Role of barrier fluctuations in tunneling in a metal

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The interaction of a tunneling particle with fluctuations of the barrier between potential wells is analyzed. This interaction is usually weak and therefore ignored, but the infrared infinity in the rescattering of electron excitations near the Fermi surface significantly strengthens the inelastic interwell transitions which result from the shaking of the barrier. This problem is closely related to the general question of the validity of replacing an electron heat reservoir by a phonon heat reservoir, since rescattering plays no role in the latter case. A simple method is developed for directly solving the kinetic problem in a case with barrier fluctuations, for an arbitrary interaction of the tunneling particle with the electrons. This method is based on the overlap integrals of the intrawell wave functions of the system. The effective scattering phase shifts must satisfy a certain condition if substantial changes in the dynamics of the system and in the structure of the ground state are to be possible in principle. This condition is found. A rigorous analysis shows, however, that there are no parameter values of the two-well problem for which the inelastic mechanism for a transition between wells, involving changes in the barrier, can become the dominant mechanism, while the coherent amplitude varies only slightly. It is thus shown that the approximate replacement of the electron reservoir by the phonon reservoir is justified in most tunneling problems.

1. INTRODUCTION

In an analysis of the tunneling of particles in a two-well potential or in a regular crystal, there are typically two mechanisms for interaction with excitations of the medium. The first is intrawell interaction, which leads to a polaron effect and which predetermines disruption of the coherent coupling between wells or dynamic destruction of a band. At higher temperatures this mechanism leads to incoherent transitions with "shaking" of the polaron "coat." The intrawell scattering does not depend on the overlap integral.

The second mechanism involves fluctuations of the barrier resulting from the interaction with electron or phonon excitations. An analysis of the tunneling in an insulator has revealed that at low temperatures and with a limited asymmetry of the wells, $\xi(T,\xi \ll \omega)$, the second mechanism always plays a minor role, a measure of which is the parameter

$$\left[\frac{(\Omega_T, \xi)_{max}}{\omega}\right]^2 \ll 1, \tag{1.1}$$

in a perturbation-theory approach. Here ω is a characteristic frequency of the motion of the tunneling particle in the potential relief, and Ω_T is the rate of decay of an element of the density matrix which is not diagonal in terms of the wells.[1]

If the interaction with phonons is strong, the existence of this second mechanism leads to a so-called fluctuational preparation of the barrier.[2] This effect is essentially an effective lowering of the potential barrier for extremal paths of the below-barrier motion. This effect may prove important in the case of pronounced fluctuational reorganization of the atomic surroundings. In this case, there is a significant renormalization of the amplitude for a tunneling transition. The probability for an inelastic transition accompanied by the excitation of the phonon subsystem through shaking of the barrier, however, remains small, also in proportion to the parameter in (1.1.)

In the case of an interaction with conduction electrons, the picture changes fundamentally. The well-known infrared infinity intensifies inelastic interwell transitions because of shaking of the barrier. This circumstance was originally pointed out by Kondo.[3] Zawadowski *et al.*[4–6] undertook a detailed analysis of this problem, using a multicomponent renormalization-group method for the partition function of the system. They found a significant increase in the role played by this mechanism during tunneling in a metal. However, the important question of whether the second mechanism can become more important than the first in an actual tunneling problem remains open.

In addition to everything else, this problem has one important aspect: The overwhelming majority of the studies[7–15] of the tunneling of a heavy "particle" in a metal have used the concept that the electronic and phonon heat reservoirs are equivalent, and the phonon reservoir has been used in the calculations. In the case of phonons, however, there is no infrared enhancement during the rescattering of excitations, so the inequality (1.1) makes it possible to ignore fluctuations of the barrier. In terms of the widely used spin Hamiltonian, the implication here is that there is no term representing an interaction with excitations of the medium which is proportional to the matrix σ_x. The question of the role of the inelastic processes associated with fluctuations of the barrier is thus related to the general questions of whether it is valid to replace the electron reservoir by the phonon reservoir.

In this paper we develop a comparatively simple method for directly solving the kinetic problem while incorporating the interaction with barrier fluctuations, for a completely arbitrary interaction of the electrons with the tunneling particle. It turns out to be possible to find the explicit relationship between the renormalized amplitude for a tunneling transition and the probability for hopping between wells, on the one hand, and the scattering phase shifts, on the other. These phase shifts are the actual physical parameters which characterize the interaction. The primary result of the analy-

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sis below is the rigorous proof that there are no parameter values for which the second mechanism outweighs the first, while the amplitude for coherent transition changes insignificantly. The proof is presented for a two-well Hamiltonian of a general type. We begin by deriving a tunneling Hamiltonian from first principles, in order to avoid any arbitrariness in the choice of a model spin Hamiltonian.

2. TUNNELING HAMILTONIAN IN THE ADIABATIC APPROXIMATION

We write the original Hamiltonian in the form ($\hbar = 1$)

$$H=H_p(\mathbf{R})+H_{el}(\mathbf{r})+V(\mathbf{r},\mathbf{R});\quad H_p=-\nabla_{\mathbf{R}}^2/2M+U(\mathbf{R}), \tag{2.1}$$

where H_p is the Hamiltonian of a particle of mass M in the potential relief $U(\mathbf{R})$, H_{el} is the Hamiltonian of the electron subsystem ($\mathbf{r}$ represents the set of variables of the electron subsystem, and $V(\mathbf{r},\mathbf{R})$ is the interaction of the particle with the electrons, given by

$$V(\mathbf{r},\mathbf{R})=\sum_{\mathbf{k}\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\exp[i(\mathbf{k}-\mathbf{k}')\mathbf{R}]a_{\mathbf{k}\sigma}^{+}a_{\mathbf{k}'\sigma}. \tag{2.2}$$

Without any loss of generality we can assume $\langle V(\mathbf{r},\mathbf{R})\rangle_{\mathbf{r}}=0$ [in the opposite case, the corresponding expectation value is incorporated in the definition of $U(\mathbf{R})$]. The presence of a barrier, whose quasiclassical effect is assumed to be large, leads to an exponentially weak tunneling coupling of the single-well wave functions of the particle, $\varphi_{is}(\mathbf{R})$ (s is the index of the level in well i). We can thus switch to an effective matrix form of the Hamiltonian H in the basis of localized wave functions $\varphi_{is}(\mathbf{R})$ of the particle in (2.1):

$$H=H_{el}+\sum_{iss'}(\varepsilon_{is}\delta_{ss'}+V^{is,is'})c_{is}^{+}c_{is'} + \sum_{\substack{isi's'\\ i\neq i'}}(V^{is,i's'}+\Delta_0^{is,i's'})c_{is}^{+}c_{i's'}, \tag{2.3}$$

where c_{is}^{+} are operators which create particles in energy levels ε_{is}.

We will be interested below in the situation in which the lower energy levels in the neighboring wells 1 and 2 are shifted by an amount which is small in comparison with the distance between energy levels in a individual well: $\xi=\varepsilon_{10}-\varepsilon_{20}\ll\omega$. We also restrict the analysis to low temperatures, $T\ll\omega$; we can thus ignore activation processes and discuss the lower levels exclusively. At first glance it would appear that these conditions are sufficient grounds for discarding all the matrix elements with $(s,s')\neq(0,0)$ from (2.3). As a result of doing so, we would find the known expression for the Hamiltonian of a particle in a two-well potential,

$$H=\tfrac{1}{2}(\xi\sigma_z+\Delta_0\sigma_x+V_z(\mathbf{r})\sigma_z+V_x(\mathbf{r})\sigma_x+V_0(\mathbf{r}))+H_{el}. \tag{2.4}$$

where

$$\Delta_0\approx\Delta_0^{10,20},\quad V_z\approx V^{10,10}-V^{20,20},$$
$$V_x\approx V^{10,20},\quad V_0\approx V^{10,10}+V^{20,20}.$$

Actually, even under the assumptions made above it is of fundamental importance to incorporate the excited states of the particle in a well. The Hamiltonian (2.4) corresponds to the inequality $\omega\gg\varepsilon_0$, where ε_0 is a characteristic energy of the electrons, on the order of the Fermi energy ε_F. This inequality means that the medium does not have time to react to the instantaneous position of the fast particle; it adjusts itself only to the state of the particle which has been established in an individual well. Actually, the opposite inequality holds for all systems (except for the tunneling of electrons themselves):

$$\omega\ll\varepsilon_0,\quad \omega\propto\varepsilon_0\varkappa^2=\varepsilon_0(m_e/M)^{1/2}, \tag{2.5}$$

where m_e is the mass of a conduction electron. As was shown in Ref. 16, in this case it is incorrect to go directly from (2.3) to (2.4). An analysis of the intrawell motion of a particle with allowance for the system of levels ε_{is} leads to a natural distinction between "fast" and "slow" excitations of the crystal.[16,17] The fast excitations, with frequencies $\delta E>\omega$, adjust adiabatically to the position of the moving particle. The slow excitations, with frequencies $\delta E<\omega$, cannot keep up with the particle, and the modified wave function of the system corresponding to them is oriented toward the center of the potential well. By virtue of (2.5), the overwhelming majority of virtual transitions in the system fall in the adiabatic category. These are the transitions which determine the energy of a state, the screening, the effective adiabatic potential, and, to a slight extent, the mass of a particle.

