Tunneling phenomena in solids

Lecture 4. Tunneling in normal-metal junctions

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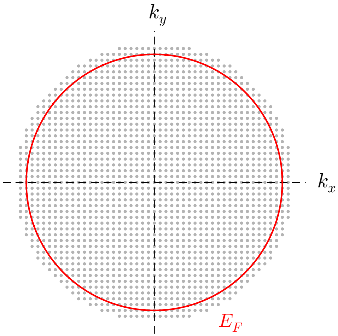
Pauli exclusion principle and Fermi surface

The Pauli exclusion principle states that two or more identical particles with half-integer spins (fermions) cannot simultaneously occupy the same quantum state within a system that obeys the laws of quantum mechanics (1925).



Periodic boundary conditions:

$$k_x L_x = 2\pi n_x \;\rightarrow\; \Delta k_x = 2\pi / L_x$$

$$k_y L_y = 2\pi n_y \;\rightarrow\; \Delta k_y = 2\pi / L_y$$

$$k_z L_z = 2\pi n_z \;\rightarrow\; \Delta k_z = 2\pi / L_z$$

Volume per a single state in k-space:

$$\Delta k_x \, \Delta k_y \, \Delta k_z = (2\pi)^3 / (L_x \, L_y \, L_z) = (2\pi)^3 / V$$

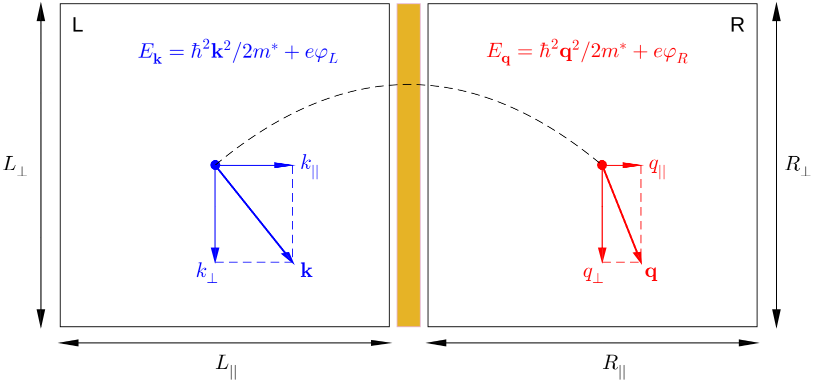
Fermi surface is the surface in reciprocal space which separates occupied from unoccupied electron states at zero temperature. The existence of a Fermi surface is a direct consequence of the Pauli exclusion principle, which allows a maximum of one electron per quantum state.

Tunneling in multi-electron systems

We consider two metal electrodes (electronic reservoirs): left (L) and right (R). For brevity, the electron momentums in the left and right electrodes are denoted by $\boldsymbol{k}$ and $\boldsymbol{q}$, respectively. Here and further we will use the notation typical for the theory of **quantum transport**:

sign «$\|$» corresponds to the direction along the current,

sign «$\perp$» corresponds to the directions along the barrier.



Tunneling current induced by single electron

Each of free electrons in $L-$electrode can be described by normalized quasiclassical wave function

$$\psi_L(x, y, z, t) = a_L \cdot e^{i\boldsymbol{k}_\perp \mathbf{r}_\perp} \cdot e^{ik_\parallel z} \cdot e^{-iE_{\boldsymbol{k}} t/\hbar},$$

where $|a_L| = \Omega_L^{-1/2}$ is normalized coefficient, $\Omega_L = L_\perp^2 L_\parallel$ is volume of $L-$electrode, $E_{\boldsymbol{k}} = \hbar^2 \boldsymbol{k}_\perp^2/2m^* + \hbar^2 k_\parallel^2/2m^* + e\varphi_L$ is the full energy of electron with wave vector $\boldsymbol{k}$ accounting electrostatic energy, m^* is effective mass.

During tunneling the longitudinal (with respect to the direction of the current) and perpendicul (with respect to the barrier) component of the probability flux is transformed as follows

$$\Pi_L = \frac{\hbar k_\parallel}{m^*} |a_L|^2 \quad \Longrightarrow \quad \Pi_R = \Pi_L \cdot \mathcal{T}_{L\to R} = \frac{\hbar k_\parallel}{m^*} \cdot \frac{1}{\Omega_L} \cdot \mathcal{T}_{L\to R} = \frac{v_{L,\parallel}}{\Omega_L} \cdot \mathcal{T}_{L\to R},$$

where $\mathcal{T} = |t|^2$ is the transmission coefficient depending only on $k_\parallel$ and the parameters of the tunneling barrier.

