Multiquantum vibrational transitions upon the resonant tunneling of electrons

F. I. Dalidchik

(Submitted 27 March 1984)
Zh. Eksp. Teor. Fiz. **87**, 1384–1399 (October 1984)

A theory of the resonant tunneling of electrons is constructed with allowance for the vibrational degrees of freedom of the scattering centers. It is shown that under the conditions of greatest physical interest the tunneling occurs through the formation and destruction of a long-lived electron-vibrational complex and can be accompanied by interesting multiquantum vibrational transitions. For the vibrational subsystem of the complex an equation of motion is found which generalizes the Born-Oppenheimer method to the case of electron resonances of the potential type. The limits of applicability are determined for the model of complex terms and the fixed-scatterers approximation. It is established that absolute transparency of barriers containing impurities is also possible for inelastic, including multiquantum, tunneling. The theory is used to evaluate the tunnel conductance of metal-insulator-metal junctions and the energy distributions of the field-emission electrons from metals containing absorbed atoms of light elements.

1. INTRODUCTION

Resonant tunneling, in particular the fact that under certain conditions particles can pass unimpeded through potential barriers of arbitrarily great height and width but having a depression in the central part with a quasistationary level $E_p = E^0 - i\Gamma$, is one of the clearest manifestations of quantum effects. As we know, the explanation of this effect draws upon many physical phenomena—tunneling transitions of electrons in solids,[1] field emission of electrons by metals containing adsorbed particles,[2] etc.

In resonant tunneling, particles with energies E close to E^0 ($|E - E^0| \lesssim \Gamma$) are trapped for a long time $t \sim 1/\Gamma$ by local centers ($e = m = h = 1$). These particles accumulate in the below-barrier region, and their subsequent breakaway from the centers gives rise to characteristic features (resonance peaks) in the tunneling spectra.

The resonance features in the tunneling spectra are observed in measurements of the conductance of metal-insulator-metal (or metal-semiconductor-metal) junctions[3–6] and in measurements of the energy distributions of field-emission electrons.[2,7,8]

There is by now a broad literature (see, e.g., Refs. 9–16) on the theory of resonant tunneling of electrons. However, in all the studies known to the author the resonant tunneling has been treated only in the approximation of fixed scatterers. Such an approach is justified if the characteristic time spent by the electron at the center is sufficiently small, i.e., if, during the lifetime of the intermediate quasistationary state, the center which has trapped the electron and which is consequently moving in a new field of forces does not have time to move from its initial position. For this we must have[1)]

$$\Gamma \gg \omega_v, \tag{1}$$

where ω_v is the characteristic frequency of the local vibrations of the center.

Condition (1) obviously does not hold in the case of rather wide (or high) potential barriers, i.e., when the effects of resonant tunneling should be most clearly manifested.

In systems with metal-insulator-metal (MIM) junctions condition (1) fails at insulator thicknesses $d > d_{\min}$, where

$$d_{min} \sim |E^0|^{-1/2} \ln(|E^0|/\omega_v).$$

Under typical experimental conditions ($E^0 \sim 4$ eV, $\omega_v \sim 0.1$–0.01 eV) one has $d_{\min} \sim 4$–5 Å, whereas for systems of practical interest $d \gtrsim 10$ Å (Ref. 1).

Condition (1) may also fail in field-emission processes, where the role of the resonant-scattering centers for tunneling electrons is played by adsorbed particles.[2] When light elements are adsorbed, $\Gamma \sim 0.1$–0.7 eV (Ref. 2) and $\omega_v \sim 0.1$–0.3 eV (Ref. 17).

For describing the resonant tunneling of electrons through wide potential barriers in which the intracenter electron-vibrational coupling is important it is necessary to go outside the framework of the fixed-scatterer approximation. A solution to this problem is proposed in the present paper, where we shall develop a method which constitutes the adiabatic (in the small parameter ω_v/ω_e, where ω_e is the characteristic frequency of electronic transitions within the center) generalization of the pole approximation of Refs. 12–15. The method leads to an equation of motion for a center in a quasistationary electronic state which is coupled to the continuum by tunneling transitions. (We shall call such systems electron-vibrational complexes, or EVCs). The derivation of Eq. (15) solves the problem of generalizing the Born-Oppenheimer approximation to electron resonances of the potential type. Here it must be stressed that the solution obtained is of interest not only for the theory of resonant tunneling; states of the EVC type are also known in other physical systems. They are formed, for example, in the resonant scattering of slow electrons by molecules (the "shape" resonances of negative molecular ions[18,19]), in the interaction of molecules with electric fields and metal surfaces, etc. At the present time such systems are frequently described using the phenomenological model of complex terms,[20] which at first glance is the most natural generalization of the adiabatic approximation to the case of decaying states of the

 0038-5646/84/100795-09$04.00

electronic subsystem. With a suitable choice of parameters this model gives results consistent with the experimental data on the resonant scattering of slow electrons by molecules. However, up till now there has been no consistent justification for such an approach, and the region of applicability of the model of complex terms remains unknown.[2)] The unfinished state of the present-day theory of electron potential resonances is obvious from the lively discussion that has recently appeared in papers on the resonant scattering of electrons by molecules.[22–25]

It is shown in the present paper that for describing EVCs one can introduce a hierarchy of adiabatic approximations. The most general of these is the approximation of a nonlocal optical potential, which is applicable under the two relatively mild conditions

$$\omega_e \gg \omega_v, \quad \omega_e \gg \Gamma.$$

The optical potential, which allows for the influence of the decays of the electronic subsystem on the vibrational degrees of freedom of the EVC, is expressed in terms of the parameters of the vibrational subsystem of the center and the electronic interactions. By analyzing the resulting expressions one can obtain as limiting cases both the model of complex terms[20] and the fixed-scatterer approximation.[9–16] Here it becomes clear that, in contrast to the prevailing view, the region of applicability of the model of complex terms depends not only on the energy parameters (ω_e, ω_v, Γ, and E) but also on the tunneling time τ. For $\omega_v \tau \gtrsim 1$ (this case corresponds to a long-lived state of the EVC) the model of complex terms does not apply. The applicability region of the fixed-scatterer approximation, in turn, is found to depend not only on the parameter ω_v/Γ but also on the electron-vibrational interaction constant α. Here the situation is analogous to that for the resonant scattering of slow electrons by molecules, considered earlier.[26]

In the following sections it will be shown that in the cases of greatest practical interest, when $\alpha \gtrsim 1$ and $\Gamma \lesssim \omega_v$, the resonant tunneling of electrons should be accompanied by interesting multiquantum vibrational transitions of the centers. Another, rather general consequence of the theory developed here is the conclusion that absolute transparency of barriers containing impurities is also possible for inelastic, including multiquantum, tunneling.

In this paper the theory of inelastic resonant tunneling is used to describe the features of the differential spectra measured in experiments on the tunneling of electrons in MIM junctions[3–6] and in experiments on the field emission of electrons by metals containing adsorbed atoms of light elements.[2,8] Analysis of the influence of the vibrational degrees of freedom of the centers on the integrated tunnel currents—in particular, analysis of temperature effects due to multiquantum transitions—is of independent interest and would appropriately be done separately.