In a sense, the particle and the adiabatic excitations which have adjusted to it form a real physical entity, whose below-barrier motion as a whole we will be studying. In general, therefore, the problem reduces to one of studying the Hamiltonian (2.1), which describes the motion of a screened particle of this sort with a mass $\tilde{M}$ in a potential $\tilde{U}(\mathbf{R})$. The definition of these quantities may be strongly influenced by part of the interaction with the medium, but the remaining interaction $\tilde{V}(\mathbf{r},\mathbf{R})$ should contain only slow excitations with energies $\delta E<\omega_c=(\varepsilon_0,\omega)_{\min}$.

A further solution of the problem is possible in the customary adiabatic approximation, under the inequality $\omega>\omega_c$. A particle spends a time $\tau\gg\omega^{-1}$ in a individual well. Over this time, the overwhelming majority of the excitations with energies $\delta E>\tau^{-1}$ adapt to the single-well situation and form a single-well wave function of the system, $\Psi_\alpha^{(i)}(\mathbf{r},\mathbf{R})$. In the original potential relief we focus on an individual well $\tilde{U}^{(i)}(\mathbf{R})$, and we continue the sides of the well in the usual manner. We denote by $H_1(\mathbf{R})$ the difference between the actual potential relief and the selected nondecay well. We then find the following expression for the matrix element for a transition from well 1 to well 2:

$$M_{\alpha\beta}=\langle\Psi_\alpha^{(1)}(\mathbf{r},\mathbf{R})|H_1(\mathbf{R})|\Psi_\beta^{(2)}(\mathbf{r},\mathbf{R})\rangle. \tag{2.6}$$

Once we know the matrix elements (2.6), both those which are and are not diagonal in the state of the medium, α, we have completely solved the tunneling problem, including the problem of a coherent transition accompanied by the formation of a band ($\alpha=\beta$), if we are dealing with a crystal.

The Hamiltonian of the single-well problem can be written in the form

$$H^i=H_p^i(\mathbf{R})+H_{el}+\tilde{V}(\mathbf{r},\mathbf{R}). \tag{2.7}$$

In the zeroth adiabatic approximation, the eigenfunctions are

$$\Psi_\alpha(\mathbf{r},\mathbf{R})=\varphi_0(\mathbf{r},\mathbf{R})\Phi_\alpha(\mathbf{r}), \tag{2.8}$$

where φ_0 and Φ_α are solutions of the equations (for the mo-

ment we will omit the index i)

$$[\hat{H}_p+\tilde{V}(\mathbf{r},\mathbf{R})]\varphi_0(\mathbf{r},\mathbf{R})=\varepsilon_0(\mathbf{r})\varphi_0(\mathbf{r},\mathbf{R});$$
$$[H_{el}+\varepsilon_0(\mathbf{r})]\Phi_\alpha(\mathbf{r})=E_\alpha\Phi_\alpha(\mathbf{r}). \tag{2.9}$$

By virtue of the conditions $\omega_c\leqslant\omega\ll\varepsilon_0$ in a metal, the energy $\varepsilon_0(\mathbf{r})$ is determined, to within an error on the order of the parameter $\varkappa^2\ll 1$, by the diagonal matrix element between unperturbed wave functions of the particle:

$$\varepsilon_0(\mathbf{r})\approx\omega+\langle 0|\tilde{V}(\mathbf{r},\mathbf{R})|0\rangle\equiv\omega+V_z(\mathbf{r},\mathbf{R}_i). \tag{2.10}$$

The scale of the change in the potential energy in a well due to the interaction with excitations, $\delta E<\omega$, is on the order of $\varepsilon_0\cdot\omega/\varepsilon_0=\omega$. The dependence of the potential $\tilde{V}(\mathbf{r},\mathbf{R})$ on the coordinate $\mathbf{R}$ is smooth (the potential varies over distances on the order of $1/k_F$). The correction to the energy (2.10) for the nonuniformity of $\tilde{V}(\mathbf{r},\mathbf{R})$ is therefore small, inproportion to the parameter $(k_Fu)^2\propto\varkappa^2$, where u is the size of wave function $\varphi_0(\mathbf{R})$ in a well. Substituting (2.8) into the definition (2.6), we find

$$M_{\alpha\beta}=\langle\Phi_\alpha^{(1)}(\mathbf{r})|J(\mathbf{r})|\Phi_\beta^{(2)}(\mathbf{r})\rangle;$$
$$J(\mathbf{r})=\langle\varphi_0(\mathbf{r},\mathbf{R})|H_1(\mathbf{R})|\varphi_0(\mathbf{r},\mathbf{R})\rangle. \tag{2.11}$$

The expression for $J(\mathbf{r})$ reflects the dependence of the tunneling amplitude for a transition on the distortions of the barrier which result from the interaction with fluctuations in the electron subsystem.[2-4] Interestingly the situation which arises is precisely the opposite of the adiabatic case: Over the time taken by the particle to pass through the barrier, the electron fluctuation remains static. The expression for $J(\mathbf{r})$ can be written in the form

$$J(\mathbf{r})=J_0e^{B(\mathbf{r})}, \tag{2.12}$$

where J_0 is the tunneling amplitude in the potential relief in the absence of fluctuations, and $B(\mathbf{r})$ is given by

$$B=\int[2M(U+\tilde{V})]^{1/2}d\mathbf{R}-\int(2MU)^{1/2}d\mathbf{R}.$$

Noting that the scale of the changes in the barrier is small in comparison with the height of the barrier, we can expand this expression. Using (2.2) for V, we then find

$$B=\sum_{\sigma\mathbf{k}\mathbf{k}'}\frac{B_{\mathbf{k}\mathbf{k}'}}{\omega}a_{\mathbf{k}\sigma}^+a_{\mathbf{k}'\sigma}. \tag{2.13}$$

The quantity $B_{kk'}$ in this expression is on the same order of magnitude as $\tilde{V}_{kk'}$. Substituting (2.12) into (2.11), we finally find

$$M_{\alpha\beta}=J_0\langle\Phi_\alpha^{(1)}(\mathbf{r})|e^{B(\mathbf{r})}|\Phi_\beta^{(2)}(\mathbf{r})\rangle. \tag{2.14}$$

It would appear at first glance that expression (2.14) is completely equivalent in terms of physical content to the spin Hamiltonian (2.4), with

$$\Delta_0=J_0,\ V_z(\mathbf{r},\mathbf{R})=V(\mathbf{r},\mathbf{R}_1)-V(\mathbf{r},\mathbf{R}_2),$$
$$V_x(\mathbf{r},\mathbf{R})=J_0(e^{B(\mathbf{r})}-1),V_0(\mathbf{r},\mathbf{R})=V(\mathbf{r},\mathbf{R}_1)+V(\mathbf{r},\mathbf{R}_2),(\delta E<\omega). \tag{2.15}$$

Note that the interaction with electrons (both V_z, on the one hand, and V_x and V_0, on the other) is cut off at energies $\delta E<\omega$ of the electron-hole pairs in (2.15), while the operator V_x may contain a component which is diagonal in the electron variables and which renormalizes J_0 (the fluctuational preparation of the barrier[2]). If we expand the exponential function at small B, i.e., if we write $\exp(B(\mathbf{r}))=1+B(\mathbf{r})$, then the corresponding Hamiltonian becomes (2.4) (see also Refs. 2 and 4–6).

