Tunnel Effect in Quantum Science

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Lecture 1

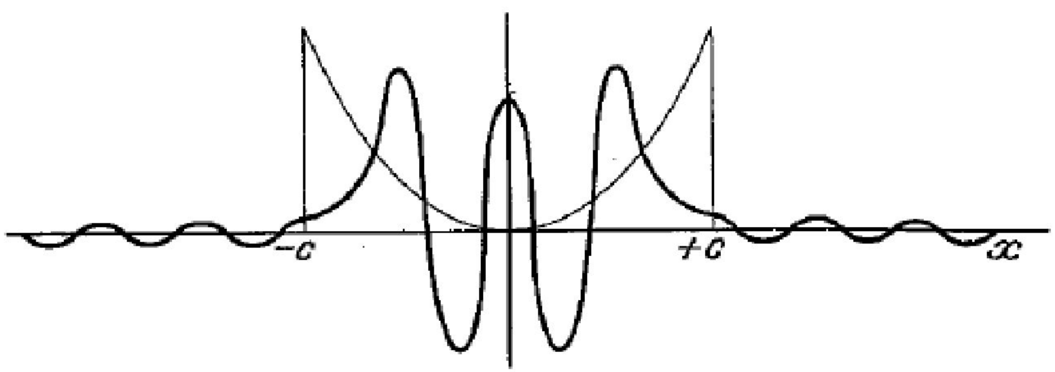
Tunnel effect is one of the most important manifestations of quantum mechanics

Zur Theorie der Schrödingerschen Gleichung.

Von **L. Mandelstam** und **M. Leontowitsch** in Moskau.

$$\psi'' + \frac{8\pi^2 m}{h^2}[E - V(x)]\,\psi = 0 \qquad (1)$$

Mit 2 Abbil

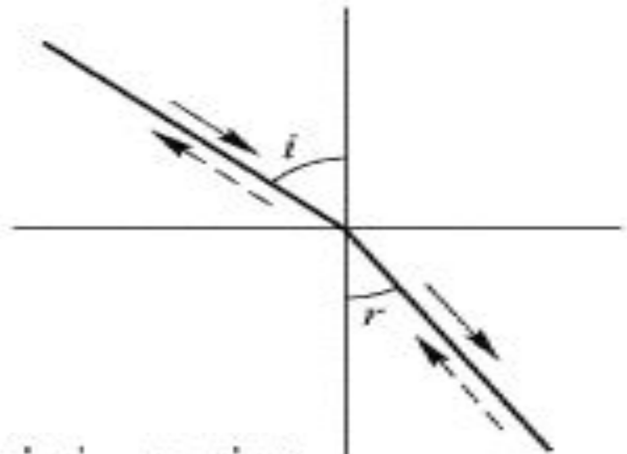


c| < c,

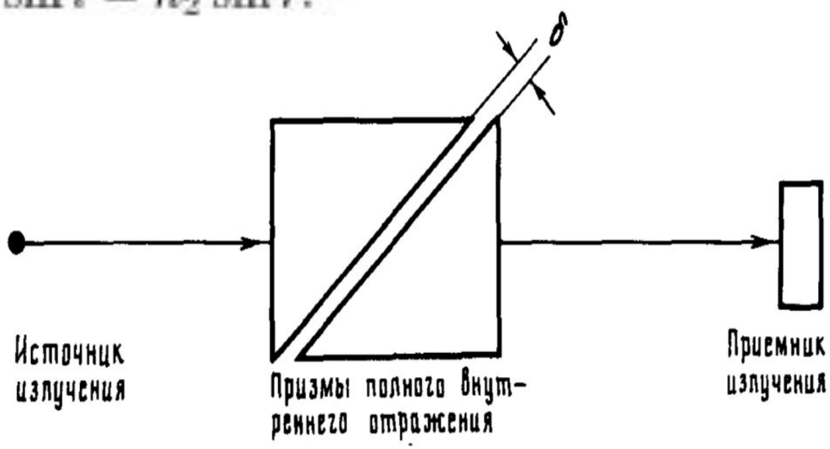
c| > c.

Fig. 2. Die stark ausgezogene Kurve stellt den Verlauf einer der Eigenfunktionen für $\lambda = 4{,}5$ dar.

Classic analogy: full internal reflection



$n_1 \sin i = n_2 \sin r.$



In the geometric optics sin(r) starts to exceed 1 when n2 is low enough. Thus, refraction becomes impossible.

Actually, electromagnetic wave penetrates into the optically more dense medium at a distance of the wave length λ. It can be found by the indicated set-up when $\delta \leq \lambda$.

Hence, a massive particle (electron, proton, etc.) directly reveals its wave properties!

Classic analogy: full internal reflection

A particularly simple qualitative demonstration of frustrated internal reflection, resembling Newton's original observation, has been described by Pohl [9] and is shown in Fig. 1.3.

If a knife blade is pressed against the outside of a glass of water and viewed through the water from above, much more of it is visible than is in actual contact with the glass. We can assume as a rough approximation that transmission is possible through a gap z one wavelength thick (cf. Equation 1.7), say 0.6 μm. If the radius of the glass is $R = 35$ mm, simple geometry shows that the radius of the visible spot x is given by

$$x \approx (2Rz)^{1/2} \approx 0.2 \text{ mm} \tag{1.8}$$

which can easily be seen.

