TUNNELING PHENOMENA IN SOLIDS

Edited by **Elias Burstein**
Department of Physics, University of Pennsylvania
and S. Lundqvist

Tunneling Phenomena in Solids

Lectures presented at the
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Edited by
ELIAS BURSTEIN
Department of Physics
University of Pennsylvania
Philadelphia, Pennsylvania

and

STIG LUNDQVIST
Institute of Theoretical Physics
Chalmers Tekniska Högskola
Göteborg, Sweden

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Foreword

The aim of this volume is to provide advanced predoctoral students and young postdoctoral physicists with an opportunity to study the concepts of tunneling phenomena in solids and the theoretical and experimental techniques for their investigation. The contributions are primarily tutorial in nature, covering theoretical and experimental aspects of electron tunneling in semiconductors, metals, and superconductors, and atomic tunneling in solids.

The work is based upon the lectures delivered at the Advanced Study Institute on "Tunneling Phenomena in Solids," held at the Danish A.E.C. Research Establishment, Risö, Denmark, June 19–30, 1967. Sponsored by the Danish Atomic Energy Commission, the Nordic Institute for Theoretical Physics (NORDITA), and the Science Affairs Division of NATO, with the cooperation of the University of Copenhagen, the Technical University of Denmark, Chalmers Institute of Technology, and the University of Pennsylvania, the lectures were presented by a distinguished panel of scientists who have made major contributions in the field. The relatively large number of lecturers was, in part, made possible by the close coordination of the Advanced Study Institute with the Second International Conference on Electron Tunneling in Solids, which was held at Risö on June 29, 30 and July 1, 1967, under the sponsorship of the U.S. Army Research Office–Durham. We are indebted to I. Giaever, E. O. Kane, J. Rowell, and J. R. Schrieffer for advice and assistance in planning the lecture program of the Institute.

The Institute was made possible through the active interest of an organizing group consisting of H. Højgard Jensen, A. Mackintosh, N. I. Meyer, M. Nielsen, and K. Saermark. The Danish Atomic Energy Commission supported the Institute financially and made available its facilities at the Risö Research Establishment. We take this opportunity to thank the Danish AEC officials for their gracious cooperation. In particular, we would like to express our gratitude to the Director of the Research Establishment, Professor T. Bjerge, for his kind interest and for being a generous and excellent host.

The heavy burden of making all the arrangements for the Institute was very ably undertaken by M. Nielsen and by the Information Officer of the Research Establishment, Mrs. J. Starcke. Dr. Nielsen and Mrs. Starcke kept the secretariat running smoothly at all times and helped the Directors of the Institute, as well as the participants, in solving the many problems that arose. We would like to express our warmest thanks to them for their patient and efficient work in following as closely as possible our intentions along a rather winding course toward a successful end.

E. BURSTEIN, Director of the Institute
S. LUNDQVIST, Associate Director of the Institute

October 20, 1968

Contents

Chapter 1

Basic Concepts of Tunneling

E. O. Kane
Bell Telephone Laboratories
Murray Hill, New Jersey

A great many of the features of tunneling phenomena in solids are essentially of a one-dimensional nature. If the tunneling barrier extends in the x direction, the momentum in the y and z directions can usually be taken to be constants of the motion, and hence are merely fixed parameters.

In this introductory chapter we will describe some of the basic concepts of tunneling by studying purely one-dimensional problems, and we may anticipate that most of our results will have a wider range of applicability to real situations than one-dimensional problems usually have.

We will, in fact, study the simplest of all one-dimensional problems, namely, square barriers and square wells in one dimension. The Schrödinger equation will have the simple form

$$\left(\frac{p^2}{2m} + V\right)\psi = E\psi, \tag{1}$$

where V is a constant in a given region. The general solution of Eq. (1) has the well-known form

$$\psi(x) = ae^{ikx} + be^{-ikx}, \tag{2}$$

$$\hbar^2 k^2/2m = E - V. \tag{3}$$

When $E - V > 0$ the wave functions are plane waves. When $E - V < 0$ we will write $k = i\varkappa$ and

$$\psi(x) = ae^{-\varkappa x} + be^{\varkappa x}. \tag{4}$$

The wave functions are now exponentially growing and decaying waves characteristic of barrier penetration problems. In the "square barrier" and

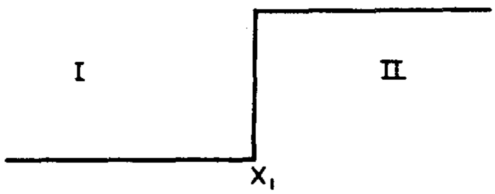

Fig. 1.