Actually, a description of the system by means of (2.14) is not identical to a description by means of (2.15), (2.4). The states of the conduction electrons, including those near ε_F, which have become modified to accommodate the position of the particle in well 1 (or 2) are determined by the phase shifts of the scattering in potential $V^{(1)}$ ($V^{(2)}$). Virtual rescattering processes over the entire conduction band are thus important in shaping the well wave functions of the system, $\Phi_\alpha^{(i)}(\mathbf{r})$ in (2.14). The only important point is that the initial and final states fall in a region $|\varepsilon|<\omega$ near the Fermi surface. The rigorous restriction $\delta E<\omega$ for intrawell interactions in Hamiltonian (2.15), (2.4) formally contradicts this requirement. Consequently, it is not possible in general to construct an effective spin Hamiltonian which is completely appropriate for the problem. Only at a small V, for which we can ignore rescattering, can we use the Hamiltonian (2.15), (2.4) to describe the two-well dynamics of a particle in a metal.

3. ELECTRON POLARON OPERATOR

The matrix element (2.14) is defined in terms of wave functions which are eigenfunctions of different Hamiltonians. As always in such situations, it is thus convenient to introduce a unitary operator Λ, which relates the representations of the wave functions $\Phi_\beta^{(1)}$ and $\Phi_\beta^{(2)}$. We make use of the circumstance that the symmetry of the problem makes it possible to retain the same notation for the states during the transport of a particle. We can then write

$$\Phi_\beta^{(2)}=\Lambda\Phi_\beta^{(1)}\equiv\Lambda|\beta\rangle, \tag{3.1}$$

and, correspondingly,

$$M_{\alpha\beta}=J_0\langle\alpha|e^B\Lambda|\beta\rangle. \tag{3.2}$$

We write the Hamiltonian of the system for the case in which the particle is in well 2 in the form ($V=V^{(2)}-V^{(1)}$)

$$H^{(2)}=H^{(1)}+V\equiv\sum_{\mathbf{k}\sigma}\varepsilon_{\mathbf{k}}a_{\mathbf{k}\sigma}^+a_{\mathbf{k}\sigma}+\sum_{\mathbf{k}\mathbf{k}'\sigma}V_{\mathbf{k}\mathbf{k}'}a_{\mathbf{k}\sigma}^+a_{\mathbf{k}'\sigma}. \tag{3.3}$$

We expand $V_{kk'}$ in some complete system of functions defined on a unit sphere, separately for the arguments $\mathbf{k}/k$ and $\mathbf{k}'/k'$. Noting that the energy $\varepsilon_{\mathbf{k}}$ is independent of the wells, we can easily show that the Hamiltonian (3.3) can be put in a diagonal form in the general case for $\mathbf{k}$ and $\mathbf{k}'$ near the Fermi surface. We can then write

$$V_{\mathbf{k}\mathbf{k}'}=\sum_jV_j(\varepsilon,\varepsilon')\Omega_j(\mathbf{k})\Omega_j^*(\mathbf{k}'). \tag{3.4}$$

If the interaction V is spherically symmetric, the index j is obviously the same as the index (l,m) of the ordinary spherical harmonics. To make the latter expansion more transparent, we assume separability of V_j:

$$V_j(\varepsilon,\varepsilon')=V_j\alpha_j^*(\varepsilon)\alpha_j(\varepsilon'), \tag{3.5}$$

where $\alpha_j(\varepsilon)$ is a smooth function of the energy, and $\alpha_j(0)=1$.

We seek the wave function $\Phi_\alpha^{(2)}$ as an expansion in states of the unperturbed Hamiltonian $H^{(1)}$. The operator Λ can then be written

$$\Lambda = S\exp\left(-\sum_{ss'}^{\alpha} C_{ss'}a_s^+ a_{s'}\right) = S\prod_{ss'}^{\alpha}(1-C_{ss'}a_s^+ a_{s'}) \qquad (3.6)$$

(S is a normalization factor). The index s in product (3.6) specifies *exclusively vacant* single-particle states in $|\alpha\rangle$, while s' specifies *exclusively occupied* states (the α on the summation sign is intended to flag this circumstance). It is this circumstance which allows us to go to the latter equality in (3.6), since the spaces $\{s\}$ and $\{s'\}$ do not overlap, and all the terms in the exponential function commute with each other.

We substitute expansion (3.6) into the Schrödinger equation

$$(H^{(1)}+V)\Phi_\beta^{(2)} = E_\beta \Phi_\beta^{(2)}, \quad [\Lambda^{-1}(H^{(1)}+V)\Lambda]_{\beta\beta'} = E_\beta \delta_{\beta\beta'}. \qquad (3.7)$$

Since the effect of the operator Λ (and of Λ^{-1}) reduces to one of simply creating independent electron-hole pairs, there is no difficulty in finding an explicit form of Eq. (3.7). A solution can be written in the form

$$E_\alpha = E_\alpha^0 - \sum_{ss'} V_{s's} C_{ss'}, \qquad (3.8)$$

$$C_{ss'} = \frac{1}{\varepsilon_s - \varepsilon_{s'}}\Big[V_{ss'} - \sum_p (1-n_p)V_{sp}C_{ps'} + \sum_{p'} n_{p'}V_{p's'}C_{sp'} - \sum_{pp'}(1-n_p)n_{p'}V_{p'p}C_{sp'}C_{ps'}\Big]. \qquad (3.9)$$

It can be concluded from the form of (3.6) that the coefficients $C_{ss'}$ mean the probability amplitude for finding in $\Phi_\alpha^{(2)}$ a state with a single electron-hole pair, $a_s^+ a_{s'}|\alpha\rangle$. It is thus no accident that relations (3.8) and (3.9) are the usual equations of perturbation theory for finding this amplitude and for finding the total energy E_α, which, in standard form, are

$$(E_\alpha - E_\beta^0)C_\beta = \sum_\gamma V_{\beta\gamma}C_\gamma.$$

A state with a single pair can be obtained through direct creation from the state $|\alpha\rangle$, through rescattering of an electron or a hole, or through annihilation of an extraneous pair from a state with two electron-hole pairs. These possibilities correspond to the order of the terms in (3.9). The fact that the amplitude for the creation of two pairs breaks up into a product of amplitudes is valid with macroscopic accuracy. On this basis we ignore the splitting of the points $p = s$ and $p' = s'$ in the last term in (3.9). Note also that the states s and p' (or p and s') belong to different subspaces, and the question of the behavior of $\varepsilon_s - \varepsilon_{p'}$ and $\varepsilon_p - \varepsilon_{s'}$ does not arise at all.

We seek a solution of Eq. (3.9) in the form

$$C_{ss'} = \sum_j \Omega_j(\mathbf{k})\Omega_j^*(\mathbf{k}')C_j(\varepsilon,\varepsilon'),$$
$$C_j(\varepsilon,\varepsilon') = \frac{V_j(\varepsilon,\varepsilon')}{\varepsilon-\varepsilon'}\xi_j(\varepsilon)\eta_j(\varepsilon'). \qquad (3.10)$$

After averaging over angles, the terms with different j split up, and we find independent equations for ξ and η (for the moment we will omit the index j):

$$\xi_\varepsilon = 1 - V\sum_{s'}\frac{n_{s'}|\alpha_{\varepsilon'}|^2}{\varepsilon'-\varepsilon}\eta_{\varepsilon'}\xi_\varepsilon,$$
$$\eta_\varepsilon = 1 - V\sum_{s'}\frac{(1-n_{s'})|\alpha_{\varepsilon'}|^2}{\varepsilon'-\varepsilon}\xi_{\varepsilon'}\eta_\varepsilon. \qquad (3.11)$$

We have obtained a system of nonlinear integral equations which entangle the mechanisms of electron and hole scattering. The system has a latent symmetry, however, which allows us to convert it into a linear system of equations. To demonstrate the point, we substitute the explicit expression for the function η from the second equation into the first part of the equation for ξ. Switching from a summation to an integration over the energy, and correspondingly introducing the state density ρ_ε in the electron subsystem and the expectation value n_ε of the occupation numbers of states with a given energy we then find

$$\xi_\varepsilon = 1 - \xi_\varepsilon V\int\frac{n_x|\alpha_x|^2}{x-\varepsilon}\rho_x\,dx + V^2\iint\rho_y\rho_x(1-n_y)|\alpha_y|^2 n_x|\alpha_x|^2\eta_x\xi_\varepsilon\xi_y\left(\frac{1}{x-\varepsilon}-\frac{1}{x-y}\right)\frac{dy\,dx}{y-\varepsilon}. \qquad (3.12)$$

