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LOCALIZED MAGNETIC STATES AND FERMI-SURFACE ANOMALIES IN TUNNELING

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(Received 6 June 1966)

The purpose of this paper is to provide a physical model for the interactions proposed by Appelbaum which he used to explain Fermi-surface anomalies in tunneling. We also evaluate these interactions and show why the anomalous conductance need not be small compared to the direct tunneling.

Appelbaum[1] has recently explained some of the anomalous variations of the tunneling conductance which are frequently observed near zero-bias voltage in terms of exchange interactions between tunneling electrons and magnetic states in, or near, the insulating layer of the tunnel junction. These anomalous variations are observed both in tunneling between degenerate semiconductors[2,3] and between metals,[4,5] and in the latter case depend to some extent on the metal, on the insulator, and on junction preparation.[5] Characteristically, in the simplest cases, a peak in conductance, logarithmic in some homogeneous function of V and T, is observed.[5]

The purpose of this Letter is to provide a physical model for the interactions postulated by Appelbaum, which also evaluates them and demonstrates why the anomalous conductance need not be small compared to the direct tunneling.

Appelbaum's explanation assumed an exchange type of interaction between a localized spin $\vec{S}$, somewhere near the tunneling layer, and electrons in the two degenerate Fermi gases described by operators $a_{k\sigma}^*, a_{k\sigma}$ for metal 1, $b_{q\sigma}^*, b_{q\sigma}$ for metal 2:

$$\mathcal{H}_{\text{int}} = \sum_{kk'\sigma\sigma'} \{\vec{S}\cdot(\vec{\tau})_{\sigma\sigma'}[J(a_{k\sigma}^* a_{k'\sigma'}) + T_J(a_{k\sigma}^* b_{k'\sigma'} + b_{k\sigma}^* a_{k'\sigma'})]\}. \quad (1)$$

(Appelbaum's Hamiltonian is symmetric in the two metals, but this is neither necessary nor, as we shall see, likely). $\vec{\tau}$ is the Pauli spin operator, and J and T_J are exchange and exchange-tunneling interactions between the local moment and the metals.

The anomalous term appears to order JT_J^2 and is, in the simplest case, of the form

$$\Delta G(0) = J\rho_a(0)[(16\pi e^2/\hbar)T_J^2 S(S+1)\rho_a(0)\rho_b(0)] \times \ln[E_0/(|eV|+kT)]. \quad (2)$$

ρ_a and ρ_b are the metallic densities of states;

E_0 is a cutoff energy for the densities and coefficients J and T_J; the Fermi energy is taken as zero; and other symbols have their usual meanings.

The model we propose is the following: On or near the surface of one of the metals we assume there are a number of quasilocalized electron orbitals φ_d. These orbitals may represent either d orbitals on impurities in the oxide (or interstitial metal atoms, if we consider a case such as Ta or Nb) or surface states on the metal extending into the oxide. The basic criteria for these states is that they be rather well localized, and that the bulk of their amplitude should be in the oxide layer where the Coulomb self-interaction cannot be screened out by the metallic electrons. One may think of these states, whether surface states[6] or impurity states,[7] as scattering resonances from the point of view of the nearer metal, and the above criteria may be stated more precisely: Their widths Δ should be rather small compared with their internal Coulomb and/or exchange interactions.

Under these circumstances a suitable approximate Hamiltonian[7] is

$$\mathcal{H}=\sum_{k\sigma}\epsilon_k a_{k\sigma}{}^* a_{k\sigma}+\sum_{q\sigma}\epsilon_q b_{q\sigma}{}^* b_{q\sigma}+\sum_{\sigma}\epsilon_d n_{d\sigma}+Un_{d\uparrow}n_{d\downarrow}$$
$$+\sum_{k\sigma}V_{kd}(a_{k\sigma}{}^* d_\sigma+d_\sigma{}^* a_{k\sigma})$$
$$+\sum_{q\sigma}T_{qd}(b_{q\sigma}{}^* d_\sigma+d_\sigma{}^* b_{q\sigma}), \qquad (3)$$

where $n_{d\sigma}=d_\sigma{}^* d_\sigma$ is the number operator for electrons in φ_d. Here ϵ_d is the energy of a single electron in the state φ_d; ϵ_d+U that necessary to add a second; and these energies should bracket the Fermi energy

$$\epsilon_d+U>0>\epsilon_d,$$

and also be large compared to the width Δ,

$$\Delta=\pi\langle|V_{kd}|^2\rangle\rho_a(0)\ll U.$$

If the thickness of the junction is t, if we assume the localized state to be on the average a distance d from metal A ($d\ll t$), and if the decay constant of the electron wave functions into the oxide is (E_C is the conduction-band level)

$$k\cong\hbar^{-1}(2m^*E_c)^{1/2},$$

V will be proportional to e^{-kd} and T to $e^{-k(t-d)}$, so their product will be of the same exponential order as the direct tunneling matrix element $T'\sim e^{-kt}$. In fact, if the localized state is to be a meaningful object, $VT/(\epsilon_d+U)$ is in a sense greater than the coresponding matrix element T' because $\epsilon_d+U<E_C$. The localized state is at a favorable energy and should represent an easy route for tunneling. Thus, such states, if present in any appreciable concentration, may carry a rather large fraction of the tunnel current.