"square well" problem which we will discuss V changes abruptly from one constant value to another. The overall wave function is then constructed out of pieces having the form of Eq. (2) by matching ψ and $d\psi/dx$ at the discontinuities of V.

The basic matching problem can be done at a potential step as shown in Fig. 1. The matching conditions are then conveniently described as a 2×2 matrix R operating on the two-dimensional vectors

$$\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} a_2 \\ b_2 \end{pmatrix}$$

which describe the wave function in regions I and II, respectively. We may write

$$\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = R_1 \begin{pmatrix} a_2 \\ b_2 \end{pmatrix}, \tag{5}$$

$$R_1 = \frac{1}{2k_1}\begin{pmatrix} (k_1 + k_2)\exp[i(-k_1+k_2)x_1] & (k_1 - k_2)\exp[i(-k_1 - k_2)x_1] \\ (k_1 - k_2)\exp[i(k_1 + k_2)x_1] & (k_1 + k_2)\exp[i(k_1 - k_2)x_1] \end{pmatrix}. \tag{6}$$

Of course, Eqs. (5) and (6) are valid for either real or imaginary values of k. The general problem of any number of square barriers or wells may then be succinctly described in terms of a chain of operators of the form R_j.

We turn first to the square barrier problem of Fig. 2. We may write the solution

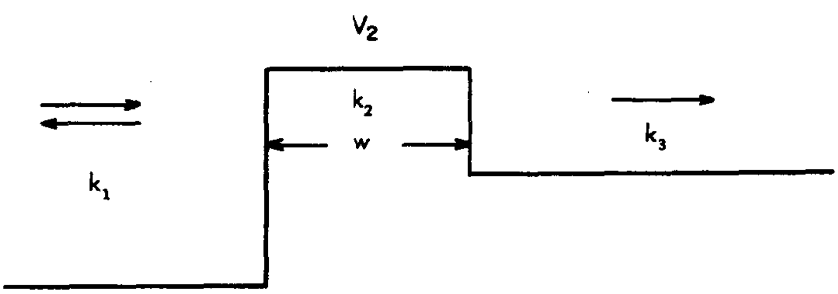

Fig. 2.

$$\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = R_1 R_2 \begin{pmatrix} a_3 \\ b_3 \end{pmatrix}. \tag{7}$$

Let us study the boundary condition of an electron incident from the left. There will be a reflected wave in region 1 but only a transmitted wave in region 3; hence $b_3 = 0$. We want a_3 in terms of a_1. Equation (7) then gives

$$a_1 = (R_1 R_2)_{11} a_3. \tag{8}$$

Explicit evaluation of (8) with the use of (6) results in

$$(R_1 R_2)_{11} = [\exp(ik_3 x_2 - ik_1 x_1)](k_1^2 + \varkappa_2^2)^{1/2}(k_3^2 + \varkappa_2^2)^{1/2} \times (e^{i\alpha} e^{\varkappa_2 w} - e^{-i\alpha} e^{-\varkappa_2 w})/(4ik_1 \varkappa_2) \tag{9}$$

$$\alpha = \tan^{-1}(\varkappa_2/k_1) + \tan^{-1}(\varkappa_2/k_3) \qquad \varkappa_2 = ik_2 \qquad w = x_2 - x_1 \tag{10}$$

We are assuming real plane waves in regions 1 and 3 and tunneling in region 2. To simplify the formula, we will neglect $e^{-\varkappa_2 w}$ in comparison to $e^{\varkappa_2 w}$; in other words, we consider only a strongly attenuating barrier. Then we have

$$a_3 = \frac{4k_1 \varkappa_2 \varphi e^{-\varkappa_2 w}}{(k_1^2 + \varkappa_2^2)^{1/2}(k_3^2 + \varkappa_2^2)^{1/2}} a_1, \tag{11}$$

$$\varphi = ie^{-i\alpha} \exp(ik_1 x_1 - ik_3 x_2); \tag{12}$$

φ is a phase factor of absolute value 1, which we ignore for the moment.