Using the first equation in (3.11) again, we can then reduce this equation to the form

$$\xi_\varepsilon = 1 - \xi_\varepsilon V\int\frac{|\alpha_x|^2}{x-\varepsilon}\rho_x\,dx + V\int\frac{(1-n_y)|\alpha_y|^2}{y-\varepsilon}\xi_y\rho_y\,dy. \qquad (3.13)$$

We have thus indeed obtained a linear integral equation for ξ. Proceeding in the same way, we find an equation for η:

$$\eta_\varepsilon = 1 - \eta_\varepsilon V\int\frac{|\alpha_x|^2}{x-\varepsilon}\rho_x\,dx + V\int\frac{n_y|\alpha_y|^2}{y-\varepsilon}\eta_y\rho_y\,dy. \qquad (3.14)$$

An important point is that ξ and η are related by the simple relation

$$\eta = \frac{G}{g\xi}; \quad G = g\left(1+V\int\frac{|\alpha_x|^2}{x-\varepsilon}\rho_x\,dx\right)^{-1}, \qquad (3.15)$$

where $g = \rho(\varepsilon_F)V$ is an interaction constant.

These equations are well known in the theory of singular integral equations and have exact quadrature solutions.[18] An equation of this type has been derived and used extensively by Nozières and De Dominicis[19] for the problem of x-ray absorption in a metal accompanied by the creation of an electron near ε_F (Ref. 20). That problem has much in common with the problem of the present paper (see also Refs. 13, 21, and 22).

As ε and $\varepsilon' \to 0$, this solution simplifies and can be written in the form

$$\xi_\varepsilon = A_0\cos\tilde{\delta}_\varepsilon\exp\omega_\varepsilon, \qquad (3.16)$$

($A_0 \propto 1$) or, for the product in (3.10),

$$\xi_\varepsilon\eta_{\varepsilon'} = \frac{G_0}{g}\frac{\cos\tilde{\delta}_\varepsilon}{\cos\tilde{\delta}_{\varepsilon'}}\exp(\omega_\varepsilon-\omega_{\varepsilon'}),$$
$$\omega_\varepsilon = \frac{1}{\pi}\int\frac{\tilde{\delta}_x}{x-\varepsilon}dx. \qquad (3.17)$$

Here

$$\tilde{\delta}_\varepsilon = \operatorname{arctg}\{\pi G_0(1-n_\varepsilon)\}. \qquad (3.18)$$

The integral in the difference $\omega_\varepsilon - \omega_{\varepsilon'}$ is determined at small values of x, so all the phases in (3.17) are determined by the value of $G_0 = G(\varepsilon = 0)$. For definiteness, we are adopting $\tilde{d}_{(G_0)} > 0$ in (3.16)–(3.18) and below. In the opposite case $\tilde{\delta} < 0$, we would have

$$\xi_\varepsilon \eta_{\varepsilon'} = \frac{G_0}{g} \frac{\cos \tilde{\delta}_{\varepsilon'}}{\cos \tilde{\delta}_\varepsilon} \exp(\omega_{\varepsilon'} - \omega_\varepsilon),$$
$$\tilde{\delta}_\varepsilon = \operatorname{arctg}(\pi G_0 n_\varepsilon). \tag{3.19}$$

At $T = 0$, these expressions take a particularly simple form. Transforming to $C_{ss'}$ in (3.10), we find

$$C(\varepsilon, \varepsilon') = \frac{V(\varepsilon, \varepsilon')}{\varepsilon - \varepsilon'} \left(\frac{\varepsilon'}{\varepsilon}\right)^{\delta/\pi} \frac{\sin \delta}{\pi g},$$
$$\delta = \operatorname{arctg} \pi G_0. \tag{3.20}$$

Here δ is the phase shift in the scattering of an electron at the Fermi surface in the potential V.

At a nonzero temperature, with

$$n_\varepsilon = [1 + \exp(\varepsilon/T)]^{-1},$$

the integral for $\omega_\varepsilon - \omega_{\varepsilon'}$ can be evaluated analytically. As a result we find

$$C_{\varepsilon\varepsilon'} = \frac{V_{\varepsilon\varepsilon'}}{\varepsilon - \varepsilon'} \frac{G \cos \tilde{\delta}_\varepsilon}{g \cos \tilde{\delta}_{\varepsilon'}} \left| \frac{\Gamma\{1/2 - (i/2\pi)[\varepsilon/T + \ln(1 - i\pi G)]\}\Gamma\{1/2 + (i/2\pi)[\varepsilon'/T + \ln(l - i\pi G)]\}}{\Gamma\{1/2 + (i/2\pi)[\varepsilon/T + \ln(1 - i\pi G)]\}\Gamma\{1/2 - (i/2\pi)[\varepsilon'/T + \ln(l - i\pi G)]\}} \right|. \tag{3.21}$$

Despite the complexity of this expression, it can be approximated by a simple expression, which is sufficient for all physical applications (we are restoring the index j):

$$C_j(\varepsilon, \varepsilon') = \frac{V_j(\varepsilon, \varepsilon')}{\varepsilon - \varepsilon'} \left[\frac{(\varepsilon', T)_{max}}{(\varepsilon, T)_{max}}\right]^{\delta_j/\pi} \frac{\sin \delta_j}{\pi g_j}. \tag{3.22}$$

The normalization factor S is equal to the overlap integral $\langle \Phi_\alpha^{(2)} | \Phi_\alpha^{(1)} \rangle$, which is calculated in the Appendix. The value found for this integral at $T = 0$ in several studies[19,23,24] is

$$S = \exp[-b \ln(\omega/\varepsilon_{min})] \equiv \exp(-\phi);$$
$$b = \sum_j (\delta_j/\pi)^2. \tag{3.23}$$

We conclude by writing a convenient expression for the operator Λ in the case of a weak interaction, in which we can ignore all electron rescattering processes. The effect is to simplify the situation in two regards. First, the amplitude $C_{ss'}$ is simply $C_{ee'} = V_{ee'}/(\varepsilon - \varepsilon')$. Second, in expression (3.6) we can lift the restrictions on the summation indices s and s' (Ref. 16):

$$\Lambda = \exp\left(-\sum_{ss'} \frac{V_{ss'}}{\varepsilon_s - \varepsilon_{s'}} a_s^+ a_{s'}\right). \tag{3.24}$$

In this form the operator Λ is unitary, so the function $\Phi_\alpha^{(2)}$ is automatically normalized.

4. EFFECT OF BARRIER FLUCTUATIONS ON A TUNNELING TRANSITION

From the results of the preceding section of this paper, we can immediately determine the effect of the fluctuational preparation of the barrier on coherent and incoherent tunneling processes. Retaining the first two terms in the expansion of the exponential function in (3.2), we find the following expression for the amplitude for coherent tunneling between wells:

$$\Delta_{coh} = \Delta_{coh}^{(0)} + J_0 \langle \beta | B\Lambda | \beta \rangle, \tag{4.1}$$

$$\Delta_{coh}^{(0)} = J_0 e^{-\phi}. \tag{4.2}$$

When the self-consistent cutoff of the infrared divergence at $\varepsilon_{min} \propto \Delta_{coh}^{(0)}$ is taken into account (Ref. 8, for example), the amplitude $\Delta_{coh}^{(0)}$ becomes

$$\Delta_{coh}^{(0)} = J_0 (J_0/\omega)^{b/(1-b)}. \tag{4.3}$$

We expand the interaction $B_{kk'}$ in (2.13), where $|\varepsilon_k|$ and $|\varepsilon_{k'}|$ are bounded by $\omega \ll \varepsilon_F$, in the same system of functions Ω_j:

$$B_{\mathbf{kk'}} = \sum_{jj'} B_{jj'} \Omega_j(\mathbf{k}) \Omega_{j'}^*(\mathbf{k'}). \tag{4.4}$$