2. RESONANT TUNNELING WITH ALLOWANCE FOR THE VIBRATIONAL DEGREES OF FREEDOM OF BELOW-BARRIER SCATTERING CENTERS (THE BORN-OPPENHEIMER APPROXIMATION)

Let us formulate and outline the solution to the problem of the resonant tunneling of electrons through a one-dimensional potential barrier $U(z)$ containing a center of three-dimensional resonant interaction described by a potential $u(\mathbf{r}, R)$. (Here and below, $\mathbf{r}$ is the coordinate of the electron, and R represents the internal variables of the center.) The Hamiltonian of the system is

$$H(\mathbf{r}, R) = -\Delta_r/2 + U(z) + \hat{h}_R + u(\mathbf{r}, R).$$

Here $\hat{h}_R$ is the Hamiltonian of the center; here it will incorporate only the vibrational degrees of freedom [$\hat{h}_R \chi_v(R) = \varepsilon(v)\chi_v(R)$]. We stress that the "shape" resonances of negative molecular ions[18,19] and the other metastable systems mentioned in the Introduction are described by just this type of Hamiltonian. Therefore, the main results of the present section will extend to these systems as well.

Electron tunneling transitions between two half-spaces separated by a barrier $U + u$ will be described by solutions of the Lippmann-Schwinger equation

$$\Psi^{(+)}_{\mathbf{k},E_z,n,v} = |\mathbf{k}, E_z, n, v\rangle + \hat{G}_U^{(+)}(E(\mathbf{k}, E_z, v))\, u \Psi^{(+)}_{\mathbf{k},E_z,n,v}. \tag{2}$$

Here

$$|\mathbf{k}, E_z, n, v\rangle = (2\pi)^{-1} e^{i\mathbf{k}\mathbf{r}} f^{(+)}_{E_z,n}(z)\chi_v(R), \qquad \mathbf{k} = (k_x, k_y, 0),$$

n is the index of the half-space, $f^{(t)}_{E,n}(z)$ are the regular solutions of the one-dimensional Schrödinger equation with potential $U(z)$:

$$f^{(+)}_{E,1}(z) \sim S_{12} \exp\{i(2(E-U_0^+))^{1/2} z\} \quad \text{for} \quad z \to +\infty,$$

$$f^{(+)}_{E,2}(z) \sim S_{21} \exp\{-i(2(E-U_0^-))^{1/2} z\} \quad \text{for} \quad z \to -\infty.$$

To simplify the notation in the intermediate expressions we have assumed

$$\lim_{z \to \pm\infty} U(z) = U_0^{\pm}.$$

The final expressions will not depend on this assumption. In Eq. (2) $E(\mathbf{k}, E_x, v) = k^2/2 + E_z + \varepsilon(v)$ is the total energy of the state under consideration, and

$$\hat{G}_U^{(+)}(E) = (E - H + u + i\eta)^{-1}, \qquad E(\mathbf{k}, E_z, v) < U(0) = 0.$$

To evaluate the tunneling currents along the positive z direction it is sufficient to know the asymptotic behavior of the solutions $\Psi^{(+)}$. It is not hard to show that the asymptotic behavior for $z \to +\infty$ is of the form

$$\Psi^{(+)}_{\mathbf{k},E_z,1,v} = |\mathbf{k}, E_z, 1, v\rangle + \frac{i}{2\pi} \sum_{v'} \int \frac{d\mathbf{k}'}{k_z^+} \chi_{v'}^*(R) \times \exp(i\mathbf{k}'\mathbf{r} + ik_z^+ z) A_{if}(E). \tag{3}$$

Here

$$k_z^+ = \left[2\left(E(\mathbf{k}, E_z, v) - U_0^+ - \frac{k'^2}{2} - \varepsilon(v')\right)\right]^{1/2}, \qquad A_{if}(E) = -\frac{1}{2\pi}\langle f | u | \Psi_i^{(+)}\rangle \tag{4}$$

is the scattering amplitude of the tunneling electron, $i = (\mathbf{k}, E_z, 1, v)$; $f = (\mathbf{k}', E_z', 2, v')$; $E(\mathbf{k}, E_z, v) = E$.

The resonant interaction of an electron with a center qualitatively alters the shape of the wavefunction in the below-barrier and above-barrier regions. This interaction clearly cannot be taken into account by the perturbation-theory methods usually used to describe nonresonant inelastic tunneling (see, e.g., Ref. 27). Calculating the amplitudes $A_{if}(E)$ is the central problem of resonant-tunneling theory.

To solve this problem we use the scattering-operator ($\hat{T}$) method.

We define the operator ($\hat{T}$) by the equation

$$\hat{T}\,|i\rangle = u\Psi_i^{(+)}. \tag{5}$$

It is easy to show (see the analogous derivation in Refs. 28–30) that the operator ($\hat{T}$) can be found from the system of equations

$$\hat{T} = \hat{t}_0 + \hat{t}_0(\hat{G}_U^{(+)} - \hat{G}_0^{(+)})\,\hat{T}, \tag{6}$$

$$\hat{t}_0 = u + u\hat{G}_0^{(+)}\hat{t}_0, \tag{6'}$$

where $\hat{G}_0^{(+)}$ can be any convenient Green function.

Resonant tunneling proceeds by means of the formation and destruction of an intermediate quasistationary state which is similar in many respects to a bound state in the field of potential $u(\mathbf{r}, R)$. It is therefore convenient to choose $\hat{G}_0^{(+)} = (E + \Delta_r/2 - \hat{h}_R + i\eta)^{-1}$, i.e., to take the operator $\hat{t}_0$ to be the scattering operator for the scattering of free electrons by the center. (Here we are in fact assuming that the potentials u and U do not overlap in space. This, however, is not a fundamental limitation, since any interaction can be written as a sum of nonoverlapping terms by introducing a suitable set of projection operators.[29] For constructing a theory it is sufficient that the interaction U be concentrated in the asymptotic region of the coordinate $\mathbf{r}$ and, consequently, cause exponentially small changes in the states corresponding to the field u.)

In the investigated energy interval ($E < 0$) the free-electron scattering operators

$$\hat{t}_0 = u + u\hat{G}_u^{(+)}u, \qquad \hat{G}_u^{(+)} = (E + \Delta_r/2 - \hat{h}_R - u + i\eta)^{-1}$$

have only real poles $E(\nu)$, which correspond to stationary levels of a complex separated from regions of infinite motion by potential barriers of unbounded width. These levels and the corresponding wavefunctions $\Phi_\nu(\mathbf{r}, R)$ for the main range of variation of the variables $\mathbf{r}$ and R can be found by the Born-Oppenheimer method:

$$\Phi_\nu(\mathbf{r}, R) = \varphi(\mathbf{r}, R)F_\nu(R), \tag{7}$$

$$\left(-\frac{\Delta_r}{2} + u(\mathbf{r}, R)\right)\varphi(\mathbf{r}, R) = E^0(R)\varphi(\mathbf{r}, R),$$

$$(\hat{h}_R + E^0(R))F_\nu(R) = E(\nu)F_\nu(R). \tag{8}$$

Using functions (7) and including in the spectral representation of the function $\hat{G}_u^{(+)}$ only a single energetically isolated term $E^0(R)$, we obtain

$$\hat{t}_0 = u\varphi\sum_\nu \frac{|\nu\rangle\langle\nu|}{E - E(\nu)}\varphi u = u\varphi(E - \hat{h}_R - E^0(R))^{-1}\varphi u,$$

$$|\nu\rangle = F_\nu(R). \tag{9}$$

Here $|E - E^0(R)| \ll \omega_e$, $R \approx R_0$, where R_0 represents the equilibrium values of the variables R for the vibrational subsystem of the complex.