Now the recent paper of Schrieffer and Wolff[8] shows formally that a canonical transformation on Eq. (3) gives precisely Appelbaum's Hamiltonian in Eq. (1). Equation (3) is identical to the usual, localized-state Hamiltonian, if we simply realize that the two types of free-electron states will interact simultaneously with the impurity and may be treated formally as though they were in the same metal, so that both J and T_J appear as parts of the exchange scattering interaction $J(\mathbf{S}_{\rm loc}\cdot\mathbf{S}_{\rm free})$. We need not repeat the derivation, but we give the following values for the constants in Eq. (1):

$$J_{kk'}=2V_{kd}V_{dk'}U/\epsilon_d(\epsilon_d+U),$$
$$T_{kk'}=2V_{kd}T_{dk'}U/\epsilon_d(\epsilon_d+U). \qquad (4)$$

With these values, and realizing that direct tunneling will be proportional to $|T'|^2\rho_a(0)\rho_b(0)$, the ratio of Appelbaum's term to direct tunneling is proportional to

$$\frac{\rho_a(0)|V|^4|T|^2}{|T'|^2}\,\frac{U^3}{\epsilon_d{}^3(\epsilon_d+U)^3}$$
$$=\left(\frac{\Delta}{U}\right)\left[\frac{|V|^2|T|^2}{\epsilon_d(\epsilon_d+U)|T'|^2}\right]\left[\frac{U^2}{\epsilon_d(\epsilon_d+U)}\right]^2. \qquad (5)$$

This is clearly highly dependent on all the parameters but need not be small: The last factor cannot be less than 16 or greater than $(U/\Delta)^2$, and the second factor is basically the ratio which is large if tunneling via the energy minimum causing the localized state is easier than direct tunneling. {Another way of putting it is that $|V|^2|T|^2[(\epsilon_d)^{-2}+(\epsilon_d+U)^{-2}]$ is the coefficient of direct, ordinary tunneling via the localized state, as may also be seen from Ref. (8).} We are left with Δ/U, and while this must be small to localize the state, it need not be much less than ~0.1. It is clear, however, that the requirement $d\ll t$ (i.e., $V\gg T$) is essential:

Localized states deep within the layer will not show the effect. If either ϵ_d or $\epsilon_d + U$ is close to the Fermi level, the effect may even become quite large with respect to direct tunneling.

Physically, what appears to be going on is that the one-electron Green's function on the "d" state is exhibiting a logarithmic peak near the Fermi surface caused by its exchange interaction with the nearby metal,[9] and tunneling to the second metal is measuring this peak in the usual way.

I am indebted to W. L. McMillan, J. M. Rowell, J. C. Phillips, Joel Appelbaum, and L. Dworin for helpful and/or stimulating discussion.

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ANOMALIES IN THE SPIN-ORBIT TERM OF THE OPTICAL MODEL POTENTIAL

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(Received 2 May 1966)

The elastic scattering of 18.5- and 20.5-MeV polarized protons from complex nuclei was studied extensively at this laboratory during the last few years.[1,2] In the course of this investigation, large differences in the polarization were observed in the scattering of 18.5-MeV protons from Ar^{40} and Ca^{40}.[3]

An automated computer search program (prepared by H. C. Volkin and C. C. Giamati of this Center) was used to analyze the polarization data from this laboratory in terms of the optical model to investigate the spin-orbit potential dependence on proton energy and target mass, and, possibly, to find an interpretation for the Ar^{40}-Ca^{40} polarization difference.

Because the differential cross-section data for each set of polarization data were lacking, the two step procedure applied by Ball[4] and Durisch and Gould[5] for studying the symmetry term has been used. First, average sets of geometric and well-depth parameters were obtained for the real and imaginary potentials from analyzing 37 polarization angular distributions at 16.5, 18.5, and 20.5 MeV, 20 differential cross sections at 17.0 and 22.2 MeV,[6,7] and six reaction cross-section data at 16.4 MeV.[8] Second, only the parameters of the spin-orbit potential were permitted to vary in searches to produce optimum fits to the polarization data. The spin-orbit parameters thus obtained have been studied for systematic tendencies.

The first step was started from the average set of parameters proposed by Rosen,[9] and various individual and simultaneous searches on different parameters were made by minimizing both χ_σ^2 and χ_p^2 with the reaction cross section serving as a guide. Two similar compromise sets of parameters were found. Set (a) produces, on the average, good fits to the polarizations and differential cross sections, but it is inferior in predicting the reaction cross sections; set (b) behaves conversely. The parameters are as follows:

V	W_D	V_{so}	a	a_I	a_{so}	r_0	r_I	r_{so}
(a) V_{Perey}[a]	$2A^{1/3}$	5.5	0.65	0.65	0.65	1.25	1.25	1.1
(b) V_{Perey}[a]	$1.5A^{1/3}+2.5$	5.5	0.65	$0.45+A/650$	0.65	1.25	1.25	1.1

[a]V_{Perey} is taken from F. G. Perey, Phys. Rev. 131, 745 (1963).

The real and imaginary well parameters of set (a) were chosen to begin step two. In this step, only the parameters of the spin-orbit potential were varied to produce optimum fits to the polarization data. The analysis under such restricted conditions was considered permissible, since it is essentially the polarization that defines the V_{so}, a_{so}, r_{so} parameter space. The optimum values for V_{so},