The fact that all the terms in the argument of the exponential function in the definition of the operator Λ in (3.6) commute (this circumstance is the basic distinctive feature of the method which we selected for constructing this operator) means that the evaluation of the matrix elements will be a simple process. In the case at hand, using (4.4), we immediately find the following expression for the second term in expression (4.1) at $T = 0$:

$$\Delta_{coh}^{(0)} 2 \sum_j \frac{B_{jj} V_j \sin \delta_j}{\omega \pi g_j} \rho^2(\varepsilon_F)$$
$$\times \int_{-\omega}^{\bullet} \int \frac{(1 - n_\varepsilon) n_{\varepsilon'} \, d\varepsilon \, d\varepsilon'}{\varepsilon - \varepsilon'} \left| \frac{\varepsilon'}{\varepsilon} \right|^{\delta_j/\pi} \tag{4.5}$$

The value of this integral is determined at the upper limits of the integration, so we find the simple estimate

$$J_0 \langle \beta | B\Lambda | \beta \rangle \propto \Delta_{coh}^{(0)} (\rho V)^2. \tag{4.6}$$

Using $\rho V \lesssim 1$, we see that the renormalization of $\Delta_{coh}^{(0)}$ is not of fundamental importance. This result continues to hold at nonzero temperatures $T \ll \omega$, since $\varepsilon, \varepsilon' \sim \omega$ are important in integral (4.5). It is easy to show that the corrections from higher-order terms in the expansion of e^B do not alter this result.

We thus conclude that the infrared catastrophe near the Fermi surface has no effect on the fluctuational preparation of the barrier in $\Delta_{coh}^{(0)}$ for an arbitrary set of scattering phase shifts.

As was shown in Refs. 17, the amplitude for a coherent transition begins to decay exponentially even at temperatures $bT \gtrsim \Delta_{coh}$. The below-barrier motion of the particles is now accompanied by an excitation of the electron subsystem, and it thereby becomes incoherent. Under these conditions the transition probability can be determined in lowest-order perturbation theory in the weak tunneling coupling:

$$W=2\pi\sum_{\alpha\beta}\rho_\alpha{}^0|M_{\alpha\beta}|^2\delta(E_\alpha-E_\beta+\xi)$$
$$=J_0{}^2\int_{-\infty}^{+\infty}dt\,e^{i\xi t}\langle\Lambda^+(t)e^{B(t)}e^B\Lambda\rangle, \quad (4.7)$$

where ρ_α^0 is the equilibrium density matrix of the conduction electrons. If we ignore the fluctuations of the barrier, we can write (see, for example, Refs. 16, 25, and 26)

$$W'=J_0{}^2\int_{-\infty}^{+\infty}dt\,e^{i\xi t-\chi(t)}, \quad (4.8)$$

$$\chi(t)=2b\int_0^\bullet\frac{dy}{y}\left[(1-\cos yt)\operatorname{cth}\frac{y}{2T}+i\sin yt\right].$$

An evaluation of this integral leads to the familiar expression[11,12,16]

$$W'=\frac{2\tilde\Delta_0{}^2(T)\Omega_T}{\xi^2+\Omega_T{}^2}\pi^{1/2}\frac{|\Gamma(1+b+i\xi/2\pi T)|^2}{\Gamma(1+b)\Gamma(1/2+b)}e^{\xi/2T}, \quad (4.9)$$
$$\tilde\Delta_0(T)=J_0(\pi T/\omega)^b, \quad \Omega_T=2\pi bT. \quad (4.10)$$

We now consider the probability for the process in which the excitation of the electron system is coupled specifically with fluctuations of the barrier. We again begin with a perturbation theory in B. We first ignore the rescattering of the electron-hole pair created by the operator B. In this case the transition probability is given by

$$W''=J_0{}^2\sum_{ss'}|B_{ss'}/\omega|^2(1-n_s)n_{s'}\int_{-\infty}^{+\infty}dt\exp[i(\xi+\varepsilon_{s'}-\varepsilon_s)t-\chi(t)]$$
$$=\sum_{ss'}|B_{ss'}/\omega|^2(1-n_s)n_{s'}W'(\xi+\varepsilon_{s'}-\varepsilon_s). \quad (4.11)$$

The integral over dt in (4.11) is determined over time scales $1/(T,\xi)_{\max}$. We single out the constant part of $\chi(t)$, which leads to renormalization of J_0 by $\tilde\Delta_0(T)$; the remainder leads to a δ-function which is smeared over a scale $\Omega_T\propto bT$. As a result we find the simple estimate ($\xi=0$)

$$W''\approx(\tilde\Delta_0/\omega)^2\Omega_T. \quad (4.12)$$

Comparing this expression with (4.9), we find the ratio

$$W''/W'\propto(\Omega_T/\omega)^2\ll1. \quad (4.13)$$

We now consider this process in the general case. We evaluate the effective matrix element $\tilde B_{ss'}$, which corresponds to a transition from well 2 to well 1, in a process accompanied by the creation of a single electron-hole pair:

$$\tilde B_{\beta\alpha}=S^{-1}\langle\beta|B\Lambda|\alpha\rangle. \quad (4.14)$$

From the definition of the operator Λ, we can easily write all possible matrix elements which lead to the state $|\beta\rangle=\alpha_s{}^+\alpha_{s'}|\alpha\rangle$:

$$\tilde B_{ss'}=B_{ss'}-\sum_k(1-n_k)B_{sk}C_{ks'}+\sum_{k'}n_{k'}B_{k's'}C_{sk'}$$
$$-\sum_{kk'}(1-n_k)n_{k'}B_{k'k}C_{ks'}C_{sk'}. \quad (4.15)$$

Substituting expressions (3.10) and (4.4) into this equation, we find

$$\tilde B_{jj'}(\varepsilon,\varepsilon')=B_{jj'}\xi_j(\varepsilon)\eta_{j'}(\varepsilon'). \quad (4.16)$$

Using (3.16), (3.17), and (3.22), we find

$$\tilde B_{jj'}(\varepsilon,\varepsilon')\approx B_{jj'}\left[\frac{\omega}{(\varepsilon,T)_{max}}\right]^{\delta_j/\pi}\left[\frac{\omega}{(\varepsilon',T)_{max}}\right]^{-\delta_{j'}/\pi}. \quad (4.17)$$

This expression demonstrates that there can be a rapid increase in the amplitude for an incoherent transition because of the fluctuations of the barrier when the rescattering of the electron and hole which are created is taken into account. This circumstance was first pointed out by Kondo.[3] Zawadowski *et al.*[4,5] undertook a detailed analysis of the renormalization of this amplitude. A result similar to (4.17) was first derived by a multicomponent renormalization-group method.

The question of the renormalization of B does not arise at all if this operator is put in diagonal form at the same time as the operator for intrawell scattering, V. For $j=j'$, the basic renormalizations cancel out.[4] In the general case, however, the operators B and V do not commute.

The transition probability determined by the amplitude $\tilde B$ is obviously given by expressions (4.10) and (4.11), with B replaced by $\tilde B$:

$$W''\approx\sum_{jj'}f_{jj'}\int_{-\omega}^{\omega}\int W'(\xi+\varepsilon'-\varepsilon)(1-n_\varepsilon)n_{\varepsilon'}\left[\frac{\omega}{(\varepsilon,T)_{max}}\right]^{2\delta_j/\pi}$$
$$\times\left[\frac{\omega}{(\varepsilon',T)_{max}}\right]^{-2\delta_{j'}/\pi}\frac{d\varepsilon\,d\varepsilon'}{\omega^2}, \quad (4.18)$$

where $f_{jj'}=\rho^2(\varepsilon_F)B_{jj'}^2$. We can estimate the relative order of magnitude of W'' even without writing an explicit expression for W'. The integral over $d\varepsilon$ and $d\varepsilon'$ is determined at energies of the electron-hole pairs on the order of $\varepsilon-\varepsilon'\propto(\xi,T)_{\max}$ (at energy transfers $E>T$, the probability W' falls of exponentially, $\propto e^{-E/T}$). We then immediately find from (4.18)

$$W''\propto W'|(\xi,T)_{max}/\omega|^{2(1-\theta)}, \quad (4.19)$$
$$\theta=(\theta_{jj'})_{max}, \quad \theta_{jj'}=(\delta_j-\delta_{j'})/\pi. \quad (4.20)$$

To evaluate the role played by the fluctuational shaking of the barrier we thus need to know the phase shifts in the scattering of electrons by the particle. Clearly, the corrections to result (4.8), (4.9) will be small as long as the relation $\theta<1$ holds.