Expression (9) differs from the pole approximation of Refs. 12–15 by the presence of a "small" (in the sense of condition $\omega_v \ll \omega_e$) operator $\hat{h}_R$ in the resonant denominator. This small operator must be introduced in order to take into account the motion of the system over the vibrational degrees of freedom. Operator (9) takes into account the adiabatic dependence of state φ on R but ignores tunnling effects. In order to take tunneling effects into consideration one must find the operator $\hat{T}$, i.e., solve Eq. (6). Let us give the final result. One can verify by direct substitution that the necessary solution is of the form

$$\hat{T} = u\varphi[E - \hat{h}_R - E^0(R) - \hat{\Omega}_R(E)]^{-1}\varphi u, \tag{10}$$

where $\hat{\Omega}_R(E)$ is an integral operator which acts only on the variable R:

$$\hat{\Omega}_R(E)F(R) = \int dR'\,\Omega(E, R, R')F(R'), \tag{11}$$

$$\Omega(E, R, R') = \langle\varphi|u(\hat{G}_U^{(+)}(E) - \hat{G}_0^{(+)}(E))u|\varphi\rangle_{\mathbf{r}}. \tag{12}$$

Here and below the symbol $\langle\ \rangle_{\mathbf{r}}$ denotes an integration over $\mathbf{r}$.

Having found the solution, we can write the amplitude $A_{if}(E)$ in the form

$$A_{if}(E) = -\frac{1}{2\pi}\langle(f)\,|u|\,\Psi_i^{\mathrm{EVC}}\rangle, \tag{13}$$

where

$$\Psi_i^{\mathrm{EVC}}(\mathbf{r}, R) = \varphi(\mathbf{r}, R)F_i(R) \tag{14}$$

is the wavefunction of the EVC.

The function $F_i(R)$ describing the vibrational subsystem of the complex satisfies the Schrödinger equation with an optical potential $\hat{\Omega}_R(E)$ and a source:

$$[E - \hat{h}_R - E^0(R) - \hat{\Omega}_R(E)]F_i(R) = a_{ie}(R)\chi_v(R). \tag{15}$$

Here

$$a_{ie}(R) = \langle\varphi|u|i_e\rangle_{\mathbf{r}}$$

is the probability amplitude for the formation of an EVC and $i_e = (\mathbf{k}, E_z, 1)$. Expression (14) and Eq. (15) generalize formula (7) and Eq. (8) to the case of electron resonances of the potential type.

Here we should stress that it is possible to approximate the solutions $\Psi_i^{(+)}(\mathbf{r}, R)$ by the EVC wavefunction only in the main range of the coordinates [the region which gives the main contribution to matrix element (4)]. In this region the improbable decays have only a slight effect on the electron density. The small parameter here is clearly Γ/ω_e, where Γ is the probability (per unit time) for the electron to break away from the complex (a rather general analytical expression for Γ will be obtained below). In the asymptotic region of the coordinate $\mathbf{r}$ (a region which, however, gives an exponentially small contribution to the transition matrix element), expression (14) does not apply. The method of adiabatic separation of variables and the method of unnormalized quasistationary states [these methods are unified by solution (10)] give approximations which are inhomogeneous with respect to $\mathbf{r}$. At large distances neither of these methods applies. This situation is manifested formally in certain mathematical difficulties such as the appearance of divergent matrix elements in the theory, preventing the direct application of standard perturbation-theory techniques (including the method of perturbed stationary states) in the case of decaying systems. The approach set forth above is free from these difficulties. The integral expressions with which this method operates contain the unknown functions $\Psi_i^{(+)}$ and $(E - H)^{-1}$ only in

combination with the interaction u. The latter is localized, and in the integration over r it singles out the finite region of space in which the EVC wave functions can be used.

Using the equalities

$$\hat{G}_U^{(+)}-\hat{G}_0^{(+)}=\hat{G}_U^{(+)}U\hat{G}_0^{(+)}, \quad \hat{G}_0^{(+)}u\varphi=\varphi[1+o(\omega_v/\omega_e)],$$

we can write the optical potential in the form

$$\hat{\Omega}_R(E)=\langle\varphi|u\hat{G}_U^{(+)}(E)U|\varphi\rangle_r, \tag{16}$$

which we shall use in analyzing the conditions of applicability of the model of complex terms. Suppose the conditions

$$E\gg\varepsilon(v), \quad \varepsilon(v)\tau_{1,2}\ll 1 \tag{17}$$

hold, indicating that the formation and destruction of the EVCs can be considered instantaneous acts with respect to the vibrations. (Here $\tau_n = dS_n(E)/dE$ is the modulus of the imaginary tunneling time of the electron through the potential barrier separating the center from the nth half-space, and $S_n(E)$ is the modulus of the imaginary action along the extremal below-barrier trajectory). Then in expression (16) we can neglect the energies $\varepsilon(v)$ and use the completeness of the system of functions $\chi_v(R)$. We have

$$\Omega(E,R,R')=\sum_v|v\rangle\langle\varphi|u\hat{g}_U^{(+)}(E-\varepsilon(v))U|\varphi\rangle_r\langle v|$$

$$\approx\Delta(E,R)\delta(R-R'). \tag{18}$$

Here

$$\hat{g}_U^{(+)}(E)=(E+\Delta_r/2-U+i\eta)^{-1},$$
$$\Delta(E,R)=\langle\varphi|u\hat{g}_U^{(+)}(E)U|\varphi\rangle_r. \tag{19}$$

In approximation (18) Eq. (15) assumes the form postulated in the model of complex terms,[19,20,23] the term of a state coupled to the continuum by tunneling transitions being given by

$$E_p(R)=E^0(R)+\Delta(E,R)\approx E^0(R)+\Delta(E^0(R),R).$$

The function $\Delta(E,R)$ gives the complex shift of the discrete level $E^0(R)$ upon allowance for electron tunneling transitions to the continuum. The problem of evaluating this function is discussed in many papers dealing with special and general questions in the theory of potential resonances (see, e.g., Refs. 31–33). For the case of one-dimensional motion this problem was solved recently in Ref. 34, in which the evolution of the wave packet in the field of a potential having a general form of the "well with barrier" shape. Expression (19) generalizes the result of Ref. 34 to the case of three dimensions.

Let us now find the relationship of operator $\hat{\Omega}_R(E)$ to the decay probability (per unit time) of the complex. Let us treat the evolution of the wave packet $\Phi(\mathbf{r},R)=\varphi(\mathbf{r},R)=F(R)$ using Eq. (15). We find

$$\Gamma=-\frac{d}{2\,dt}\ln\sum_v|\langle\Phi_v|\exp(-i\hat{H}_Rt)|\Phi\rangle|^2$$

$$=-\langle F|\operatorname{Im}\hat{\Omega}_R(E)|F\rangle. \tag{20}$$

(Here $\hat{H}_R=\hat{h}_R+E^0(R)+\hat{\Omega}_R(E)$ is the Hamiltonian of the vibrational subsystem of the EVC.)

