EUROPHYSICS LETTERS 1 August 2001

Europhys. Lett., **55** (3), pp. 404–410 (2001)

Tunneling of Bloch electrons through vacuum barrier

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(received 4 December 2000; accepted in final form 17 May 2001)

PACS. 73.40.Gk – Tunneling.

Abstract. – Tunneling of Bloch electrons through a vacuum barrier introduces new physical effects in comparison with the textbook case of free (plane wave) electrons. For the latter, the exponential decay rate in the vacuum is minimal for electrons with the parallel component of momentum $\boldsymbol{k}_{\parallel} = 0$, and the prefactor is defined by the electron momentum component in the normal to the surface direction. However, the decay rate of Bloch electrons may be minimal at an arbitrary $\boldsymbol{k}_{\parallel}$ ("hot spots"), and the prefactor is determined by the electron's group velocity, rather than by its quasimomentum. We illustrate this by first-principles calculations for (110) Pd surface.

There is a general feeling in the applied-physics community nowadays that the next decade will bespeak an advent of magnetoelectronics, exploiting spin, rather than charge, degrees of freedom [1]. Many of such spintronic devices are based on the phenomenon of quantum tunneling, and specifically on the difference between tunneling currents in different spin channels. This opens up a possibility to control the electric properties via magnetic field. In view of all that, an explosion of publication on spin-polarized tunneling, which started around 1995, is not surprising at all.

Interestingly, despite the fact that tunnelling is one of the best studied phenomena in quantum mechanics, there is still substantial diversity in microscopic understanding of tunneling in real systems. Tunneling problems are very easily solved in one dimension and for free electrons; but it is not so obvious how this is related to real systems, and how to incorporate the effects of realistic electronic structure. This is the reason why most theoretical papers use the free-electron model, that is, the electronic wave functions that are plane waves and a spherical Fermi surface. The deviations of the wave function from the single plane-wave form, and of the Fermi surface from a sphere, are very often crucial for understanding the physics of tunneling. In particular, a totally counterintuitive result has been observed in some recent calculations [2], when the electrons with nonzero quasimomentum parallel to the interface had a larger probablility to tunnel through a vacuum barrier compared to those with zero parallel quasimomentum. It was also pointed out [3] that electrons in different Bloch states with the same energy and quasimomentum may, in principle, have different decay rates in vacuum: another counterintuitive result. In this regard, it is important to establish a formal theory for tunneling of Bloch electrons through a vacuum barrier, elucidating the qualitatively new aspects of this process as opposed to the free-electron tunneling, particularly because only the latter is discussed in the classical textbooks. This is the goal of the current paper.

The simplest case of a tunneling contact is the so-called Sharvin contact [4], which is essentially an orifice between two metals (or a metal and the vacuum), whose size is smaller than the mean free path of electrons in the bulk. All electrons with the a positive projection onto the current direction (which we will denote as x) pass through the contact. Conductance of a Sharvin contact between two identical metals is

$$G = \frac{e^2}{\hbar}\frac{1}{2}\langle N|v_x|\rangle\, A, \tag{1}$$

where A is the contact area, N is the volume density of electronic states at the Fermi level, v is the Fermi velocity, and brackets denote Fermi surface averaging:

$$\frac{1}{2}\langle N|v_x|\rangle = \frac{1}{\Omega}\sum_{\boldsymbol{k}i\sigma}\delta(\epsilon_{\boldsymbol{k}i\sigma}-E_{\rm F})v_{\boldsymbol{k}i\sigma,x} = \frac{1}{(2\pi)^3}\sum_{i\sigma}\int\frac{{\rm d}S_{\rm F}}{|v_{\boldsymbol{k}i\sigma}|}v_{\boldsymbol{k}i\sigma,x}\,. \tag{2}$$

Integration and summations are over the states with $v_{\boldsymbol{k}i\sigma,x} > 0$, and Ω is the unit cell volume [5,6]. $\boldsymbol{k}$, i, and σ denote the quasimomentum, the band index, and the spin of an electron, respectively. This formula can be derived by considering the voltage-induced shift of the Fermi surface [6], but there is a more instructive derivation starting from the Landauer-Buttiker formula for the conductance of a single ballistic electron, $G_0 = e^2/h$. In this formalism, the total conductance is equal to G_0 times the number of conductivity channels, $N_{\rm cc}$, which is defined as the number of electrons that can pass through the contact. Assuming that the translational symmetry in the interface plane is not violated, we observe that the quasimomentum in this plane, $\boldsymbol{k}_\parallel$, is conserved, and $N_{\rm cc}$ is the number of quantum-mechanically allowed $\boldsymbol{k}_\parallel$'s. Thus $N_{\rm cc}$ is given by the total area of the contact times the density of the two-dimensional quasimomenta. The latter is simply $S_x/(2\pi)^2$, where S_x is the area of the projection of the bulk Fermi surface onto the contact plane. Thus