The appearance of a transmitted beam of finite intensity is not the only phenomenon associated with frustrated internal reflection. A detailed treatment shows that both the

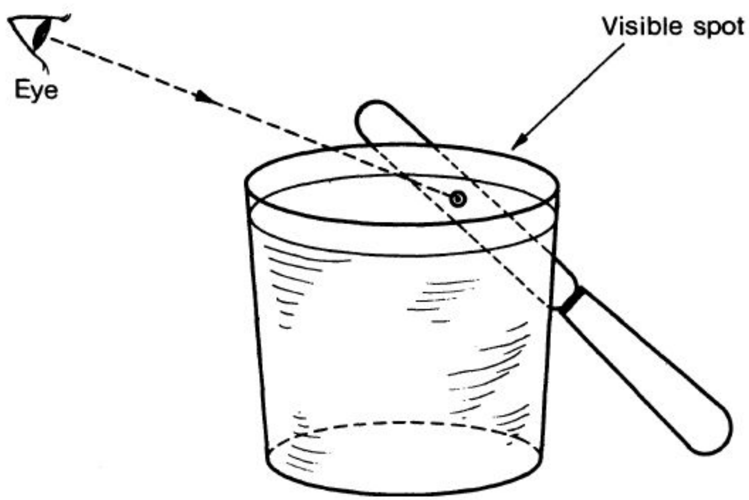
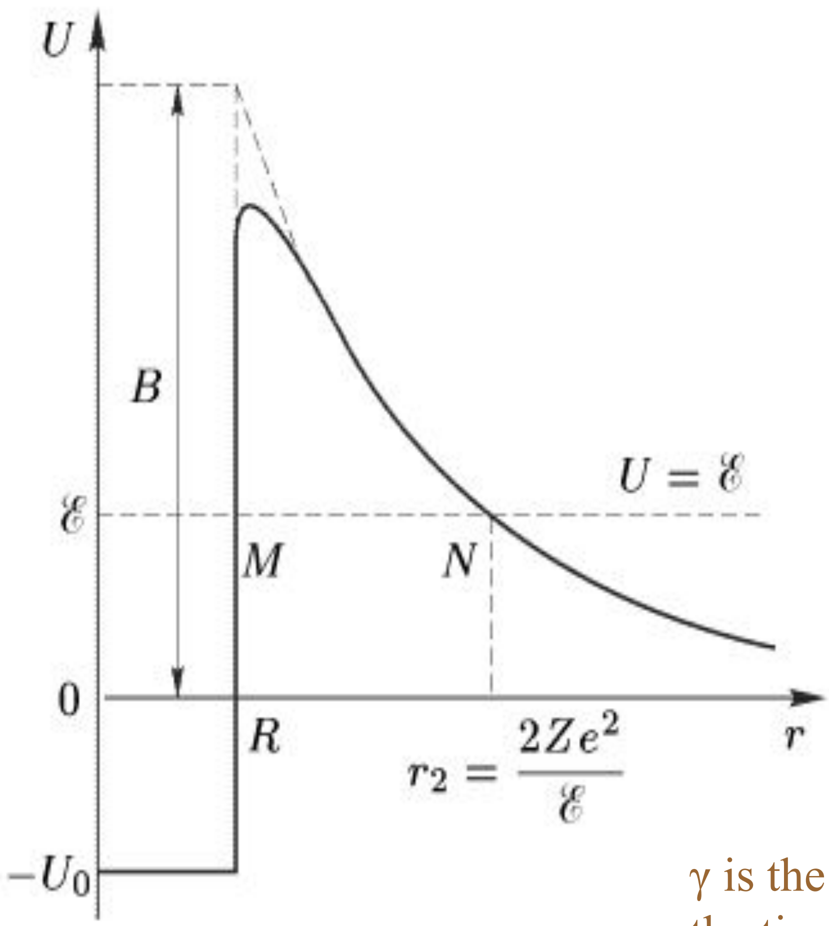


Fig. 1.3 Demonstration of the optical analogue of the tunnel effect

Examples of tunnel phenomena: α-decay of heavy nuclei



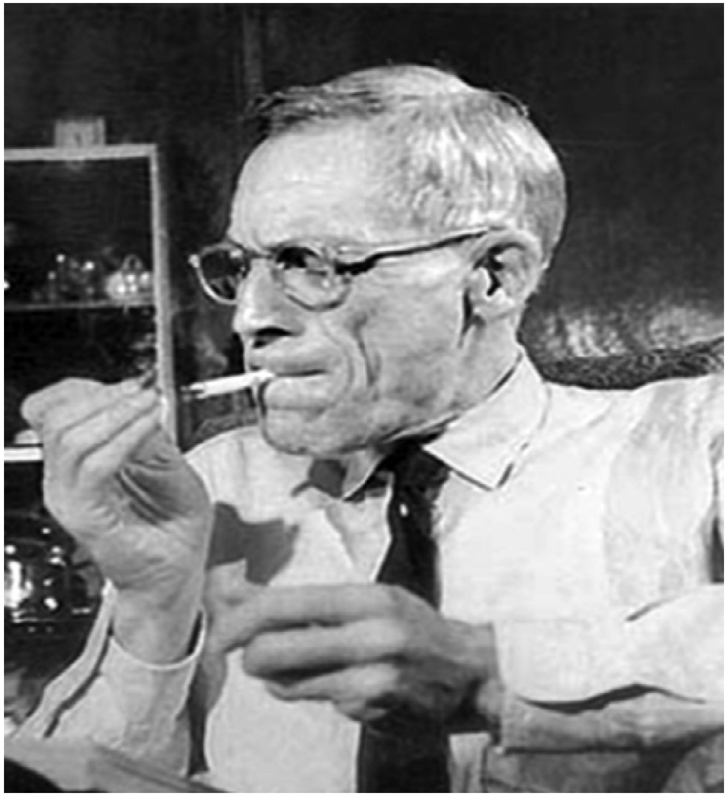
Potential energy of the particle inside and outside the atomic nucleus:

$$U(r) = \begin{cases} U_0 = \text{const} & r < R, \\ zZe^2/r & r > R, \end{cases}$$

$$\gamma = \frac{2R\sqrt{2mB}}{\hbar}\left(\sqrt{\frac{B}{\mathscr{E}}}\arccos\sqrt{\frac{\mathscr{E}}{B}} - \sqrt{1-\frac{\mathscr{E}}{B}}\right)$$