Let us now use expression (12) and the spectral representation of the Green function $G_U^{(+)}$ and take into account that $\operatorname{Im}\hat{G}_0^{(+)}=0$ in the energy interval under consideration. We then find a relation between the damping operator $\operatorname{Im}\hat{\Omega}_R(E)$ and the source functions appearing in Eq. (15):

$$\operatorname{Im}\hat{\Omega}_R(E)=-\pi\sum_{n,v}\int\frac{d\mathbf{k}\,dE_z}{k_z^n}\delta\left(E-\varepsilon(v)-\frac{k^2}{2}-E_z\right)$$

$$\times a_{j_e}(R)|v\rangle\langle v|a_{j_e}^*(R'), \tag{21}$$

$$k_z^n=[2(E_z-U_0^n)]^{1/2}, \quad \operatorname{Im}k_z^n=0, \quad U_0^{1,2}=U_0^{\pm}, \quad j_e=(\mathbf{k},E_z,n).$$

The optical potential given by formulas (11), (12), and (16) is analytic in the upper half of the energy plane. It can be shown that its real and imaginary parts are related to each other by dispersion relations which, unlike those of Ref. 21, do not contain divergent integrals.

3. ANALYSIS OF PARTICULAR AND LIMITING CASES. ABSOLUTE TRANSPARENCY IN INELASTIC TUNNELING

Here we consider several limiting and particular cases which illustrate the role of the vibrational degrees of freedom of the centers in the resonant tunneling of electrons.

Let us suppose that the potential barriers separating the EVC from the regions of infinite motion have rather low permeabilities and that

$$|E-E(v)|\leqslant|\langle v|\hat{\Omega}_R(E)|v\rangle|\ll|E-E(v')|, \quad v\neq v'.$$

Then expressions (14) and (15) imply

$$\Psi_{(i)}^{\mathrm{EVC}}(r,R)=\frac{\langle\Phi_v|u|(i)\rangle}{E-E(v)-\Delta_v(E)}\Phi_v(r,R), \tag{22}$$

$$\Delta_v(E)=\langle v|\hat{\Omega}_R(E)|v\rangle.$$

In the approximation under discussion decays do not affect the motion of the complex over the vibrational degrees of freedom. The resonant-tunneling amplitudes in this case assume the form of composite matrix elements:

$$A_{if}(E)=-\frac{1}{2\pi}\frac{\langle(f)|u|\Phi_v\rangle\langle\Phi_v|u|i\rangle}{E-\bar{E}(v)+i\Gamma(v)},$$
$$\bar{E}(v)=E(v)+\operatorname{Re}\Delta_v(E), \quad \Gamma(v)=-\operatorname{Im}\Delta_v(E).$$

Accordingly, the resonant-tunneling probabilities $W_{if}=|A_{if}|^2$ can be evaluated by the Breit-Wigner formula:

$$W_{if}=\gamma_i(v)\gamma_f(v)\{[E-\bar{E}(v)]^2+\Gamma^2(v)\}^{-1}, \tag{23}$$

where

$$\gamma_{i,f}(v)=\frac{1}{2\pi}|\langle\Phi_v|u|i,f\rangle|^2 \tag{24}$$

are the partial widths corresponding to the formation and decay of the EVCs. In the present limiting case these events can be considered independent, i.e., an EVC is a long-lived electron-vibrational compound state. (A rigorous applicability criterion for the compound-state approximation is given below.)

Using Eq. (21), we find a relation between $\gamma(v)$ and $\Gamma(v)$:

$$\Gamma(v)=\sum_{v,n}\int\frac{d\mathbf{k}\,dE_z}{k_z^n}\delta\left(E(v)-\frac{k^2}{2}-E_z-\varepsilon(v)\right)\gamma_{\mathbf{k},E_z,n,v}(v).$$

In the Condon approximation

$$\gamma_{\mathbf{k},E_z,n,v}(\nu)=\gamma_n^0(\mathbf{k})\langle v|\nu\rangle^2\exp\left(2(E(\nu)-E(0)-\varepsilon(v))\tau_n\right), \tag{26}$$

where

$$\gamma_n^0(\mathbf{k})=\pi\left|\left\langle\varphi|u|\mathbf{k},E(0)-\frac{k^2}{2},n\right\rangle_r^0\right|^2 \tag{27}$$

are the electron particle widths calculated in the fixed-scatterer model,

$$\gamma_n^0(\mathbf{k})\propto\exp\left\{-2S_n\left(E(0)-\frac{k^2}{2}\right)\right\};$$

$$\Gamma(\nu)=\sum_n\Gamma_n(0)M_\nu(\tau_n), \tag{28}$$

$$\Gamma_n(0)=\int\frac{d\mathbf{k}}{k_z^n}\gamma_n^0(k)\approx\frac{\pi\gamma_n^0(0)}{\tau_n[2(E(0)-U_0^n)]^{1/2}}, \tag{29}$$

$$M_\nu(\tau_n)=\exp\{2(E(\nu)-E(0))\tau_n\}\sum_v\langle v|\nu\rangle^2\exp(-2\varepsilon(v)\tau_n).$$

The factors M_ν take into account the influence of the electron-vibrational exchange of energy on the rate of destruction of the EVC. For a harmonic vibration model these factors have been calculated and analyzed in Refs. 35–37. It is easy to se that for $|E(\nu)-E(0)|\tau_n\ll 1$, $\varepsilon(v)\tau_n\ll 1$, $M_\nu\approx 1$, i.e., at small values of τ_ν, the electron-vibrational coupling is unimportant. At sufficiently large $\tau_n[\sim 1/\varepsilon(v)]$, however, the electron-vibrational exchange of energy has a strong effect on the probabilities of formation and destruction of EVC states.

According to formulas (23) and (26) the relative probabilities of resonant tunneling via different channels is determined by the factor $\langle\nu|v'\rangle^2\exp(-\varepsilon(v')\tau_2)$. It follows that for $v\neq 0$, $\alpha\neq 0$, $\varepsilon(v)\tau_2>1$, resonant tunneling always takes place via superelastic channels, i.e., is accompanied by an increase in the electron energy. For $v=0$, $\langle\nu|v\rangle\sim\langle\nu|v'\rangle$, $\varepsilon(v')\tau_2\lesssim 1$ the elastic and inelastic resonant-tunneling probabilities are of the same order, and for $\langle\nu|v\rangle\gg\langle\nu|0\rangle$, $\varepsilon(v')\tau_2\lesssim 1$ the most probable channels for resonant tunneling correspond to a loss of electron energy. It is important that in all these cases an appreciable change in the energy of the vibrational subsystem is possible, i.e., resonant tunneling can be accompanied by intense multiquantum transitions.