$$G = \frac{e^2}{h}\frac{S_x A}{(2\pi)^2} \equiv \frac{e^2}{\hbar}\frac{1}{2}\langle N|v_x|\rangle\, A. \tag{3}$$

This is an important result. To the best of our knowledge, Walter Harrison was the first to spell it out in 1961 [7], and there is no lack of more recent papers manifesting proper understanding of this issue (*e.g.*, ref. [8]). However, till now many otherwise correct and useful papers erroneously identify the number of conductivity channels and the density of states at the Fermi level, that is

$$\underbrace{\boxed{N_{\rm cc} \propto N(E_{\rm F})}}_{\textit{incorrect}!} = \frac{1}{\Omega}\sum_{\boldsymbol{k}i\sigma}\delta(\epsilon_{\boldsymbol{k}i\sigma}-E_{\rm F}) = \frac{1}{(2\pi)^3}\sum_{i\sigma}\int\frac{{\rm d}S_{\rm F}}{|v_{\boldsymbol{k}i\sigma}|}\,. \tag{4}$$

Equation (3) is the basis for all more sophisticated expressions describing various aspects of quantum tunneling. None of them may explicitly depend on the bulk density of states. It may, however, be that instead of the straight $\langle N|v_x|\rangle$ averaging, one has to compute a weighted average, with the weights coming from tunneling matrix elements, or other additional physics.

Equation (3) takes care of one important difference between the free electrons and the Bloch electrons: deviation of the Fermi surface from a sphere, for $S_x \neq \pi k_{\rm F}^2$. Another important difference that is often neglected is that between the group velocity $\hbar^{-1}{\rm d}\epsilon_{\boldsymbol{k}}/{\rm d}\boldsymbol{k}$ and the phase velocity $\hbar\boldsymbol{k}/m_0$. One can get some qualitative understanding of the role that this fact plays in tunneling by considering a simplified model, where electrons in metal are approximated by free electrons with an effective mass. While this model is too crude for a quantitative

analysis of real metals, it has one great advantage: in this approximation, the phase velocity, $(\hbar \boldsymbol{k}/m_0)$, is different from the group velocity, $(\mathrm{d}\epsilon_{\boldsymbol{k}}/\hbar \mathrm{d}\boldsymbol{k})$. The standard formula (see, *e.g.*, ref. [9]) for the transparency of a symmetric rectangular barrier can be written in terms of either velocity, but only the formulation in terms of the group velocity remains correct for an arbitrary effective mass:

$$D(\boldsymbol{k}) = \frac{4m_0^2\hbar^2K^2v_{\mathrm{L}}v_{\mathrm{R}}}{\hbar^2m_0^2K^2(v_{\mathrm{L}}+v_{\mathrm{R}})^2 + (\hbar^2K^2+m_0^2v_{\mathrm{L}}^2)(\hbar^2K^2+m_0^2v_{\mathrm{R}}^2)\sinh(dK)^2}, \tag{5}$$

where $v_{\mathrm{L(R)}}$ stands for ($\boldsymbol{k}$-dependent) Fermi velocity in the left and in the right leads, and the imaginary quasimomentum $\hbar K$ is calculated from the energy conservation condition,

$$U + \hbar^2[\boldsymbol{k}_\parallel^2 - K^2]/2m_0 = E\,,$$

where m_0 is the free-electron mass, U is the barrier height, and d is its thickness.

The physical reason that one has to use group velocities, and not wave vectors, is very profound and extends well beyound the limited scope of the effective mass model: these factors appear in eq. (5) as a result of matching the gradients of the wave functions at the interface, and the gradient is, in fact, the velocity operator. Another way to express the same idea is to recall the physical meaning of the usual quantum-mechanical requirement that the wave functions be smooth: it is needed to ensure the flux continuity and, therefore, particle conservation [10]. On the other hand, the expression for K includes the *momentum*, $\boldsymbol{k}_\parallel$, and the *free* electron mass, m_0, because it comes from the solution of the Schrödinger equation inside the barrier (in vacuum) [11]. We will discuss below how the exponential part of eq. (5) should be modified when going beyond the effective mass approximation; however, the presence of the group velocities in the prefactors is universal.