γ is the probability of the α-particle escape during the time unit

Scientists, who discovered the tunnel effect



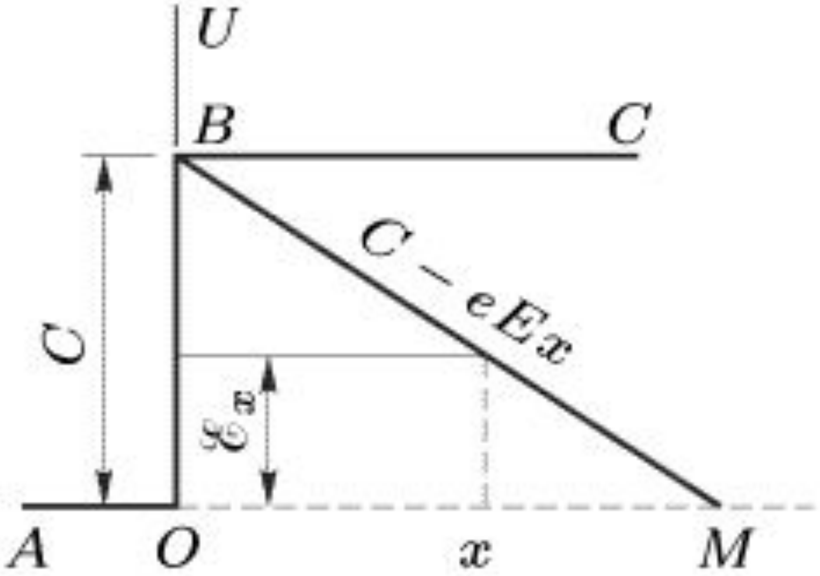
Михаил Александрович Леонтович
(07.03.1903 – 30.03.1981)

Леонид Исаакович Мандельштам*
(1879 – 1944)

Scientists, who discovered the tunnel effect

Георгий Антонович Гамов

Cold emission of metal electrons



$$U(x) = \begin{cases} 0 & x < 0, \\ C - eEx & x > 0. \end{cases}$$

Cold emission current $I(E) = I_0 \overline{D} = A e^{-E_0/E}$

E is the external electrostatic field

Cold emission of metal electrons

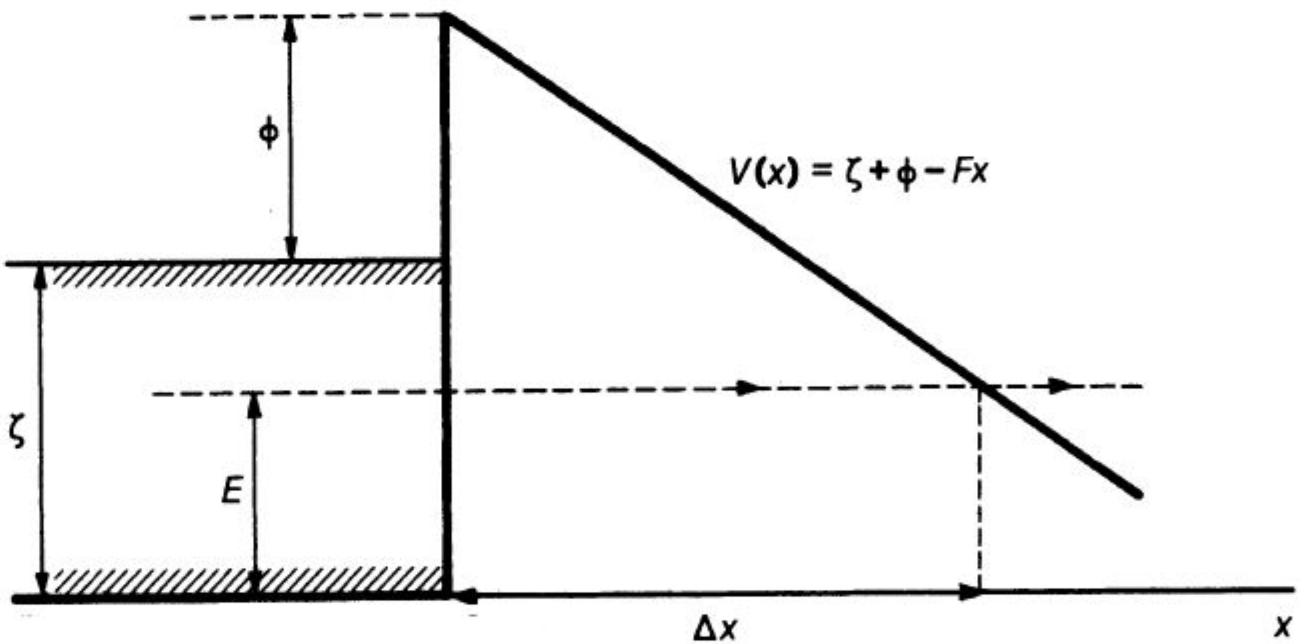
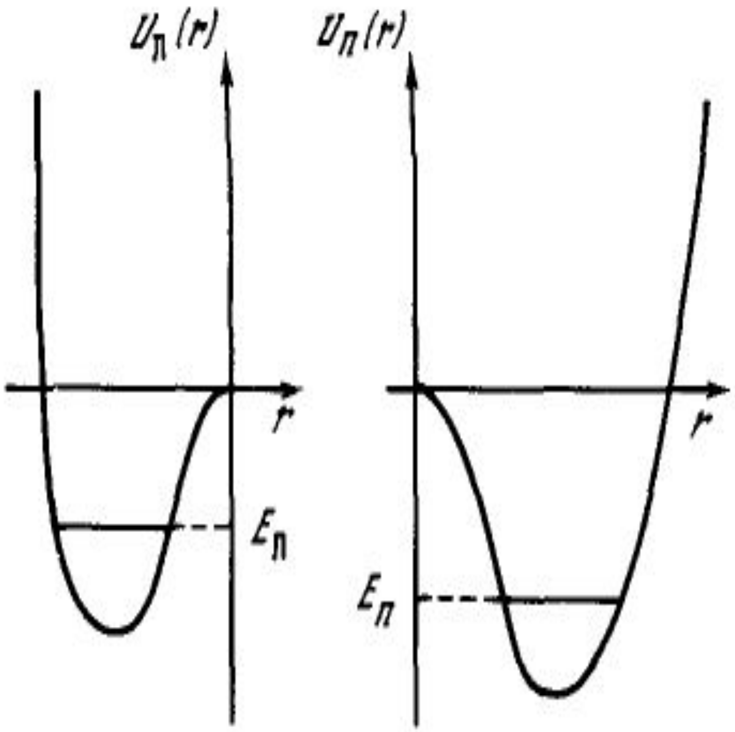