The expressions we have obtained also enable us to conclude that, under certain conditions, inelastic resonant tunneling occurs without damping. In fact, let us suppose that $S_1(E)=S_2(E)$. Then for $E=\bar{E}(\nu)$, $[\varepsilon(v)+k^2]\tau_n\ll 1$ the probabilities (23) do not contain an exponentially small factor. In other words, absolute transparency, which has previously been discussed only for elastic processes,[1,9,13,15] is also possible during inelastic tunneling. We shall show below that it is this effect that makes for observable inelastic-resonance anomalies in the tunnel conductance of MIM systems.[3–6]

Let us now consider the opposite case—that of short-lived EVC states—and take the limiting transition to the fixed-scatterer approximation.[9–16] Suppose that condition (1) is satisfied. Then the operator $\hat{h}_R$ appearing in expression (10) can be considered small, and, using the Condon approximation to evaluate $\hat{\Omega}_R$ and a_{j_e} one can expand the operator $(E-\hat{H}_R)^{-1}$ in a series in terms proportional to $\hat{h}_R$ and R. (Here the equilibrium values of R for the vibrational subsystem of the center are taken to be zero.) Finally, we get

$$W_{if}=\frac{\gamma_1^0(\mathbf{k})\gamma_2^0(\mathbf{k}')}{[E-\mathrm{Re}\,E_p(0)]^2+\Gamma^2(0)}|M_{vv'}(E)|^2. \tag{30}$$

Here, $\Gamma(0)=-\mathrm{Im}E_p(0)$,

$$M_{vv'}(E)=\delta_{vv'}\left(1+\frac{\varepsilon(v)}{E-E_p(0)}+\ldots\right)+\frac{fa_{vv'}}{E-E_p(0)}+\ldots,$$

$$f=\left(\frac{dE^0}{dR}\right)_{R=0},\qquad a_{vv'}=\langle v|R|v'\rangle. \tag{31}$$

The fixed-scatterer approximation,[9–16] which obviously admits only elastic tunneling, gives the first term in expansion (31). The corrections which arise upon allowance for the vibrational degrees of freedom of the center contain not only the energy $\varepsilon(v)$ but also the force f acting on the nucleus of a center in a quasistationary state. The applicability region of the fixed-scatterer model is thus limited by the conditions $\omega_v\ll\Gamma$, $\alpha\omega_v\ll\Gamma$ ($\alpha\sim fa_{vv_1}/\omega_v$), which can be combined as $\Gamma\gg\omega_v(1+\alpha)$.

This is probably an appropriate place to emphasize that the fixed-scatterer approximation (30), (31), the model of complex terms (17)–(19), and the optical potential method (10)–(12) form a hierarchy of adiabatic approximations. This hierarchy is possible because the decaying electronic states are characterized not only by frequencies ω_e but also by substantially smaller parameters Γ and τ^{-1}. The values of ω_e, ω_v, Γ, and τ are limited only by the conditions $\omega_v\ll\omega_e$, $\Gamma,\ll\omega_e$, and $\Gamma\tau\ll 1$. The relationship between the decay parameters and the vibrational frequencies can be arbitrary.

In the Condon approximation under conditions (17) the rate of destruction of the EVCs is constant. In this case the operator $(E-\hat{H}_R)^{-1}$ appearing in (10) can be written in the spectral representation

$$(E-\hat{H}_R)^{-1}=\sum_\nu\frac{|\nu\rangle\langle\nu|}{E-\bar{E}(\nu)+i\Gamma},$$

which is valid for arbitrary values of the parameter ω/Γ. Then it follows from (13)–(15) and (28) that

$$W_{if}=\frac{\gamma_1^0(\mathbf{k})\gamma_2^0(\mathbf{k}')}{\Gamma^2}|K_{vv'}(x)|^2, \tag{32}$$

where $\Gamma=\Gamma_1(0)+\Gamma_2(0)$, and

$$K_{vv'}(x)=\sum_\nu\frac{\langle v|\nu\rangle\langle\nu|v'\rangle}{x-x(\nu)+i} \tag{33}$$

are vibrational factors which take into account the displacement of the center during the lifetime of the EVC, $x=E/\Gamma$, and $x(\nu)=\bar{E}(\nu)/\Gamma$. For the harmonic vibrational model

$$\hat{h}_R=-\frac{d^2}{2M\,dR^2}+\frac{M\omega^2(R-R_0)^2}{2},$$

$$\hat{H}_R=-\frac{d^2}{2MdR^2}+\frac{M\omega^2R^2}{2}+\bar{E}(0)-i\Gamma, \tag{34}$$

$$\bar{E}(\nu)=E(0)+\omega\left(\nu+\frac{1}{2}\right)$$

the factors $K_{vv'}(x)$ have been evaluated and analyzed in Ref. 26. Using the results of that study, one can determine rigorous applicability criteria for the various limiting cases and

elucidate the dependence of W_{if} on E for $\Gamma \sim \omega$.

Under the condition

$$|E-\bar{E}(v)+i\Gamma| \ll \frac{\omega e^{-\alpha}}{v!}(1+\alpha^2)\alpha^v, \quad \alpha = \frac{M\omega R_0^2}{2} \tag{35}$$

the model of an electron-vibrational compound state is valid:

$$|K_{vv'}(x)|^2 = \frac{\langle v|v\rangle^2\langle v|v'\rangle^2}{[x-x(v)]^2+1}. \tag{36}$$

We note that the applicability regions of formulas (36) and (23) overlap. The more general expressions (23)–(29) allow one to escape the restriction $\varepsilon(v)\tau_n \ll 1$.

For $\Gamma \gtrsim \omega$, $\Gamma \gtrsim \alpha\omega(1+|v-v'|)$

$$|K_{vv'}(x)|^2 = \frac{(v_>)!\,(\alpha\omega^2/\Gamma^2)^{|v-v'|}}{(v_<)!\,[(x-\bar{x}(0))^2+1]^{|v-v'|+1}},$$

$$\bar{x}(0) = \frac{E(0)}{\Gamma}, \quad v_{\gtrless} = \max_{\min}(v, v').$$

In this limiting case the resonant tunneling takes place mainly via elastic channels. The inelastic-tunneling probabilities are proportional to the small factor $(\alpha\omega^2/\Gamma^2)^{|v-v'|}$ and have a non-Lorentzian energy dependence.

At $\Gamma \sim \omega$ the factors $K_{vv'}(x)$ for $|v-v'| \lesssim \alpha$, $0 < x \lesssim \alpha$ have values $\propto e^{-\alpha}$ and undergo regular oscillations with a common period $\delta x \sim 1$ (see Fig. 1 of Ref. 26).

Finally, we note that in expression (32) the exponentially small quantities appear only in combinations of electronic widths. For $S_1(E) = S_2(E)$, $k'^2\tau_1 \ll 1$, $k'^2\tau_2 \ll 1$ the exponentially small factors (proportional to the permeability factors of the potential barriers separating the EVCs from the regions of infinite motion) exactly cancel, i.e., absolute transparency is possible at any values of ω/Γ.