5. RESTRICTION ON THE EFFECTIVE SCATTERING PHASE SHIFTS ($|\delta^{\text{eff}}|\leqslant\pi/2$)

Are there restrictions on the parameter θ? What are the scale values of this quantity in actual physical models? To answer these questions we begin with an analysis of a case which is a natural one for the two-well problem

$$V_{\mathbf{kk'}}^{(1)}=V_1, \quad V_{\mathbf{kk'}}^{(2)}=V_1e^{i(\mathbf{k}-\mathbf{k'})\mathbf{R}}. \quad (5.1)$$

Here is an outline of the order of steps in the proof which we present in this section of the paper. After finding the original interaction at each well, we switch from a plane-wave representation to a representation of the eigenfunctions of Hamiltonian $H^{(1)}$ in accordance with (3.3), and we write the difference between the interactions in the wells, $V=V^{(2)}-V^{(1)}$, in this basis. Expressions (3.16)–(3.21) for the amplitudes $C_{\varepsilon\varepsilon'}$ are completely determined by the one-

electron scattering phase shifts δ^{eff}. There is accordingly no need to resolve the problem of constructing the operator Λ in each specific case; it is sufficient to examine the one-electron problem of scattering by an effective potential V. For clarity, we present a systematic solution of the Schrödinger equation for the particular case of the interactioin (5.1), which contains only a single scattering phase shift, and for a potential of a general type.

In the particular case (5.1) it is convenient to introduce a simple system of only two orthogonal angular functions,

$$\Omega_1(\mathbf{k})=1, \quad \Omega_2(\mathbf{k})=(e^{i\mathbf{kR}}-h)/(1-h^2)^{1/2}, \tag{5.2}$$

$$h=\int e^{i\mathbf{kR}}\frac{d\sigma_{\mathbf{k}}}{4\pi}=\sin(k_F R)/k_F R, \tag{5.3}$$

which is sufficient for picking out the angular part of interaction (5.1). In this basis, the difference $V^{(2)}-V^{(1)}$ takes the form

$$V_{\mathbf{kk}'}=\sum_{ij}^{2}\Omega_i(\mathbf{k})\Omega_j^*(\mathbf{k}')V_{ij}, \quad \mathscr{V}=V\begin{bmatrix}-1 & x\\ x & 1\end{bmatrix}, \tag{5.4}$$

where V_{ij} are the elements of the matrix $\mathscr{V}$. Here

$$V=V_1(1-h^2), \quad x=h/(1-h^2)^{1/2}. \tag{5.5}$$

We switch from a plane-wave representation $\varphi^{(0)}$, in which the interaction (5.1) is written, to a representation in terms of eigenfunctions of Hamiltonian $H^{(1)}$, as is assumed in (3.3):

$$\varphi_\varepsilon^{(i)}=\sum_{\varepsilon_1}\gamma_{\varepsilon\varepsilon_1}^{(i)}\varphi_{\varepsilon_1}^{(0)}, \quad i=1.2. \tag{5.6}$$

In the $i=1$ channel, in which the scattering by the particle involves a phase shift $\delta^{(1)}$, the Schrödinger equation leads to the known solution (Ref. 27, for example)

$$\gamma_{\varepsilon\varepsilon_1}^{(i)}=\frac{\cos\delta_\varepsilon^{(1)}}{\rho_\varepsilon}\left[\delta(\varepsilon-\varepsilon_1)+\frac{\operatorname{tg}\delta_\varepsilon^{(1)}}{\pi}\frac{P}{\varepsilon-\varepsilon_1}\right], \tag{5.7}$$

where $\delta^{(1)}$ is related to V_1 by [cf. (3.15), (3.20)]

$$\delta^{(1)}=\operatorname{arctg}\pi G_1, \quad G_1=\rho_\varepsilon V_1\left(1+V_1\int\frac{\rho_x}{x-\varepsilon}dx\right)^{-1}. \tag{5.8}$$

The absence of scattering in channel 2 obviously leads to $\gamma_{\varepsilon\varepsilon_1}^{(2)}=\rho_\varepsilon^{-1}\delta(\varepsilon-\varepsilon_1)$.

In the new representation, matrix elements (5.4) immediately become

$$\tilde{V}_{ij}(\varepsilon,\varepsilon')=V_{ij}\alpha_\varepsilon^{(i)}\alpha_{\varepsilon'}^{(j)}, \tag{5.9}$$

where we have the following expression for $\alpha^{(i)}$, found with the help of (5.7):

$$\alpha_\varepsilon^{(1)}=\sum_{\varepsilon_1}\gamma_{\varepsilon\varepsilon_1}^{(1)}=\frac{\sin\delta_\varepsilon^{(1)}}{\pi\rho_\varepsilon V_1}, \quad \alpha_\varepsilon^{(2)}=1. \tag{5.10}$$

In evaluating the integral over ε_1 in the principal-value sense, we made use of its relationship with $\delta^{(1)}$ which follows from (5.8).

We now seek the phase shift δ^{eff} which appears in the expression for the operator Λ [the transformed interaction (5.9) leads to the appearance of two effective phase shifts]. The corresponding Schrödinger equation, in matrix form, can be written

$$(E-\varepsilon_1)\gamma_{E\varepsilon_1}=\sum_{\varepsilon_2}\tilde{\mathscr{V}}(\varepsilon_1,\varepsilon_2)\gamma_{E\varepsilon_2}. \tag{5.11}$$

The vector γ is a column vector here. The solution of Eq. (5.11) has the same structure for γ as (5.7), and this structure is characteristic in general of the scattering problem. We accordingly seek a solution for $E=0$ which corresponds to scattering by electrons on the Fermi surface in the form ($\gamma_{0\varepsilon}\equiv\gamma_\varepsilon$)

$$\gamma_{\varepsilon_1}=\left[\delta(\varepsilon_1)-z\frac{P}{\varepsilon_1}\right]\begin{bmatrix}\gamma_1\alpha_{\varepsilon_1}^{(1)}\\ \gamma_2\end{bmatrix}, \quad z=\frac{\operatorname{tg}\delta^{eff}}{\pi}, \tag{5.12}$$

$\delta^{\text{eff}}=\delta_{\text{eff}}(E=0)$. Substituting (5.12) into (5.11), and solving the resulting homogeneous system of equations, we find

$$[z(1-gQ)+g|\alpha_0^{(1)}|^2][z(1+gI)-g] -g^2x^2(|\alpha_0^{(1)}|^2-zQ)(1-zI)=0, \tag{5.13}$$

where

$$Q=\rho_0^{-1}\int|\alpha_x^{(1)}|^2\rho_x\frac{dx}{x}, \quad I=\rho_0^{-1}\int\rho_x\frac{dx}{x}, \quad g=\rho_0 V\equiv g_1(1-h^2). \tag{5.14}$$

Solution (5.13) must give us the values of δ^{eff} which determine the quantity θ in which we are interested. However, before we simplify this problem and determine the value of the constant Q, we will make use of the following simple arguments. We assume that there is no interaction of the particle with the electrons in well 2. On the other hand, a formal solution of this problem in this case leads to an effective interaction

$$\tilde{V}_{ij}(\varepsilon,\varepsilon')=-V_1\alpha_\varepsilon^{(1)}\alpha_{\varepsilon'}^{(1)}\delta_{i1}\delta_{j1},$$

which in turn leads to the scattering phase shift [see (3.15), (3.20)]

$$\operatorname{tg}\delta^{eff}/\pi=-g_1|\alpha_0^{(1)}|^2/(1-g_1Q). \tag{5.15}$$

On the other hand, since we are actually making the inverse transformation from the φ_ε representation to the plane-wave representation, we naturally have $\delta^{\text{eff}}=-\delta^{(1)}$. We then find the following result from (5.15) and (5.8):

$$Q=g_1^{-1}-|\alpha_0^{(1)}|^2G_1^{-1}. \tag{5.16}$$

Substituting this value into (5.13), and making use of the obvious relation between parameters $1+G_1g_1I=g_1$ which follows from (5.8), we find a solution of the quadratic equation in the form

$$\operatorname{tg}\delta^{eff}=\pm(1-h^2)^{1/2}\operatorname{tg}\delta^{(1)}/(1+h^2\operatorname{tg}^2\delta^{(1)})^{1/2}. \tag{5.17}$$