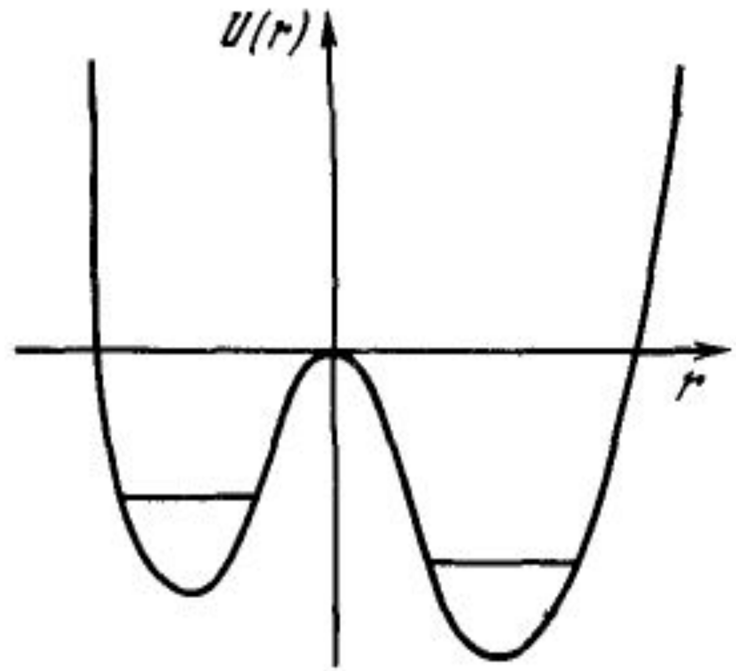
Fig. 1.4 Field-assisted emission of electrons from metals. The shaded area represents the Fermi band

$$j = A\exp[-B(\zeta + \phi - E)^{3/2}/F]$$

Oscillation of a particle between two potential wells

Initially the particle is in the left well





Separate wells

$$U^{п,п}_{лп} = \int dx\, \Psi_л\, U_{л,п}\, \Psi_п$$

$$\Delta E = E_л - E_п$$

Coupled wells

$$S = \int dx\, \Psi_л\, \Psi_п$$

Oscillation of a particle between two potential wells

Results of calculation:

W(*t*) is a probability of the particle to occur in the left well at the moment *t*

$$U^{\text{п},\text{п}}_{\text{лп}} = \int dx\, \dot{\Psi}_{\text{л}}\, U_{\text{л},\text{п}}\, \Psi_{\text{п}}$$

Limiting cases:

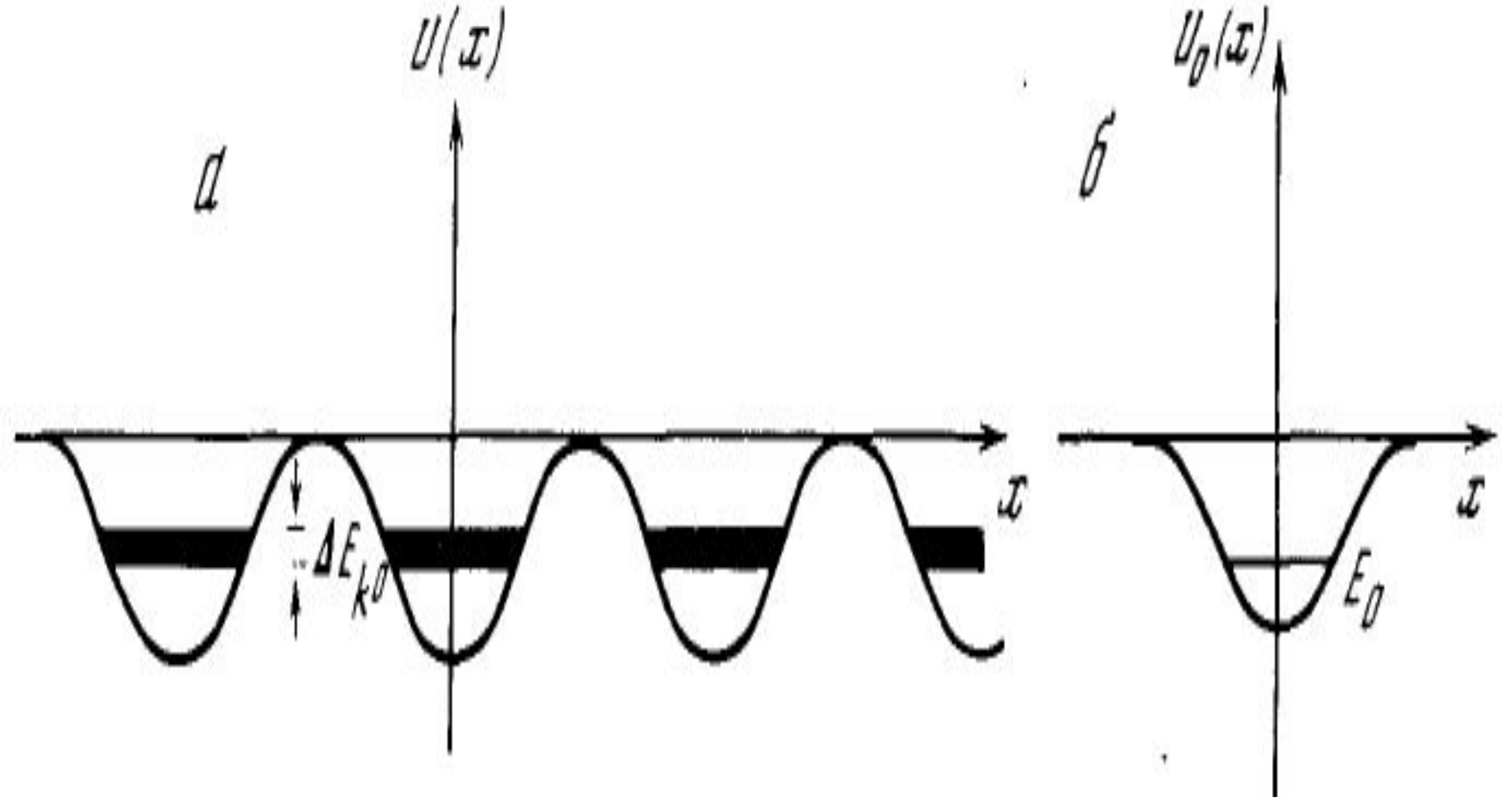
1. $\Delta E \doteq 0$ $$W(t) = 1 - \sin^2\left(\sqrt{U^{\text{л}}_{\text{лп}}\, U^{\text{п}}_{\text{лп}}}\; t/\hbar\right)$$

The particle spends equal times in both wells

2. $\Delta E^2 \gg 4U^{\text{л}}_{\text{лп}}\, U^{\text{п}}_{\text{лп}}$ $$W(t) = 1 - \frac{4U^{\text{л}}_{\text{лп}}\, U^{\text{п}}_{\text{лп}}}{\Delta E^2} \sin^2 \frac{\Delta E t}{2\hbar}$$

The particle is predominately in the left well

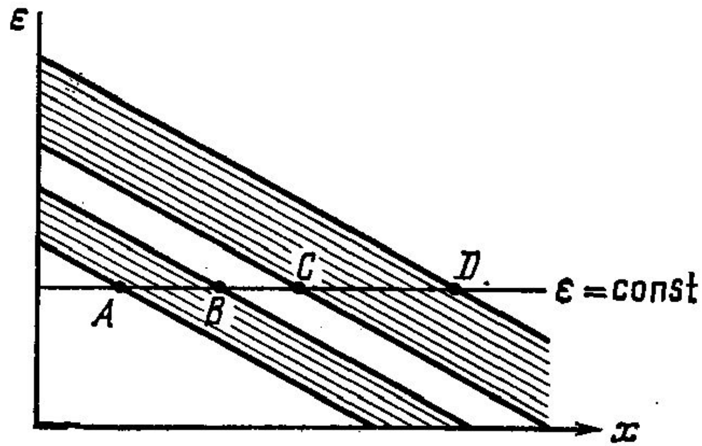
Tunneling in the periodic lattice; electron band formation



One-dimensional periodic lattice potential

ΔE_{k0} is the bandwidth

Franz-Keldysh effect



$$\alpha_E \sim \exp\left[-\gamma \frac{(\omega_G - \omega)^{3/2}}{E}\right]$$

$$\omega_G = \varepsilon_G/\hbar$$

Tunneling probability *W*(B→C) from the valence band AB into the conductance band CD is proportional to exp{$-c[\varepsilon_g]^{3/2}/E$}, where ε_g is the forbidden-gap width. This is Zener effect. It changes the coefficient α_E of the light absorption in a semiconductor in the homogeneous electric field *E*. This is Franz-Keldysh effect.

Tunneling in chemistry

The preceding chapter deals with the permeability of one-dimensional barriers to particles of specified energy W. Under normal conditions a chemical reaction involves a large number of systems covering a range of energies, and in this context a more realistic model consists of a stream of particles in thermal equilibrium impinging on a barrier. The simplest form of energy distribution in such a stream is given by

$$\frac{\mathrm{d}N}{N} = \frac{1}{\mathrm{k}T} \mathrm{e}^{-W/\mathrm{k}T} \mathrm{d}W \qquad (3.1)$$

in which $\mathrm{d}N/N$ is the fraction of particles having energies between W and $W + \mathrm{d}W$.