4. RESONANCE FEATURES IN THE TUNNELING SPECTRA. COMPARISON OF THEORY AND EXPERIMENT

Here we use the results obtained for the purpose of analyzing the features of the tunnel conductance of MIM junctions[3–6] and energy distributions of field-emission electrons.[2,8]

Differential conductance of MIM systems

In the single-particle approximation the tunneling current of electrons passing through an MIM contact and undergoing single scattering in the below-barrier region by an impurity atom (or defect) can be evaluated by the formula

$$j(V) = 2\int dE \sum_{v,v'} n(v)\,dz\,d\mathbf{k}\,d\mathbf{k}' f_1(E)\,[1-f_2(E + \varepsilon(v)-\varepsilon(v')+V)]\frac{|A_{if}(E+\varepsilon(v), z)|^2}{k_z^{(+)}k_z^{(-)}}. \tag{37}$$

Here $E = k^2/2 + E_z$, $V \geqslant 0$ is the potential difference applied to the contact, $n(v)$ is the bulk concentration of centers in state v, $f_{1,2}(E)$ are the Fermi distributions of the electrons for the emitter metal and second metal, respectively, $A_{if}(E,z)$ are the scattering amplitudes for tunneling electrons, and z is the coordinate of the center. In the derivation of formula (37) we used Eq. (2) of Ref. 38 and the asymptotic formula (37) of the present paper and called for a summation over vibrational quantum numbers and an averaging over random spatial distribution of centers in the barrier.

In what follows we are interested only in the resonant electrons, which for wide barriers represent the predominant contribution not only in the total current $j(V)$ but also in the differential conductance $G(V) = dj/dV$. We use the harmonic model (34) and, following Refs. 12 and 13, incorporate the dependence of the electron parameters on z and V. Let us take

$$(E-\hat{H}_R)^{-1} = \sum_v \frac{|v\rangle\langle v|}{E-E(v, V, z)+i\Gamma(z)},$$

$$E(v, V, z) = E(v) - Vz/d,$$

$$E(v) = E(0)+v\omega; \quad v = 0, 1, 2, \ldots \tag{38}$$

($0 \leq x \leq d$, where d is the thickness of the insulating layer), and

$$\Gamma(z) = \Gamma_1(z)+\Gamma_2(z),$$

$$\Gamma_1(z) = \Gamma_1(0)\exp(-2S_1(E, z)),$$

$$\Gamma_2(z) = \Gamma_2(d)\exp(-2S_2(E, z)) \tag{39}$$

and consider the low-temperature case, setting $f_{1,2}(E) = \eta(E_F - E)$, where E_F is the Fermi energy, $\eta(E)$ is the step function, and $n(v) = n\delta_{v0}$. Then it follows from expressions (32), (37)–(39) that

$$G(V) = \frac{n}{2}\sum_v \eta(V-\varepsilon(v))\left[\langle D_{0v}(E_F-V+\varepsilon(v), V, z)\rangle_z + \frac{1}{d}\langle zD_{0v}(E_F, V, z)\rangle_z - \frac{1}{d}\langle zD_{0v}(E_F-V+\varepsilon(v), V, z)\rangle_z\right], \tag{40}$$

where

$$D_{0v}(E, V, z) = 4\frac{\Gamma_1(z)\Gamma_2(z)}{\Gamma^2(z)}|K_{0v}(x(E, V, z))|^2, \tag{41}$$

$$x(E, V, z) = (E-E(0)-zV/d)/\Gamma(z),$$

$$\langle z^n D_{0v}(E, V, z)\rangle = \int_0^d z^n D_{0v}(E, V, z)\,dz. \tag{42}$$

It is easily seen that the main contribution to the integral in (42) is from the neighborhood of the point z_0 for which the resonant tunneling occurs without damping: $\Gamma_1(z_0) = \Gamma_2(z_0)$, $z_0 \approx d/2$.

Let us consider two limiting cases. Suppose d is sufficiently small that $\Gamma(d/2) \gtrsim \alpha\omega_v$. Then, neglecting inelastic-tunneling currents and using formula (3), we obtain

$$G(V) = \frac{n}{p}[J(\xi(E_F, V, a))+J(\xi(E_F-V, V, a))], \tag{43}$$

where

$$J(\xi, a) = \int_{-\infty}^{\infty}\frac{dx}{(\xi+ax)^2+4\operatorname{ch}^2 x},$$

$$\xi(E, V) = \frac{E-E(0)+V/2}{\Gamma(d/2)}, \quad a = \frac{V}{pd\Gamma(d/2)},$$

$$p = \frac{\partial S_1}{\partial z}\Big|_{z_0}, \quad pd \gg 1. \tag{44}$$

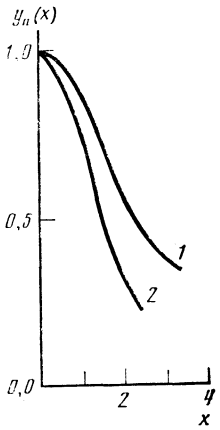

FIG. 1. The dependence of $J(\xi, a)$ on ξ. Curve 1) the function $y_1(x) = \frac{3}{4}J(x,0)$; curve 2) the function $y_2(x) = (8/\pi)^{1/2}aJ(\xi, a)$. Here $x = \xi_a$, $a \gg 1$.

As a function of ξ, integral (44) has a symmetric peak at zero, with a length and shape which depend on the parameter a (see Fig. 1). For $a \ll 1$ and $a \gg 1$ one easily obtains the asymptotic expressions

$$J(\xi, a) = [\xi^2(\xi^2+4)]^{1/2} \ln \frac{\xi^2+3+[\xi^2(\xi^2+4)]^{1/2}}{\xi^2+3-[\xi^2(\xi^2+4)]^{1/2}}, \quad a \ll 1,$$

$$J(\xi, a) = (\pi/8)^{1/2}\left[a \operatorname{ch}\left(\frac{\xi}{a}\right)\right]^{-1}, \quad a \gg 1.$$

We see that in the present case the conductance of the contact as a function of V can have only one resonance peak, described by either the first or second term of expression (43). In the first case the resonant increase in the conductance arises when the level $E(0, V, d/2)$ passes through the Fermi level of the emitter metal; the corresponding resonance value of the voltage is $V_p = 2(E(0) - E_F)$. In the second case the peak arises when the level $E(0, V, d/2)$ passes through the Fermi boundary of the metal having the larger electrostatic potential; here $V_p = 2(E_F - E(0))$.

Let us now consider the most interesting case—that of rather thick insulating layers, when the resonant tunneling of electrons should be accompanied by interesting multiquantum vibrational transitions of the centers of interaction. Let $\Gamma(d/2)$ be sufficiently small that condition (35) holds. Then, using formulas (40), (41), and (23), we obtain

$$G(V) = \frac{n}{p}\sum_{v,\nu} \eta(V-\varepsilon(v))\langle 0|\nu\rangle^2\langle\nu|v\rangle^2[J(\xi_\nu(E_F, V), a) + J(\xi_\nu(E-V+\varepsilon(v), V), a)]. \quad (45)$$

Here

$$\xi_\nu(E, V) = \frac{E-E(\nu)+V/2}{\Gamma(d/2)}, \quad \nu = 0, 1, \ldots .$$

Comparison of expressions (43) and (45) shows that allowance for the vibrational degrees of freedom of the centers leads to a qualitative change in the spectrum of the features appearing in the tunnel conductance of the contact. First, jumps appear in the spectrum, corresponding to the opening of the inelastic-tunneling channels; here, in resonant tunneling, unlike the familiar case of the nonresonant interaction,[27] one can also observe multiquantum features. Second, the resonance peaks are grouped into series obeying the combination relations

$$V_p^{(1)}(\nu) = 2(E(\nu)-E_F), \quad \text{if} \quad E(\nu) > E_F,$$

$$V_p(\nu) = 2(E_F+\varepsilon(v)-E(\nu)), \quad \nu = 0, 1, \ldots, \quad \text{if} \quad E(\nu) < E_F.$$

The peaks of the first series correspond to a resonant increase in the probability of formation of an EVC upon passagae of the Fermi boundary of the emitter metal through the level $(E(\nu, V, d/2)$. The second group of peaks arises from EVC states which for $V = 0$ lie below the Fermi level of the emitter metal. These features correspond to resonance peaks of the energy distributions of the electrons released in the decay of the EVCs.