If we then find the quantity $b=(\delta_1^{\text{eff}}/\pi)^2+(\delta_2^{\text{eff}}/\pi)^2$, which determines the value of overlap integral (3.23), we immediately arrive at the result which was first found by Yamada *et al.*[24,26]

Examining the interaction in the form in (5.1), we easily conclude that in the limit $\mathbf{R}\to 0$ the phase shifts δ_i^{eff} also tend toward zero. If they did not, we would have the paradoxical result that the overlap integral did not become unity in the limit $\mathbf{R}\to 0$. It follows that at small values of $\mathbf{R}$ the value of the phase shift must be determined by the branch of the arctangent between $-\pi/2$ and $\pi/2$. A question of funda-

mental importance which arises here is whether the phase shift can reach a value $|\delta^{\text{eff}}| > \pi/2$ for arbitrary values of the parameters. With a continuous functional dependence $\delta^{\text{eff}}(\mathbf{R})$, which is physically obvious, the meaning would be that $z = \tan\delta^{\text{eff}}/\pi$ would become infinite at some point. It follows from the result (5.17), however, that for any arbitrary finite $\tan\delta^{(1)}$ we will not have the corresponding result $z \to \infty$. There exist singular points, at which we have $\delta^{(1)} = \pi/2$ and $h(\mathbf{R}) = 0$ simultaneously, and at which the solution δ^{eff} is tangent to the value $\pi/2$. Our assertion of tangency follows from the continuity of δ^{eff} as a function of $\delta^{(1)}$. The motion away from $\delta^{(1)} = 0$ tells us that the solution belongs to the same branch of the arctangent.

We thus arrive at the important conclusion that for one arbitrary scattering phase shift we have $|\delta^{\text{eff}}| \leqslant \pi/2$ (cf. Refs. 24 and 28). The restriction $\theta \leqslant 1$ then follows immediately.

This result is actually more general in nature since it remains valid in the case in which the scattering by an individual center is determined by several phase shifts. All the arguments concerning the behavior of the phase shifts δ^{eff} in the limit $\mathbf{R} \to 0$ or $\delta^{(i)} \to 0$ naturally continue to hold, predetermining that the solution for δ^{eff} belongs to the same arctangent branch $(-\pi/2, \pi/2)$. As a result, again in the more general case we are faced with the question of whether one of the phase shifts δ^{eff} might become greater than $\pi/2$ in magnitude at intermediate values of the parameters.

For the general case we write the interaction in the form

$$V_{\mathbf{kk}'}^{(1)} = \sum_{j=lm} V_j Y_j(\mathbf{k}) Y_j^*(\mathbf{k}'),$$

$$V_{\mathbf{kk}'}^{(2)} = V_{\mathbf{kk}'}^{(1)} \exp[i(\mathbf{k}-\mathbf{k}')\mathbf{R}]. \tag{5.18}$$

Since the choice of a special system of angular functions does not facilitate a search for the phase shifts δ^{eff} for an arbitrary number of scattering channels, we retain the basis of ordinary spherical harmonics $Y_j(\mathbf{k}) = Y_{lm}(\mathbf{k})$. In this basis the elements of the matrix $\mathscr{V}$ are

$$V_{ii'} = \sum_j e_{ij} V_j e_{ji'}^+ - V_i \delta_{ii'}, \tag{5.19}$$

where

$$e_{ij} = \int \frac{d\mathbf{o}_\mathbf{k}}{4\pi} Y_i^*(\mathbf{k}) e^{i\mathbf{kR}} Y_j(\mathbf{k}), \quad e^+ = e^{-1}. \tag{5.20}$$

The transformation to the representation of eigenfunctions of Hamiltonian $H^{(1)}$ is made in accordance with (5.9), (5.10). Now i and j are arbitrary, and the $\alpha_e^{(i)}$ are different from unity for only those i (j) for which V_i in (5.18) are nonzero. We again seek a solution of the Schrödinger equation (5.11) with $E = 0$ in the form in (5.12); now γ_{ε_i} is now a column of arbitrary order with elements $\gamma_i \alpha_{\varepsilon_i}^{(i)}$. As a result we find a homogeneous system of equations for determining γ_i:

$$z\gamma_i = \sum_{i'} \Big(\sum_j e_{ij} g_j e_{ji'}^+ - g_i \delta_{ii'} \Big) \times [\,|\alpha_0^{(i')}|^2 - z(g_{i'}^{-1} - |\alpha_0^{(i')}|^2/G_{i'})\,]\gamma_{i'}, \tag{5.21}$$

where $g_j = \rho_0 V_j$, and G_i is given by (5.8). In evaluating the integral in the principal-value sense, we used relation (5.16), which obviously holds for each of the functions $\alpha_\varepsilon^{(i)}$.

We transform the expression on the right side of (5.21) by making use of the relationship between $\alpha_0^{(i)}$ in (5.10) and G_i in (5.8). Moving the term proportional to $\delta_{ii'}$ to the left side of the equation, we have

$$(z+G_i)\gamma_i = \sum_{ji'} e_{ij} g_j e_{ji'}^+ [1 - G_{i'} I - z(\pi^2 G_{i'} + I)]\gamma_{i'}. \tag{5.22}$$

We introduce

$$K_n = \sum_{i'} e_{ni'}^+ \gamma_{i'}, \quad U_n = \sum_{i'} e_{ni'}^+ G_{i'} \gamma_{i'}. \tag{5.23}$$

Multiplying both sides of (5.22) by e_{ni}^+ from the left, and summing over i, we find

$$K_n = \frac{(1+\pi^2 G_n z)}{G_n - z} U_n. \tag{5.24}$$

We can simplify the right side of Eq. (5.22) by making use of the relationship (5.24). After some simple manipulations, we finally find

$$\frac{z+G_i}{1+\pi^2 z^2}\gamma_i = \sum_{ji'} e_{ij} e_{ji'}^+ \frac{G_j G_{i'}}{G_j - z}\gamma_{i'}. \tag{5.25}$$

Significantly, the system (5.25) contains only a number of equations which is equal to the number of independent scattering channels in the potential $V^{(1)}$. Actually, the symmetry dictated by the shift factor $\exp[i(\mathbf{k}-\mathbf{k}')\mathbf{R}]$—if $\mathbf{R}$ is adopted as the polar axis—predetermines the breakup of Eqs. (5.25) into independent subsystems, each characterized by its own azimuthal quantum number m. In particular, with $G_{lm} = G_{l0}\delta_{l|0}$ we find from (5.25)

$$(G_{l_0}^2 - z^2)/(1+\pi^2 z^2) = e_{l_0 m}^2 G_{l_0}^2,$$
$$e_{l_0 m} = \int \frac{d\mathbf{o}_\mathbf{k}}{4\pi} |Y_{l_0 m}(\mathbf{k})|^2 e^{i\mathbf{kR}}, \tag{5.26}$$

which naturally leads to a result analogous to (5.17).

Taking the limit $z \to \infty$ in (5.25), we find that the determinant of the system becomes

$$D = \det \Big| \delta_{ii'} + \pi^2 \sum_j e_{ij} G_j e_{ji'}^+ G_{i'} \Big|. \tag{5.27}$$

Can the determinant (5.27) vanish, and if so under what conditions? Let us assume that the two orbital scattering channels l_1 and l_2 in (5.18) are nonzero. Simple calculations then lead to the expression

$$D = |(-1)^{l_1 - l_2} - \pi^2 G_1 G_2 (e_{11}e_{22} - e_{12}e_{21})|^2 + |(-1)^{l_1 - l_2}\pi G_1 e_{11} - \pi G_2 e_{22}|^2. \tag{5.28}$$

We see that we have $D = 0$ only under the condition that each of the terms vanishes separately. In the three-dimensional space of the parameters $(\delta^{(1)}, \delta^{(2)}, \mathbf{R})$, these two conditions determine a line of singular points. Significantly, in three-dimensional space this line cannot prevent the continuous attainment of any point in the parameter space if one starts from the origin, where $\delta^{\text{eff}} = 0$. It follows immediately from the continuity of solution δ^{eff} that the phase shifts δ^{eff} always remain on the arctangent branch $-\pi/2 \leqslant \delta^{\text{eff}} \leqslant \pi/2$. Again in this case, we thus have $\theta \leqslant 1$.