The conductance of a contact described by eq. (5) is given by the appropriately modified eq. (1):

$$G = \frac{e^2}{\hbar}\frac{A}{\Omega}\sum_{\boldsymbol{k}}\delta(\epsilon_{\boldsymbol{k}} - E_{\mathrm{F}})v_{\boldsymbol{k}x}D(\boldsymbol{k})\,. \tag{6}$$

It is instructive to consider the last formula in some limiting cases. First, let us consider a *specular* barrier. It is defined by the limit $U \to \infty$, $d \to 0$, $Ud = V$. Then $K \to \sqrt{2m_0U/\hbar^2}$ and

$$D(\boldsymbol{k}) = \frac{4\hbar^2v_{\mathrm{L}}v_{\mathrm{R}}}{\hbar^2(v_{\mathrm{L}}+v_{\mathrm{R}})^2 + 4V^2}, \tag{7}$$

Note that in the literature the ratio $V/\hbar v_x = Z$ is commonly used to characterize the barrier strength. In principle, this quantity is different for different electrons, as v_x depends on $\boldsymbol{k}$**.** In the limit of low transparency, $Z \gg 1$, $D(\boldsymbol{k}) = \hbar^2v_{\mathrm{L}}v_{\mathrm{R}}/V^2$. Substituting this into eq. (6), we find that the total current is proportional to

$$\sum_{\boldsymbol{k}}\delta(\epsilon_{\boldsymbol{k}} - E_{\mathrm{F}})v_{\boldsymbol{k}x}v_{\mathrm{L}}v_{\mathrm{R}}, \tag{8}$$

where summation is, of course, over those $\boldsymbol{k}$ that are allowed in both left and right lead. Roughly speaking, the total conductance is defined by the smaller of the two $\langle Nv_x^2\rangle$'s, that is, by $\min\left(\langle Nv_x^2\rangle_{\mathrm{L}}, \langle Nv_x^2\rangle_{\mathrm{R}}\right)$. In the high-transparency limit D is still smaller than 1, $D = 4v_{\mathrm{L}}v_{\mathrm{R}}/(v_{\mathrm{L}}+v_{\mathrm{R}})^2$, (the so-called Fermi velocity mismatch), but in most cases this is not a large effect: a factor of two mismatch reduces D by only 10%.

In the case of a thick barrier, defined as $dK \gg 1$, eq. (5) can be expanded in $\hbar^2 k_\parallel^2/4m_0(U - E_\mathrm{F})$, and the transparency is

$$D(\boldsymbol{k}) = \frac{2m_0^2(U-E_\mathrm{F})v_\mathrm{L}v_\mathrm{R}}{(U-E_\mathrm{F}+m_0v_\mathrm{L}^2/2)(U-E_\mathrm{F}+m_0v_\mathrm{R}^2/2)} \exp[-2d^2W] \exp\left[-\frac{k_\parallel^2}{W}\right], \tag{9}$$

where $\sqrt{2m_0(U-E_0)}/\hbar d = W \ll k^2$ (thick barrier limit). W does not depend on $\boldsymbol{k}$**.** The tunneling current is proportional to

$$J \propto \sum_{\boldsymbol{k}_\parallel} \frac{2m_0^2(U-E_\mathrm{F})v_\mathrm{L}v_\mathrm{R}}{(U-E_\mathrm{F}+m_0v_\mathrm{L}^2/2)(U-E_\mathrm{F}+m_0v_\mathrm{R}^2/2)} \exp\left[-\frac{k^2}{W}\right]. \tag{10}$$

Let $\boldsymbol{k}_n$ be the set of points on the Fermi surface where $\boldsymbol{k}_\parallel = 0$ (note that for Bloch electrons beyond the effective mass approximation tunneling from some of these points may be suppressed by symmetry, as discussed later in the paper). Except in the exponent, we can put $\boldsymbol{k}_\parallel$ to zero,

$$\begin{aligned} J &\propto \frac{1}{(2\pi)^3} \sum_n \left\{ \int \mathrm{d}^2k \exp\left[-\frac{k^2}{W}\right] \right\} \frac{2m_0^2(U-E_\mathrm{F})v_\mathrm{L}v_\mathrm{R}}{(U-E_\mathrm{F}+m_0v_\mathrm{L}^2/2)(U-E_\mathrm{F}+m_0v_\mathrm{R}^2/2)} \qquad (11) \\ &\propto \sum_n \frac{v_\mathrm{L}}{m_0\hbar^2v_\mathrm{L}^2/2+U-E_\mathrm{F}} \frac{v_\mathrm{R}}{m_0\hbar^2v_\mathrm{R}^2/2+U-E_\mathrm{F}}. \end{aligned}$$