The quantity of physical interest that we wish to compute is the ratio of the transmitted current j_3 to the incident current j_1,

$$j_1 = (\hbar k_1/m) \mid a_1 \mid^2; \qquad j_3 = \hbar k_3/m \mid a_3 \mid^2. \tag{13}$$

We find

$$\frac{j_3}{j_1} = \frac{16 k_1 k_3 \varkappa_2^2}{(k_1^2 + \varkappa_2^2)(k_3^2 + \varkappa_2^2)} e^{-2\varkappa_2 w}, \tag{14}$$

$$\hbar^2 \varkappa_2^2/2m = V_2 - E. \tag{15}$$

The dominant feature of Eq. (14) is, of course, the barrier penetration factor $e^{-2\varkappa_2 w}$. In typical problems of interest this factor may be 10^{-5}–10^{-10}, so that it tends to dominate the prefactor. In more realistic problems this factor can seldom be calculated accurately, so that usually any experimental determination of the prefactor is doubtful or impossible.

Tunneling is one of the simplest examples of a truly quantum mechanical phenomenon. In classical physics a particle whose energy is less than the height of a potential barrier can never pass through it.

We note that Eq. (14) shows that the barrier transmission is symmetric in the indices 1 and 3. This means that the barrier transmission is the same for currents incident from the right or left, as we would expect. We may also compute the incident current per unit energy if we assume that the states on the left and right are quantized in a box and occupied with an occupancy factor $f(E)$. The incident current is given by

$$\Delta j_1(E) = |a|^2 \frac{\hbar k_1}{m} \frac{dn}{dE} \Delta E f_1(E). \tag{16}$$

Box normalization gives $|a|^2 = 1/L_1$, where L_1 is the length of the box. The density of states in one dimension without spin is

$$dn/dE = mL_1/2\pi\hbar^2 k_1; \tag{17}$$

hence (16) becomes

$$\Delta j_1(E) = [f_1(E)/2\pi\hbar]\, \Delta E. \tag{18}$$

In equilibrium $f_1(E) = f_3(E)$; hence the current per unit energy incident on the barrier from either side of the barrier is the same. By the symmetry of Eq. (14), the transmitted currents per unit energy are also the same, and equilibrium is maintained, as we should expect.

We may also note that Eq. (14) shows that the transmitted current goes continuously to zero as either k_1 or k_3 approaches zero. This is in contrast to simple calculations of tunneling in p–n junctions, which showed a discontinuous change in the transmitted current at the band edge ([1]). A more careful treatment by Shuey ([2]) showed that in the junction problem also the current goes continuously to zero at the band edge.

We now investigate a little more closely the character of the attenuating states $ae^{-\varkappa x}$ and $be^{+\varkappa x}$ in the barrier. We use the expression for the particle current operator

$$j(x) = \frac{-i\hbar}{2m} \left(\psi^*(x) \frac{d\psi}{dx} - \psi(x) \frac{d\psi^*}{dx} \right). \tag{19}$$

We see immediately that $ae^{-\varkappa x}$ or $be^{\varkappa x}$ by themselves carry zero current. In combination

$$j(x) = (i\hbar\varkappa/m)(ab^* - ba^*). \tag{20}$$

We can use this property to develop an effective Hamiltonian theory of tunneling in a manner first described by Bardeen ([3]).

The smallness of the right-hand sides of Eqs. (11) or (14) suggests that a perturbation treatment of tunneling would be very appropriate. However, there is no obvious way of introducing a term in the Hamiltonian which can be treated as small. Bardeen took a different approach. Instead of introducing states which are the exact solutions of an approximate Hamiltonian, he introduced approximate solutions of the exact Hamiltonian. Following Bardeen, we choose the states

$$\psi_r(x) = b_{2r} e^{\varkappa_2 x}; \qquad x \leq x_2, \tag{21}$$

$$\psi_2(x) = a_{2l} e^{-\varkappa_2 x}; \qquad x \geq x_1; \tag{22}$$

ψ_r is to be matched to the correct solution for $x \geq x_2$ but is to decay in the region $x \leq x_1$ instead of satisfying the Schrödinger equation. Similarly, ψ_l continues to decay for $x \geq x_2$. Then ψ_r is a correct solution of H for $x \geq x_1$ and ψ_l is correct for $x \leq x_2$. We assume an electron is initially in ψ_l and compute its transition rate into state ψ_r. We write

$$\psi = c(t)\psi_l e^{-iE_l t} + d(t)\psi_r e^{-iE_r t} \tag{23}$$

and substitute in the Schrödinger equation

$$\begin{aligned} i\dot{c}\psi_l e^{-iE_l t} + c\psi_l E_l e^{-iE_l t} + i\dot{d}\psi_r e^{-iE_r t} + d\psi_r E_r e^{-iE_r t} \\ = ce^{-iE_l t} H\psi_l + de^{-iE_r t} H\psi_r. \end{aligned} \tag{24}$$