The results of recently published experiments on electron tunneling in the systems Mg–MgO–M, where M = Mg, Bi, Pb at $T = 1.5$K (Ref. 3), Al–Al_2O_3–M, where M = Ag, Au, Sn, Pb, Pd at $T = 1.2$–4.2 K, and Ag–PgI_2–Ag at $T = 4.2$ K (Ref. 6) support this conclusion of the theory. These systems, whose insulating layers could, under the conditions of fabrication of the contacts, contain uncontrolled impurities (or defects), did in fact exhibit a series of inelastic-resonance features, which in certain cases were almost equidistant and had half-widths ~ 1 mV.

Resonant field emission

In the single-particle approximation the current density of field-emission electrons scattered in the below-barrier region by single adatoms and having energy E in the final state is described by the expression

$$\frac{dj}{dE} = 2\sum_{v,v'} n(v')f(E+\varepsilon(v')-\varepsilon(v)) \times \int \frac{d\mathbf{k}\,d\mathbf{k}'}{k_z^{(+)}k_z^{(-)}} |A_{if}(E+\varepsilon(v'))|^2. \quad (46)$$

Here $n(v)$ is the surface density of adatoms in vibrational state v,

$$k_z^{(+)} = \left[2\left(E - \frac{k^{1/2}}{2} - U_0^+\right)\right]^{1/2},$$

$$k_z^{(-)} = \left[2\left(E - \frac{k^2}{2} + \varepsilon(v') - \varepsilon(v) - U_0^-\right)\right]^{1/2}.$$

In deriving formula (46) we used the familiar expressions for the density of field-emission currents (given, e.g., in Ref. 2) and formula (3) of the present paper, called for the summation and averaging of the field-emission current over the vibrational quantum numbers of the adatoms, and averaged the current over the random position of the adatoms on the adsorption plane $z = z_a$.

In what follows we will only be interested in the case of resonant field emission, which is realized if the adatom has a quasistationary electronic term $E^0(R)$ in the vicinity of E_F.[2,10–12] (The single-quantum excitation of the vibrations of the adatoms in nonresonant field emission has been considered in Ref. 39).

We use the Condon approximation and consider the case of low temperatures, assuming that there are no vibrationally excited particles at the surface. Then expressions (32), (33), and (46) imply:

$$\frac{dj}{dE}=2n(0)\frac{\Gamma_1\Gamma_2}{\Gamma^2}\sum_v \eta(E_F-E-\varepsilon(v))\left|K_{0v}\left(\frac{E+\varepsilon(v)}{\Gamma}\right)\right|^2. \tag{47}$$

Here $\Gamma=\Gamma_1+\Gamma_2$, where Γ_n are the decay widths of the quasistationary level of the adatom for the cases when the electron escapes into the metal (Γ_1) and vacuum (Γ_2). Under typical experimental conditions one has $\sigma|z_a|\ll\varphi$, where σ is the strength of the electronic field and φ is the electronic work function of the emitter. Here

$$S_1(E)\approx|z_a|(2|E|)^{1/2},\quad S_2(E)\approx\frac{2(|E|)^{1/2}}{3\sigma},$$

$$\Gamma_n=C_n\exp\{-2S_n(E_F-E+\varphi)\},$$

where C_n are relatively unimportant pre-exponential factors which vary slowly with the energy.

Formula (47) predicts two types of features in the field-emission spectra: threshold jumps [at $E=E_F-\varepsilon(v)$, $v=0, 1, 2,...$] and resonance peaks [at $E=E(\nu)-\varepsilon(v)$, if $\Gamma\ll\omega_v$] or oscillations [if $\Gamma\sim\omega_v$].

To illustrate the effect of vibrational transitions of the adatoms on the resonance features of the field-emission spectra, we have calculated the enhancement factor $R(E)=dj/dE)/(dj^0/dE)$, which is ordinarily separated out in the processing of experimental data.[2] The distribution of dj^0/dE corresponds to field emission from a metal surface without adatoms:

$$\frac{dj^0}{dE}=\frac{\pi\eta(E_F-E)}{2\tau_2}\exp\{-2(S_1(\varphi+E_F-E)+S_2(\varphi+E_F-E)\}. \tag{48}$$

The results of our calculations on the basis of formulas (47), (48), and (33) for the harmonic-vibration model (34) are given in Fig. 2. The calculations were done using $\omega=0.1$ eV (Ref. 17), $E_F-E(0)=2\omega$, $\Gamma=0.7\omega$, and $\alpha=1$. For comparison, Fig. 2 also shows the experimental data obtained in Ref. 8 for the surface $W(100)$, D and the results of calculations done without allowance for the electron-vibrational coupling (for $\alpha=0$). One can see that the latter disagree qualitatively with experiment. Comparison of the theoretical and experimental spectra permits estimation of the main parametes of the $W(100)$, D system: $\Gamma=0.07$ eV, $\alpha\approx1$. One can also conclude that the feature observed at $E_F-E=0.05$ eV is oscillatory in character [this peak was reproduced in the calculations by an oscillatory vibrational factor $K_{00}(E/\Gamma)$].

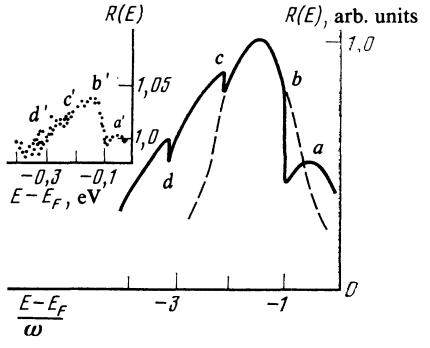

FIG. 2. The factor $R(E)$ calculated according to formulas (33), (47), and (48) for a harmonic-vibration model with $E_F-E(0)=2\omega$, $\Gamma=0.7\omega$, $\alpha=1$. Peak (a) is an interference feature corresponding to oscillations of the current of elastically tunneling electrons. The threshold jumps labeled by the letters b, c, and d correspond to single-quantum (b), two-quantum (c), and three-quantum (d) vibrational transitions of the adatoms. The dashed line is the theoretical curve for $\alpha=0$. The inset shows the experimental data of Ref. 8 for the surface $W(100)$, D.