All factors omitted in this expression are $\boldsymbol{k}_\parallel$-independent. One should not be confused by the fact that, unlike eq. (8), the numerator here does not have the third velocity. We have reduced our problem to an effective 1D problem, in which case the role of the density of states is played by the inverse velocity. Correspondingly, the product Nv cancels out.

Equations (8), (9) emphasize the role of kinematics in tunneling. For instance, the long-standing problem of the reversed (compared to the density of states) spin polarization of the $3d$ ferromagnets is entirely explained in terms of kinematics. Direct calculations show that s-like electrons in Fe, Co and Ni have much larger Fermi velocity than d-like electrons. Taking this fact into account brings the calculated spin polarization to a very good agreement with experiment, without making any additional assumptions about the character of the surface states [6, 12]. This is by no means surprising: the bulk transport is controlled by the same factor $\langle Nv_x^2 \rangle$, and the Ohmic current in these metals is carried predominantly by s-like electrons. It is only natural that in another transport phenomenon, tunneling, these electrons also play the leading role. We would like to emphasize that the effect considered above (as opposed to another effect discussed later in the paper) is not related to the s or d symmetry of the wave functions, but to the group velocities in the respective bands. In other cases the "light" and the "heavy" bands may not be directly related to the angular symmetry of the wave functions. For example, in $SrRuO_3$ both spin-up and spin-down Fermi surfaces are made up by Ru t_{2g} d-electrons, but the average group velocity in the spin-majority channel is twice smaller than that in the spin-minority one [13]. As a result, although the spin polarization of the density of states is positive, $N_\uparrow > N_\downarrow$, while the transport spin polarization is negative, $\langle Nv \rangle_\uparrow < \langle Nv \rangle_\downarrow$ [14].

Now we have some understanding of the two remarkable differences between the free electrons and the Bloch electrons: the effect of the Fermi surface geometry and the difference between the group and the phase velocities. There is, however, yet another, extremely important, dissimilarity between the two systems, recently pointed out by Butler [3]: the difference

between the momentum and the quasimomentum. In order to discuss this difference, and its physical consequences, let us consider reflection of an individual Bloch wave from a metal surface. Let x be the direction normal to the surface, and $\boldsymbol{r}$ the coordinate in the surface plane. At $x < 0$ we have a metal, and vacuum at $x > 0$. The vacuum potential is again U, and the Fermi energy is E. Since we have perfect in-plane periodicity, the wave function at any x can be classified by $\boldsymbol{k}_\parallel$, and is given by

$$\psi(\boldsymbol{k}_\parallel, x, \boldsymbol{r}_\parallel) = \sum_{\boldsymbol{G}} \exp[i(\boldsymbol{k}_\parallel + \boldsymbol{G})\boldsymbol{r}_\parallel] F_{\boldsymbol{G}}(\boldsymbol{k}_\parallel, x). \tag{12}$$

The quasimomentum in the surface plane, $\hbar\boldsymbol{k}_\parallel$, is conserved, as well as the energy. In vacuum, the solution of the Schrödinger equation is

$$\psi^T(\boldsymbol{k}_\parallel, x, \boldsymbol{r}_\parallel) = \sum_{\boldsymbol{G}} \alpha_{\boldsymbol{G}} \exp[i(\boldsymbol{k}_\parallel + \boldsymbol{G})\boldsymbol{r}_\parallel] \exp[-K_{\boldsymbol{G}} x]\,, \tag{13}$$

where $\boldsymbol{G}$ is the 2D reciprocal lattice vector, and K_G is now defined by taking into account the kinetic energy associated with the given reciprocal lattice vector, $U + \hbar^2[\boldsymbol{k}_\parallel^2 - K_{\boldsymbol{G}}^2]/2m_0 = E$. An incoming Bloch wave with a given $\boldsymbol{k}$ penetrates into the barrier as a linear combination (13) with the coefficients $\alpha_{\boldsymbol{G}}$ defined by matching conditions, set by the requirement of continuity of the wave function and its derivative:

$$\begin{aligned}
\sum_{\boldsymbol{G}} F_{\boldsymbol{G}}(0) \exp[i(\boldsymbol{k}_\parallel + \boldsymbol{G})\boldsymbol{r}_\parallel] &= \sum_{\boldsymbol{G}} \alpha_{\boldsymbol{G}} \exp[i(\boldsymbol{k}_\parallel + \boldsymbol{G})\boldsymbol{r}_\parallel]\,, \\
\sum_{\boldsymbol{G}} F'_{\boldsymbol{G}}(0) \exp[i(\boldsymbol{k}_\parallel + \boldsymbol{G})\boldsymbol{r}_\parallel] &= -\sum_{\boldsymbol{G}} \alpha_{\boldsymbol{G}} K_{\boldsymbol{G}} \exp[i(\boldsymbol{k}_\parallel + \boldsymbol{G})\boldsymbol{r}_\parallel]\,,
\end{aligned}$$

since this has to hold for any $\boldsymbol{r}_\parallel$, $\alpha_{\boldsymbol{G}} = F_{\boldsymbol{G}}(0)$, and $F'_{\boldsymbol{G}}(0) = -\alpha_{\boldsymbol{G}} K_{\boldsymbol{G}}$ for each $\boldsymbol{G}$**.** Thus

$$F_{\boldsymbol{G}}(0) K_{\boldsymbol{G}} + F'_{\boldsymbol{G}}(0) = 0. \tag{14}$$

A *bulk* electronic Bloch wave, progagating in the x-direction, is given by eq. (12) again, where now $F_{\boldsymbol{G}}^{\mathrm{bulk}}(\boldsymbol{k}_\parallel, x) = u_{\boldsymbol{G},k_x}(x) \exp[ik_x x]$, and $u_{\boldsymbol{G},k_x}(x)$ is periodic in x. If the wave functions still had the same form at $x = 0$, *i.e.*, at the interface, one would write for the incident and the reflected wave together a linear combination of the bulk states with the energy E and the quasimomentum in the plane $\hbar\boldsymbol{k}_\parallel$,

$$F_{\boldsymbol{G}}(x) = u_{\boldsymbol{G},k_x}(x) \exp[ik_x x] + a u_{\boldsymbol{G},-k_x}(x) \exp[-ik_x x]\,. \tag{15}$$

But then we would have only one free parameter, a, to satisfy eq. (14) for all $\boldsymbol{G}$'s, which is obviously impossible. The answer is that $F_{\boldsymbol{G}}(x)$ has the form (15) only far away from the surface, while near the surface it is distorted as required by eq. (14). This emphasizes once again the role of surface states in tunneling. In fact, one of the ways to realize the necessity of forming the surface states is that the bulk Bloch functions, in general, cannot be augmented continuously and smoothly into vacuum.

In the case of a thick barrier, the actual tunneling current will be defined by that component of the wave function (13) which has the smallest K, that is, by the one with $\boldsymbol{G} = \boldsymbol{0}$**.** The amplitude of this evanescent wave is set by $\alpha_{\boldsymbol{0}}$. As pointed out by Butler [3], $\boldsymbol{k}_\parallel = \boldsymbol{0}$ is a high-symmetry direction (ΓX), and the electronic states possess certain symmetry in the yz-plane. In particular, $\alpha_{\boldsymbol{0}}$ for some states may vanish by symmetry, in which case the decay rate K will be defined by the smallest G allowed by symmetry. Since we consider now a

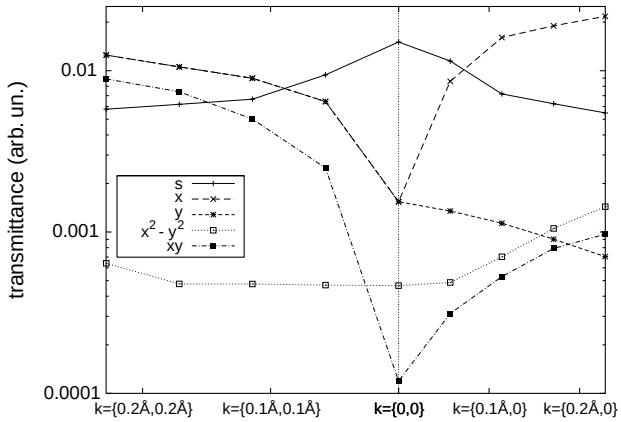

Fig. 1 – Average decay rate of the occupied bulk states of Pd metal into a vacuum barrier, for different $\boldsymbol{k}_\parallel$ and the (110) surface.