This expression is exact only when the energy is expressible as the sum of two terms, each of which is proportional either to the square of a momentum (as in any form of kinetic energy) or to the square of a co-ordinate (as in the potential energy of a harmonic oscillator). It is therefore not strictly applicable to a stream of particles moving in one dimension, as envisaged here. However, two square terms are involved in many situations relevant to chemical kinetics, for example the total energy (kinetic plus potential) of a harmonic oscillator, or the relative kinetic energy along the line of the centres of two colliding particles. It is therefore reasonable to use the simple type of Boltzmann distribution given by Equation 3.1 in applications to chemical kinetics.

Tunneling in chemistry

If J_0 is the total flux of particles striking the left-hand side of the barrier and $G(W)$ the permeability for an energy W, the rate J at which particles appear on the right-hand side of the barrier is given by

$$J = \frac{J_0}{\mathbf{k}T}\int_0^\infty G(W)\mathrm{e}^{-W/\mathbf{k}T}\,\mathrm{d}W. \tag{3.2}$$

If classical mechanics were obeyed we should have $G(W) = 0$ for $W < V_0$ and $G(W) = 1$ for $W > V_0$, where V_0 is the potential energy at the top of the barrier. The classical rate J_c is therefore

$$J_c = \frac{J_0}{\mathbf{k}T}\int_{V_0}^\infty \mathrm{e}^{-W/\mathbf{k}T}\,\mathrm{d}W = J_0\mathrm{e}^{-V_0/\mathbf{k}T}. \tag{3.3}$$

By combining Equations 3.2 and 3.3 we can formulate a *tunnel correction* Q_t which is the ratio of the quantum-mechanical rate to the classical rate, i.e.

$$Q_t = \frac{J}{J_c} = \frac{\mathrm{e}^{V_0/\mathbf{k}T}}{\mathbf{k}T}\int_0^\infty G(W)\mathrm{e}^{-W/\mathbf{k}T}\,\mathrm{d}W. \tag{3.4}$$

The integrand in Equation 3.4 contains two opposing factors, $\exp(-W/\mathbf{k}T)$ which increases with decreasing W, and $G(W)$ which decreases with decreasing W. The product $G(W)\exp(-W/\mathbf{k}T)$ represents the distribution of transmitted particles as a function of energy.

Tunneling in chemistry

The tunnel correction must have the same value for both the forward and the reverse reaction, so that for an endothermic reaction the appropriate barrier height is equal to the height of the barrier for the reverse process. This is illustrated in Fig. 3.4, which shows that only that portion of the barrier which lies above both the initial and the final states is available for tunnelling. This portion is greatest when the reaction is thermoneutral, leading to a maximum tunnel correction for this configuration.

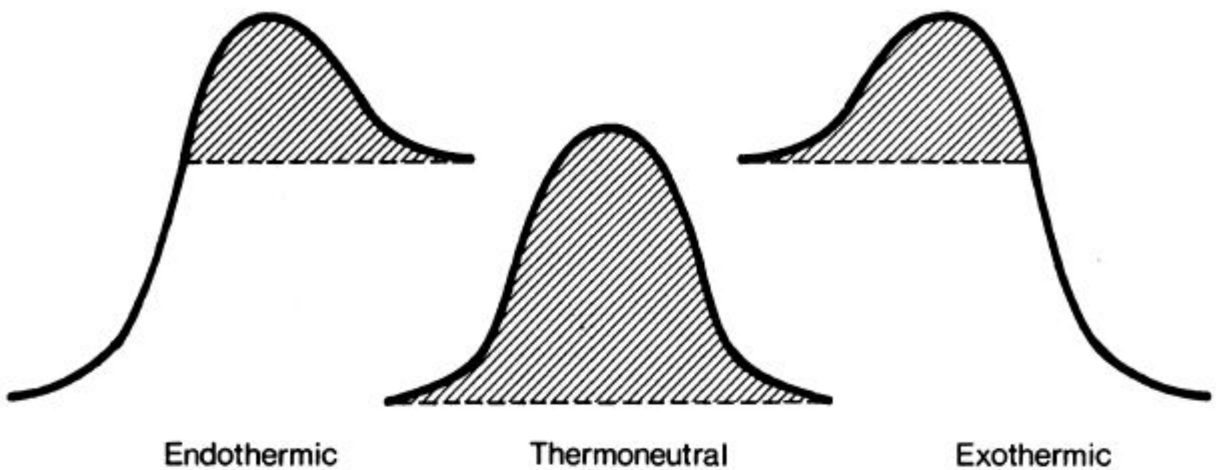
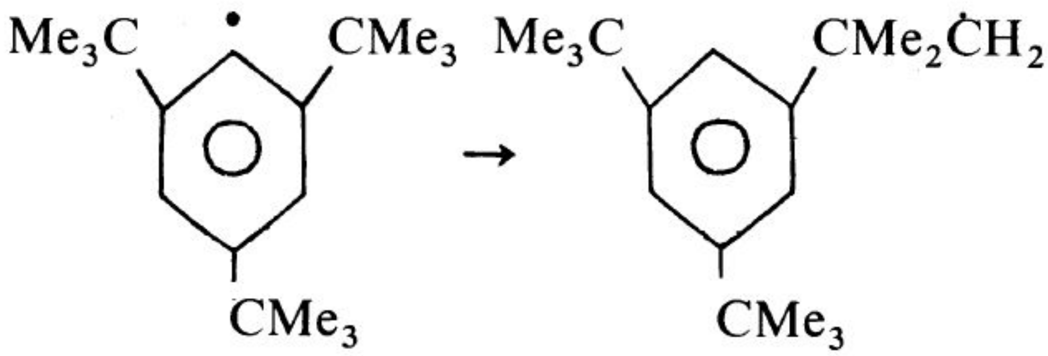


