whose magnitude in the first approximation will be linear in V and of opposite sign. This gap perturbation will then induce oscillations in the density of states whose amplitude is linear in V, so that to first order, an ordinary potential perturbation can give rise to a Tomasch effect.

[1] W. L. McMillan and P. W. Anderson, Phys. Rev. Letters 16, 85 (1966).

[2] W. J. Tomasch, Phys. Rev. Letters 15, 672 (1965); 16, 16 (1966).

[3] W. J. Tomasch and T. Wolfram, Phys. Rev. Letters 16, 352 (1966).

[4] See Ref. 2 and also W. J. Tomasch, to be published, and Bull. Am. Phys. Soc. 11, 190 (1966).

[5] Y. Nambu, Phys. Rev. 17, 648 (1960).

[6] See, for example, P. L. Richards and M. Tinkham, Phys. Rev. 119, 575 (1960). Some more recent experiments have failed to show the precursor [L. H. Palmer, thesis, University of California, 1966 (unpublished)], so that the reality of the effect is subject to question.

OBSERVATION OF RESONANT STRUCTURES AT 20- TO 23-MeV EXCITATION IN Si^{30} THROUGH THE REACTION $Mg^{26}(\alpha, \alpha)Mg^{26}$†

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Recently, large fluctuations in nuclear cross sections have been observed for many reactions at high excitations where the ratio of average compound nucleus width to average compound nucleus spacing, $\langle\Gamma_{CN}\rangle/\langle D_{CN}\rangle$, is larger than unity. Such data have been extensively analyzed in terms of the Ericson fluctuation theory[1] to extract such nuclear parameters as $\langle\Gamma_{CN}\rangle$. Block and Feshbach[2] and Kerman, Rodberg, and Young[3] have suggested that some of the structure might be due to particularly simple modes of excitation of the nucleus, e.g., two-particle, one-hole (2p1h) states. These states would have unique angular momentum and parity and would have widths which are intermediate between those of the states of the com-