The general nature of this analysis means that we can draw the conclusion that the result found here continues to

hold in the case of an arbitrary number of phase shifts, if the vanishing of determinant (5.28) requires the satisfaction of at least two independent conditions. We can show that this is indeed the situation in the general case. We write the spherical harmonics in the form

$$Y_{lm}=i^l\Theta_{lm}e^{im\varphi}/(2\pi)^{1/2}. \tag{5.29}$$

In this case it is easy to show that the following relations hold:

$$e_{ij}=e_{ij}^*,\ e_{ji}=(-1)^{l_i+l_j}e_{ij}. \tag{5.30}$$

We introduce the two complex matrices

$$A_{ij}=(-1)^{l_i}\delta_{ij}+i\pi e_{ij}G_j,\quad B_{ij}=(-1)^{l_i}\delta_{ij}-i\pi e_{ij}^+G_j. \tag{5.31}$$

Their product is equal to a matrix whose determinant figures in (5.27). Hence

$$D=\det|A_{ij}|\det|B_{ij}|=D_AD_B. \tag{5.32}$$

A sufficient condition for the vanishing of D is that one of the determinants vanish. It then follows from the fact that matrices A and B are complex that it is necessary in general to satisfy two independent conditions in order to satisfy the equality $D=0$.

This result may be thought of as the following theorem in scattering theory. We denote by $S(0)$ and $S(\mathbf{R})$ some ordinary S matrices which are determined by scattering by a potential center at the origin of coordinates and at the point $\mathbf{R}$, respectively. It can then be asserted that the matrix $S(\mathbf{R})S(0)^{-1}$ has the following properties after it is diagonalized (i.e., after the eigenvalue problem is solved):

$$[S(\mathbf{R})S(0)^{-1}]_{ii}=\exp(2i\delta_i^{eff}),\quad |\delta_i^{eff}|\leqslant\pi/2. \tag{5.33}$$

We have been discussing the case in which we expanded the exponential operator e^B to first order in B. It turns out that the initial small value of the phase volume of a pair created in the course of a transition, $((T,\xi)_{\max}/\omega)^2$, is not canceled by an increase in the effective amplitude due to rescattering processes ($\theta<1$) in any (ii') channel. It is easy to see that the higher-order terms in the expansion of e^B will not change this result. Specifically, processes of the type

$$\sum_{ns}\frac{\tilde B_{p_s}^{\ ln}\tilde B_{sp'}^{nl'}}{\omega}=\eta_l(p)\xi_{l'}(p')\times\sum_n\frac{B^{ln}B^{nl'}}{\omega}\sum_s(1-n_s)\eta_n(s)\xi_n(s)\propto\tilde B_{pp'}^{ll'}$$

do not change the scale of the amplitude $\tilde B^{ll'}$ [according to (3.15, we have $\eta_n(S)\xi_n(S)=G_n/g_n$]. On the other hand, processes in which two or more pairs are created simultaneously near ε_F can clearly be discarded, by virtue of the parameter $((T,\xi)_{\max}/\omega)^{4(1-\theta)}\ll 1$.

6. CONCLUDING REMARKS

In summary, for an interaction between electrons and a particle in an individual well which is spherically symmetric and otherwise arbitrary it is not possible to ensure $\theta>1$. This result means that the contribution of inelastic processes due to shaking of the barrier remains small, despite the strengthening of these processes by the infrared infinity near ε_F. Actually, this contribution can never exceed the inelastic contribution associated with the shaking of the electron-hole coat, W'. For this reason, in analyzing the tunneling of a heavy particle in a two-well relief or in a metallic matrix it is legitimate, in a first approximation, to consider only the intrawell interaction with conduction electrons. On the other hand, although the electron and phonon heat reservoirs are nonequivalent, the replacement of one by the other is an approximate procedure justified by a small value of the parameter

$$[(T,\xi)_{max}/\omega]^{2(1-\theta)}. \tag{6.1}$$

This condition is definitely weaker than (1.1).

We have found proof of the restriction $|\delta^{\text{eff}}|\leqslant\pi/2$ for a potential of the general type in (5.18), which is characteristic of an impurity particle in a metal. The proof was based on the translational properties of (5.18). In Josephson junctions the interaction of the quantum variable φ—the difference between the phases of the order parameter at the junction—and conduction electrons takes a different form. In a very simple model we would have[9,10]

$$V(\mathbf{r},\varphi)=V(r)e^{i\varphi/2}. \tag{6.2}$$

The arbitrary nature of the amplitude $V(\mathbf{r})$ and the change in the sign of the interaction during tunneling from the position $\varphi=0$ to the position $\varphi=2\pi$ create favorable conditions for large values of the effective scattering phase shifts $\delta^{\text{eff}}>\pi/2$. It might appear that the condition $\theta>1$ could be satisfied quite easily under these conditions. However, that is not the case. The interaction (6.2) has the property that as the quantity φ is varied the angular dependence of the matrix elements $V_{kk'}$ on the Fermi surface does not change. This result means in turn that both the intrawell interaction $V_{kk'}^{(i)}$ and the interaction with barrier fluctuations, $B_{kk'}$, simultaneously become diagonal (this is the so-called commutative model[4-6]). According to (4.20), however, we would then have $\theta=0$ identically, regardless of the size of the scattering phase shifts.

APPENDIX

To calculate the normalization $S\text{-}\exp(-\phi)$, we differentiate the condition

$$\langle\alpha|\Lambda^+\Lambda|\alpha\rangle=1 \tag{A1}$$

with respect to the parameter δ_j. Making use of the definition of the operator Λ, (3.6), we find (for simplicity we are omitting the index j and the spherical harmonics Ω_j; incorporating them is trivial)

$$\frac{\partial\phi}{\partial\delta}=\operatorname{Re}\sum_{ss'}^{\alpha}\left[\frac{\partial C_{ss'}}{\partial\delta}\langle\alpha|\Lambda^+a_s^+a_{s'}\Lambda|\alpha\rangle\right]$$
$$\equiv\sum_{\varepsilon\varepsilon'}^{\alpha}\left[\frac{\partial C_{\varepsilon\varepsilon'}}{\partial\delta}\langle\Phi_\alpha^{(2)}|a_\varepsilon^+a_{\varepsilon'}|\Phi_\alpha^{(2)}\rangle\right]. \tag{A2}$$

Since explicit expressions for the amplitudes $C_{\varepsilon\varepsilon'}$ are known (Sec. 3), it is sufficient to determine the one-particle operator $\alpha_\varepsilon^+\alpha_{\varepsilon'}$ in terms of eigenfunctions of the Hamiltonian $H^{(2)}$. We switch from one representation to another by means of the coefficients $\gamma_{x\varepsilon}$ in (5.6), (5.7):

$$\gamma_{x\varepsilon}=\frac{\cos\delta}{\rho_0}\left[\delta(x-\varepsilon)+\frac{\operatorname{tg}\delta}{\pi}\frac{P}{x-\varepsilon}\right], \tag{A3}$$

We then immediately find the following result for the second factor in square brackets in (A2):

$$\langle \Phi_\alpha^{(2)} | a_\varepsilon^+ a_{\varepsilon'} | \Phi_\alpha^{(2)} \rangle = \sum_\varkappa n_\varkappa \gamma_{\varkappa\varepsilon} \gamma_{\varkappa\varepsilon'}. \tag{A4}$$

At $T=0$, it is an elementary matter to evaluate the integral in (A4); the result is

$$\frac{1}{\pi\rho_0} \frac{\sin\delta}{\varepsilon-\varepsilon'} \left[\cos\delta + \frac{\sin\delta}{\pi} \ln|\varepsilon'/\varepsilon| \right]. \tag{A5}$$

Substituting (A5) into (A2), and using tabulated energy integrals, we finally find

$$\frac{\partial\phi}{\partial\delta} = \frac{\delta}{\pi^2} \int_0^\omega \frac{d\varepsilon}{\varepsilon}, \qquad \phi = {}^1/_2 \left[\frac{\delta}{\pi} \right]^2 \ln \frac{\omega}{\varepsilon_{min}}. \tag{A6}$$

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