Since $c \approx 1$, $d \approx 0$, we will set $d = 0$, $\dot{c} = 0$, $c = 1$ in Eq. (24) [$\dot{c} \approx 0$ follows from normalization, $(d/dt)(cc^* + dd^*) = 0$]. Equation (24) then becomes

$$i\dot{d}\psi_r e^{-iE_r t} = (H - E_l)\psi_l e^{-iE_l t}, \tag{25}$$

or

$$i\dot{d} = \int \psi_r^*(H - E_l)\psi_l \, dx \exp[i(E_r - E_l)t]. \tag{26}$$

We assume ψ_l and ψ_r are normalized.

If $H = H_0 + H_1$, as in ordinary perturbation theory, and $H_0\psi_l = E_l\psi_l$, we have

$$\int \psi_r^*(H - E_l)\psi_l \, dx = \int \psi_r^* H_1 \psi_l \, dx. \tag{27}$$

Accordingly, we identify

$$T_{rl} = \int \psi_r^*(H - E_l)\psi_l \, dx \tag{28}$$

as the effective matrix element for tunneling.

The integral in Eq. (28) gives a nonzero contribution only for $x > x_2$. We can symmetrize Eq. (28) by writing

$$T_{rl} = \int_{x_B}^{\infty} \psi_r^*(H - E_l)\psi_l - \psi_l(H - E_r)\psi_r^* \, dx, \qquad x_1 \leq x_B \leq x_2, \tag{29}$$

since the added term is zero for the range of integration $x \geq x_1$. The lower limit of the integral can take any value in the barrier since the integrand is zero there. Integrating Eq. (29) by parts gives

$$T_{rl} = -\frac{\hbar^2}{2m}\left(\psi_r^* \frac{d\psi_l}{dx} - \psi_l \frac{d\psi_r^*}{dx}\right)_{x_B}, \tag{30}$$

or

$$T_{rl} = -i\hbar j_{rl}, \tag{31}$$

where j_{rl} is the current operator as given in Eq. (19) evaluated at any point in the barrier. Using Eqs. (21) and (22), we have

$$T_{rl} = (\hbar^2 \varkappa_2 / m) b_{2r}^* a_{2l}. \tag{32}$$

We will now use this tunneling matrix element to calculate the tunnel current from the effective Hamiltonian viewpoint. Noting that $a_{2r} = b_{2l} = 0$, we use Eq. (5) to relate a_{1l} to a_{2l} and b_{2r} to a_{3r}. This gives

$$|T_{rl}|^2 = \frac{\hbar^4 \varkappa_2^2}{m^2} \frac{16 k_1^2 k_3^2 |a_{1l}|^2 |a_{3r}|^2 e^{-2\varkappa_2 w}}{(k_1^2 + \varkappa_2^2)(k_3^2 + \varkappa_2^2)}. \tag{33}$$

The current incident on the barrier, j_l, is

$$j_l = (\hbar k_1 / m) |a_{1l}|^2. \tag{34}$$

The transmitted current, j_t, is given by

$$j_t = w = \frac{2\pi}{\hbar} |T_{rl}|^2 \frac{dn}{dE_r}, \tag{35}$$

using the "golden rule" of first-order time-dependent perturbation theory. Using Eq. (17) we have

$$|a_{3r}|^2 \frac{dn}{dE_r} = \frac{m}{2\pi\hbar^2 k_3}. \tag{36}$$

Substituting (33), (34), and (36) in (35), we verify that we obtain Eq. (14). Hence the effective Hamiltonian approach gives the same result for the tunnel current as the simple matching procedure.

The "effective tunneling Hamiltonian" provides a justification for the often-quoted assumption that the tunnel current is proportional to the density of states. However, we see from the matrix element of Eq. (33) that other terms in the exponential prefactor are equally important, so that the final result in Eq. (14) does not bear any simple relation to the density of states in Eq. (36). Hence the use of tunneling measurements as a quantitative probe of the density of states must be regarded with caution. However, it is a well-known fact that superconducting tunneling does quite accurately reflect the density of states. This has been justified theoretically, using the effective tunneling Hamiltonian, by Bardeen and others. This is discussed a great deal more elsewhere in this book.