5. CONCLUSION

In the above calculations we have not considered the possibility of vibrational relaxation of the center, i.e., we have in fact assumed that the lifetime of the EVCs is shorter than the characteristic values for relaxational processes. At low temperatures the lowest excited states of the centers relax over a time $t_r\sim10^{-11}$–10^{-12} sec; for $\nu\geqslant3$ the time t_r is considerably larger.[40] It follows that the need to include relaxational processes can arise only for systems which can be described in the compound-state approximation. In this limiting case one can discern an analogy with the resonant scattering of light; this analogy is convenient for generalizing the results obtained above. An exposition of the theory of resonant tunneling under conditions of rapid vibrational relaxation of the centers of interaction is beyond the scope of this paper. We shall only remark that allowance for relaxation is not important for describing the features that correspond to the formation of EVCs in the ground or highly excited states. The character of the changes in the features which correspond to decays of rapidly relaxing EVC states is also qualitatively clear. These changes can be taken into account phenomenologically by replacing the decay width Γ by the sum $\Gamma+t_r^{-1}$. Experimentally, the influence of relaxational processes on resonant tunneling can be studied by varying the thickness of the insulating layer.

I am grateful to V. M. Agranovich and all the participants of his seminar for discussing the results of this study.

[1)] A sufficient condition, which depends on the electron-vibrational interaction constant α, will be obtained below.

[2)] To avoid misunderstandings we stress here that we are considering electron resonances which decay by a tunneling mechanism. For such resonances the familiar Fano-Feshbach method does not apply. Attempts at a nonsystematic description of potential resonances in the framework of the configurational interaction method lead to divergences which can be eliminated by a cutoff.[21]

[1]L. Esaki, Long journey into tunneling (Nobel Lecture, Dec. 13, 1973).
[2]J. W. Gadzuk and E. W. Plummer, Rev. Mod. Phys. **45**, 487 (1973).
[3]J. G. Adler and J. Straus, Phys. Rev. B **13**, 1377 (1976).
[4]N. Christen and N. E. Christen, Solid State Commun. **127**, 1259 (1980).
[5]Y. Skarlatos and R. C. Barker, J. Appl. Phys. **47**, 4593 (1976).
[6]J. Rauluskiewicz and Y. Nashino, Physica B **99**, 371 (1980).
[7]E. W. Plummer and R. D. Young, Phys. Rev. B **1**, 2088 (1970).
[8]E. W. Plummer and A. E. Bell, J. Vac. Sci. Technol. **9**, 588 (1972).
[9]L. V. Iogansen, Zh. Eksp. Teor. Fiz. **45**, 207 (1963) [Sov. Phys. JETP **18**, 146 (1964)].
[10]C. B. Duke and M. E. Alferieff, J. Chem. Phys. **46**, 923 (1967).
[11]J. P. Hurrault, J. Phys. (Paris) **32**, 421 (1971).
[12]R. J. Combescot, J. Phys. C **4**, 2611 (1971).

[13]A. V. Chaplik and M. V. Éntin, Zh. Eksp. Teor. Fiz. **67**, 208 (1974) [Sov. Phys. JETP **40**, 106 (1974)].
[14]H. Knauer, G. Richter, and P. Seidal, Phys. Status Solidi **44**, 303 (1977).
[15]I. M. Lifshitz and V. Ya. Kirpichenkov, Zh. Eksp. Teor. Fiz. **77**, 989 (1979) [Sov. Phys. JETP **50**, 499 (1979)].
[16]X. Aymerich-Humet and F. Serra-Mestres, Phys. Status Solidi A **54**, 655 (1979).
[17]W. Ho, R. F. Willis, and E. W. Plummer, Phys. Rev. B **21**, 4202 (1980).
[18]G. Schulz, Rev. Mod. Phys. **45**, 378 (1973).
[19]G. F. Drukarev, Stolknoveniya Elektronov s Atomami i Molekulami [Electron Collisions with Atoms and Molecules], Nauka, Moscow (1978).
[20]A. Herzenberg, J. Phys. B **1**, 548 (1968).
[21]W. Domcke and L. Cedarbaum, J. Phys. B **14**, 2829 (1980).
[22]B. J. Schneider, Phys. Rev. A **14**, 1923 (1976).
[23]L. Dubé and A. Herzenberg, Phys. Rev. A **20**, 194 (1979).
[24]A. A. Radtsig and O. B. Firsov, Zh. Eksp. Teor. Fiz. **77**, 1313 (1979) [Sov. Phys. JETP **50**, 660 (1979)].
[25]A. Hazi, T. N. Rescigno, and M. Curillo, Phys. Rev. A **23**, 1089 (1981).
[26]G. V. Golubkov, F. I. Dalidchik, and G. K. Ivanov, Zh. Eksp. Teor. Fiz. **73**, 439 (1977) [Sov. Phys. JETP **46**, 230 (1977)].
[27]J. Lambe and R. C. Jaklevic, in: Tunneling Phenomena in Solids (Proc. NATO Advanced Study Institute, Risö, Denmark, 1967; ed. by E. Burstein and S. Lundqvist), Plenum Press, New York (1969), p. 233, 243 [Russian translation: Mir. Moscow (1973)].
[28]F. I. Dalidchik, Teor. Eksp. Khim. **10**, 579 (1974).
[29]F. I. Dalidchik, Yad. Fiz. **21**, 51 (1975) [Sov. J. Nucl. Phys. **21**, 26 (1975)].
[30]F. I. Dalidchik, in: Teoreticheskie Problemy Khimicheskoi Fiziki [Theoretical Problems in Chemical Physics], Nauka, Moscow (1982), p. 102.
[31]A. I. Baz', Appendix to Russian translation [IL, Moscow (1961)] of book by E. C. Titchmarsh: Eigenfunction Expansions Associated with Second-Order Differential Equations, Part 2, Oxford Univ. Press (1958).
[32]S. G. Kadmenskii and V. I. Furman, Fiz. Elem. Chastits At. Yadra **6**, 469 (1975) [Sov. J. Part. Nucl. **6**, 189 (1975)].
[33]D. F. Jackson and M. Rhoades-Brown, Ann. Phys. (N.Y.) **105**, 151 (1977).
[34]E. R. Lubenets, Teor. Mat. Fiz. **32**, 279 (1977).
[35]F. I. Dalidchik and V. Z. Slonim, Teor. Eksp. Khim. **14**, 617 (1978).
[36]F. I. Dalidchik, Teor. Eksp. Khim. **15**, 130 (1979).
[37]F. I. Dalidchik, Zh. Eksp. Teor. Fiz. **74**, 472 (1978) [Sov. Phys. JETP **47**, 247 (1978)].
[38]C. B. Duke, in: Tunneling Phenomena in Solids (Proc. NATO Advanced Study Institute, Risö, Denmark, 1967; ed. by E. Burstein and S. Lundqvist), Plenum Press, New York (1969), p. 405 [Russian translation: Mir, Moscow (1973)].
[39]D. J. Flood, J. Chem. Phys. **52**, 1355 (1970).
[40]A. A. Ovchinnikov and N. S. Erikhman, Usp. Fiz. Nauk **138**, 289 (1982) [Sov. Phys. Usp. **25**, 738 (1982)].

Translated by Steve Torstveit