Fig. 3.4 Region available for tunnelling in endothermic, thermoneutral and exothermic reactions

Tunneling in chemistry

I – H



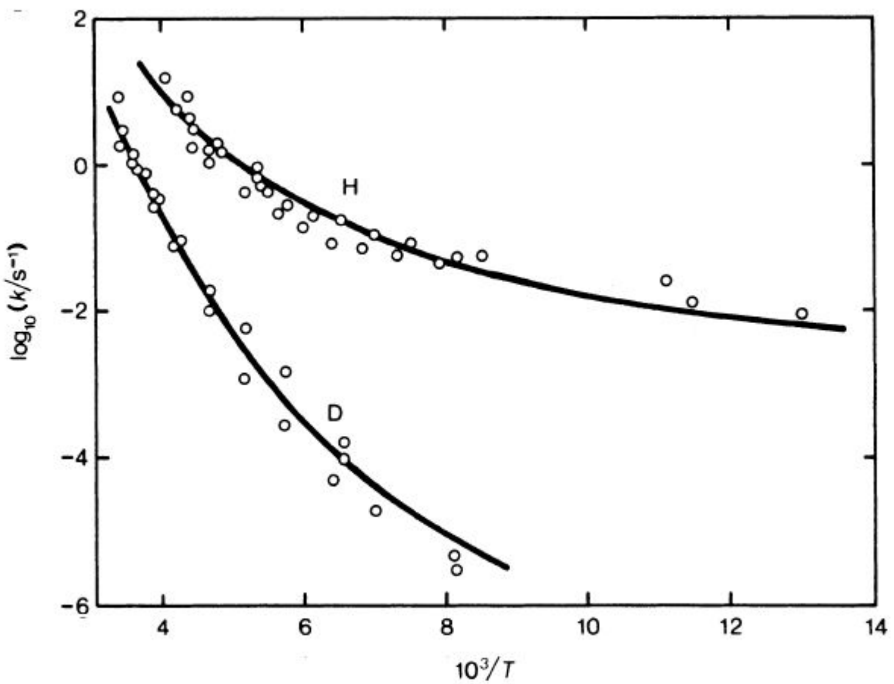


Fig. 5.1 Arrhenius plot for the isomerization of 2,4,6,-tri-*t*-butylphenyl and its completely deuterated analogue (data from [231–233])

Single-electron tunneling

The single-electronics is based on a group of physical effects with a common origin: a substantial charging of relatively large conducting objects (containing up to billions of free electrons) by addition/subtraction of one of the electrons (for the case of superconductors, a single Cooper pair or a electron-like quasi-particle). These effects are possible because the negative electric charge of the background electrons is completely compensated by the positive charge of the nuclei, but the charge of the new electron is not. Therefore, transfer of the electron causes a change

$$\Delta\mu = e^2/C \tag{1}$$

in the electro-chemical potential of the conductor, where C is its electric capacitance. For a ball with the radius of 1 μm in air, C is of the order of 10^{-16} F, so that $\Delta\mu$ is of the order of 1 meV. Thus, if the scale of thermal fluctuations k_BT is well below $\Delta\mu$ ($T \ll 10$ K in the above example) the single-electron charging can have profound effects on the electron transport properties of systems including small conductors.

For the simplest system of two small conductors separated by a tunnel barrier the orthodox theory gives a very simple prediction [1]: if the capacitance C of the system as a capacitor and the tunnel conductance G of the junction are small enough

$$C \ll e^2/k_BT, \tag{2}$$

$$G \ll e^2/\hbar, \tag{3}$$

the tunneling is vanishing within the following range

$$-\frac{e}{2} < Q < \frac{e}{2} \tag{4}$$

of the initial electric charge of the system. Physics of this so-called "Coulomb blockade of tunneling" [6] is very simple: if condition (3) is satisfied, the dominating term in the system energy is just the charging energy $Q^2/2C$. It is straightforward to get convinced that within the Coulomb blockade range (4) tunneling of an electron (i.e. the change $Q \to Q \pm e$) is energy-unfavorable, so that at low temperatures (3) this process is impossible.

Single-electron tunneling

The physical origin of the Coulomb blockade of single-electron tunneling is quite simple. In a current-biased junction, each tunneling event leads to a change of the Coulomb energy $E_0 = Q^2/2C$ (Fig. 1)

$$\Delta E_0 = \frac{(Q \pm e)^2}{2C} - \frac{Q^2}{2C} = \frac{e}{C}\left(Q \pm \frac{e}{2}\right) \tag{39}$$

If an initial charge Q is within the limits given by (4) this energy change is positive for any sign of $\Delta Q = \pm e$, and hence at low temperatures (2) tunneling events are virtually impossible.