We turn now to the much discussed question of how long it takes an electron to tunnel through a barrier. We refer to Fig. 2 and represent the electron in region 1 by a wave packet with average momentum k_1 and energy $E_1 = E(k_1)$:

$$\psi_i(x, t) = \exp[i(k_1 x - E_1 t)/\hbar] \times \int_{-\infty}^{\infty} \exp i(k - k_1)(x - v_1 t)] \exp -(k - k_1)^2] \, dk, \quad (37)$$

where we have used

$$E(k) \approx E(k_1) + (k - k_1)(dE/dk)_{k_1}, \quad (38)$$

$$v \equiv \frac{1}{\hbar} \frac{dE}{dk} = \frac{\hbar k}{m}. \quad (39)$$

Equation (39) is the usual definition of the group velocity. Carrying out the integration in Eq. (37) gives

$$\psi_i(x, t) = \exp[i(k_1 x - E_1 t)/\hbar] \exp[- \tfrac{1}{4}(x - vt)^2]. \quad (40)$$

Equation (40) shows that the packet moves with group velocity v, in agreement with what we expect from the classical limit. Since the kinetic energy of the wave packet is clearly positive, we cannot use it to localize the electron in the barrier region because the electron would then automatically have an energy greater than the barrier height. What we can do is look at the packet in region 3 beyond the barrier and compute its time dependence there. We use Eq. (11) to get the transmitted packet in terms of the incident packet. To simplify matters, we set $k_3 = k_1$. Then Eq. (12) shows that the plane wave $\exp\{i[kx - E(k)t/\hbar]\}$ on the left of the junction has the form $Aie^{-i\alpha}\exp\{i[k(x - w) - E(k)t/\hbar]\}$ on the right. Ignoring the phase term $ie^{-i\alpha}$, which does not depend on the junction thickness, we see that the electron has "lost," or rather failed to accumulate, the phase ikw in passing through the barrier. This is, of course, due to the real character of the x dependence in the barrier region as given in Eq. (4). If we ignore the k dependence of $Ae^{-i\alpha}$, the transmitted wave packet ψ_t can be written

$$\psi_t(x_1t) = A\exp\{i[k_1(x - w) - Et/\hbar]\}\exp[-\tfrac{1}{2}(x - w - vt)^2]. \quad (41)$$

The lack of phase change in traversing the barrier has advanced the transmitted packet by the junction width w relative to the incident packet. In other words, it appears that the packet has traversed the barrier in zero time or with infinite velocity.

There is no contradiction between this relation and relativistic limitations, because it was derived from the Schrödinger equation, which is only exact if the speed of light is made to approach infinity. This curious result is another way in which tunneling defies classical analogy.

It should not be concluded from this result that tunneling is a very rapid process. It is, in fact, very slow, as indicated by the very weak tunneling matrix element in Eq. (33). We can indicate the slowness of the tunneling process by solving the two-well problem shown in Fig. 3.

We use Eqs. (5) and (6) to write

$$\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = R_1R_2R_3R_4\begin{pmatrix} a_5 \\ b_5 \end{pmatrix}. \quad (42)$$

The eigenvalue condition results from the requirement that only attenuating states exist in regions 1 and 5. That is, $a_1 = b_5 = 0$. This gives the eigenvalue equation

$$(R_1R_2R_3R_4)_{11} = 0. \quad (43)$$

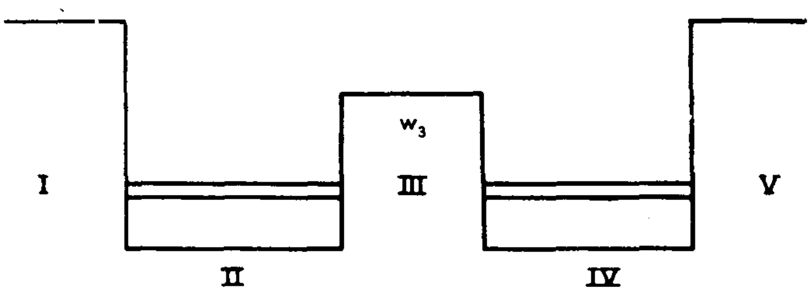

Fig. 3.