thick barrier, this essentially means that tunnelling from such a band will be defined not by the $\boldsymbol{k}_\parallel = \mathbf{0}$ state, but, rather counterintuitively, by general (not high-symmetry) points in the 2D Brillouin zone (as confirmed by actual calculations [2]). Indeed, consider a band where by symmetry $F_0(0,x) = 0$ at $\boldsymbol{k}_\parallel = \mathbf{0}$. At $\boldsymbol{k}_\parallel \neq \mathbf{0}$ thus $F_0(\boldsymbol{k}_\parallel, x) = F_0''(\mathbf{0},x)k_\parallel^2$, while $K = \sqrt{2m_0(U-E)/\hbar^2 + k^2} \approx \sqrt{2m_0(U-E)}/\hbar + \hbar k_\parallel^2/2\sqrt{2m_0(U-E)} = K_0 + k_\parallel^2/2K_0$. The optimal distance from the zone center that gives maximal contribution to the tunneling current can be estimated by maximizing with respect to $k_\parallel$ of

$$F_0''(\mathbf{0},x)k_\parallel^2 \exp[-K_0 d - k_\parallel^2 d/2K_0]\,, \tag{16}$$

where d is the barrier thickness, which gives $k_\parallel \sim \sqrt{2K_0/d}$. For Fe, for instance, $K_0 \approx 0.6$ a.u., about the same as the ΓX distance. Thus for a barrier, say, of 5 lattice parameters, $k_\parallel \sim 0.2$ a.u., a sizeable distance from the center of the Brillouin zone. Yet another counterintuitive result is that one can define to physically different the low transparency limits: a thick, but low-height barrier, or a high, but thin barrier. In the former case tunneling is predominantly from the states infinitely close to the zone center. In the latter it occurs far away from the zone center, possibly at the zone boundary. This is the effect observed in refs. [2], and in our calculations below.

The described situation is fairly universal. Most transition metals interfaces have bands of different symmetry near the Fermi level. Two remarks are important when speaking about real systems, though. First, it is not only the difference between s states and higher moments that is important, but also between different higher-moment states, as illustrated below. Second, one should not confuse the bulk symmetry and the surface symmetry. For instance, electronic states that are s or $d_{3z^2-r^2}$ in the bulk have the same (s) surface symmetry. To illustrate this on a realistic example, we performed linear muffin tin orbital calculations for Pd metal (110) surface, using a supercell of 5 Pd layers, and 7 empty sphere layers, and monitoring the intensity of the occupied bulk states in the middle empty sphere layer. The results are shown in fig. 1, where the intensity is averaged over all occupied states of a given 2D symmetry. First of all, we observe that at the zone center the s states, which have a $\boldsymbol{G} = 0$ component, decay much slower than all others states. The next highest transparency corresponds to the p_x and p_y states, where the lowest allowed reciprocal lattice vector is $G_1 = 2\pi/a$ (a being the

surface lattice vector). The Bloch waves with $d_{x^2-y^2}$ symmetry include combinations of two reciprocal lattice vectors, G_x and G_y, and thus decay faster than $p_{x,y}$ states. The states with the d_{xy} symmetry have an even faster decay rate, because they lack both $G = 0$ and $G = G_1$ component. However, when we move away from the zone center, selection rules are lifted and the other states start to pick up, and in fact for the wave vectors shown in fig. 1 the slowest decay rate appears for the states with the p_x symmetry, at $\boldsymbol{k}_\parallel = \{0.1, 0\}2\pi/a$.

To conclude, we discussed here three new effects which appear in tunneling of the Bloch electrons through a vacuum barrier, as compared with the textbook case of free-electron (plane wave) tunneling. These effects are due to i) complexity of the Fermi surface geometry ("fermiology"), ii) difference between the group and the phase velocities of a Bloch electron, and iii) nonconservation of the parallel component of electron momentum (and conservation of its quasimomentum). Each effect influences the tunneling current in its own way, and, as a result, even for the most simple case of a vacuum barrier, the tunneling of the Bloch electrons appears to be qualitatively different from the free-electron tunneling.

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Discussions with J. KUDRNOVSKY and I. MERTIG in Schwäbisch Gmünd in August 2000 stimulated this work. Many helpful discussions with B. NADGORNY and W. BUTLER are also gratefully acknowledged.

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