Correct formula:

$\Delta E = e(e/2 \pm Q)/C$

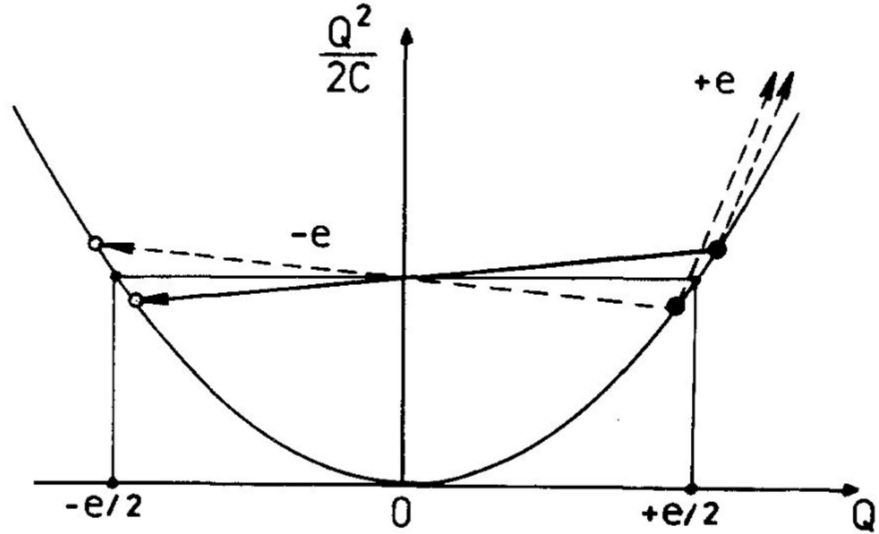


Fig. 1. Energy diagram illustrating the origin of the Coulomb blockade of the single-electrons tunneling in a small, current-biased junction. (—) Transitions favorable with regard to energy; (- -)unfavorable transitions. At low temperatures only the former transitions are possible, so that for $|Q| < e/2$ all transitions are blocked.

Single-electron tunneling

As noted in the Introduction, the final results depend substantialy on the properties of the eigenvalue spectra of the operator Q. Since, according to (3), tunneling leads only to discrete charge transfer ($\Delta Q = \pm e$), one might assume that the operator $Q = Q - Q_0$ takes on only discrete values ne. This assumption is actually correct when Q is the charge on an isolated conductor connected to the "outside world" only via the tunnel current. This is the case, for example, for a metal granule in the oxide layer of a tunnel junction,[6–8] which leads in particular to oscillatory (e-periodic) dependence of the properties of such structures on the values of Q_0 observed in experiment.[7]

A more realistic situation for an ordinary tunnel junction, however, is one in which it is shunted by an albeit small but finite metallic-type conductance G_s (this shunting is necessary at the very least for the measurement of the electrodynamic characteristics of the junction). The electric charge is transported through such a "shunt" as a result of small displacements of a large number of carriers, so that this charge is not discrete in the scale of e.

$$H = \mathcal{J}(Q) + H_T + H_1\{k_1\} + H_2\{k_2\} + H_S\{k_S\} - I\phi, \qquad (3)$$

where H_T is expressed by Equation (1), while

$$\mathcal{J}(Q) = \frac{Q^2}{2C}, \qquad \phi = \int V dt, \qquad V = Q/C,$$

$$I = I_0(t) - I_S\{k_S\}. \qquad (4)$$

The operator Q of the electric charge of the junction can be expressed via the same creation and annihilation operators as H_T:

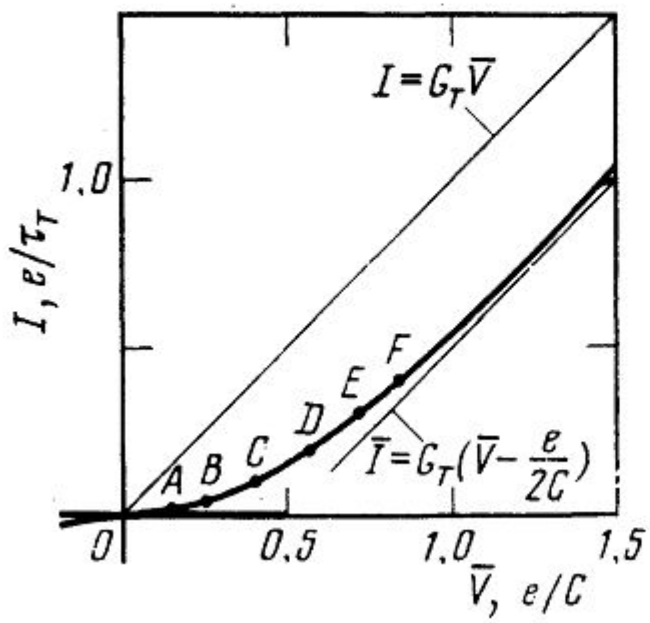
$$Q = -\frac{e}{2}\left(\sum_{k_1} c^{\dagger}_{k_1} c_{k_1} - \sum_{k_2} c^{\dagger}_{k_2} c_{k_2}\right) + \text{const.}, \qquad (5)$$

so that H_T and Q do not commute. One can readily prove that the following commutation relations are valid for an arbitrary function $F(Q)$:

$$H_{\pm} F(Q) = F(Q \pm e) H_{\pm}. \qquad (6)$$

The Hamiltonians H_1, H_2, and H_S describe the energy of the internal degrees of freedom $\{k_1\}$, $\{k_2\}$, and $\{k_S\}$ of the two electrodes of the junction and of the "shunt" G_S, respectively. The last term in Equation (3) describes the interaction of the junction with the current I (Figure 1).

Single-electron tunneling



The volt-ampere characteristic of the junction then tends toward the linear asymptotic relation

$$\overline{V}=G_T^{-1}\overline{I}+\frac{e}{2c}\operatorname{sign}\overline{I}. \tag{43}$$