Each of free electrons in $L-$electrode can induce the current inside $R-$electrode equal to $e\,(v_{L,\parallel}/\Omega_L)\,\mathcal{T}_{L\to R}$.

Each of free electrons in $R-$electrode can induce the current inside $L-$electrode equal to $e\,(v_{R,\parallel}/\Omega_R)\,\mathcal{T}_{R\to L}$.

Full tunneling current induced by all electrons

A necessary condition for the appearance of the tunnel current is that the quantum state with a given $\boldsymbol{k}$ in the emitter should be occupied, while the quantum state with a given $\boldsymbol{q}$ in the collector should be free. Consequently, the density of the tunnel current taking into account spin degeneracy and filling factors equal to

$$j_{L\to R} = 2 \cdot \sum_{\boldsymbol{k}} e\,\frac{v_{L,\parallel}}{\Omega_L} \cdot \mathcal{T}_{L\to R} \cdot f_L(E_{\boldsymbol{k}}) \left\{1 - f_R(E_{\boldsymbol{q}})\right\}, \quad \text{provided that} \quad v_{L,\parallel} > 0,$$

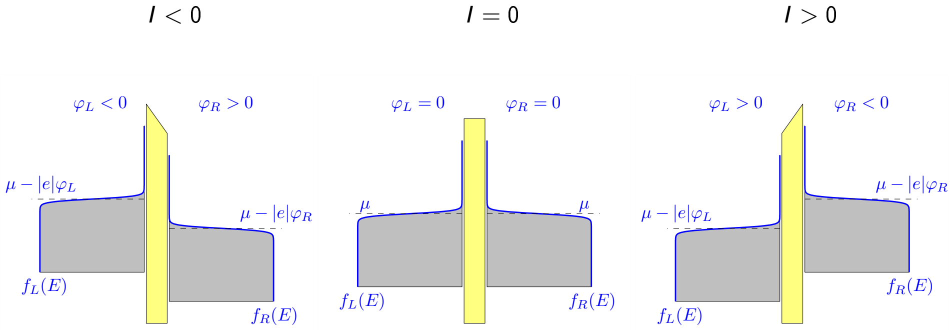
$$j_{R\to L} = 2 \cdot \sum_{\boldsymbol{q}} e\,\frac{v_{R,\parallel}}{\Omega_R} \cdot \mathcal{T}_{R\to L} \cdot f_R(E_{\boldsymbol{q}}) \left\{1 - f_L(E_{\boldsymbol{k}})\right\}, \quad \text{provided that} \quad v_{R,\parallel} < 0.$$

We assume that the filling factors are close to the equilibrium Fermi-Dirac distribution (k_B is Boltzmann constant and Θ is absolute temperature)

$$f_L(E) = \left(1 + e^{\left(E-(\mu_L+e\varphi_L)\right)/k_B\Theta}\right)^{-1} \quad \text{and} \quad f_R(E) = \left(1 + e^{\left(E-(\mu_R+e\varphi_R)\right)/k_B\Theta}\right)^{-1}.$$

where φ_L and φ_R are electrical potential of $L-$ and $R-$ reserviors; $\tilde{\mu}_L = \mu_L + e\varphi_L$ and $\tilde{\mu}_R = \mu_R + e\varphi_R$ are electrochemical potential of $L-$ and $R-$ reserviors.

Band structure of tunneling junction



Reminder: $e = -|e|$.

Electrochemical potential

$$\tilde{\mu} = \mu + e\varphi = \mu - |e|\varphi$$

corresponds to the maximal energy of the occupied states at low temperatures (including the effect of electrostatic energy).

Simplifying assumptions

Burstein and Lundquist, Tunneling phenomena in solids. New York, Plenum Press, 1969

1. Conservation of the total energy of tunneling particle $E_{\boldsymbol{k}} = E_{\boldsymbol{q}}$ (elastic tunneling).

2. For simplicity, we assume equal temperatures and chemical potentials of both electrodes $(\mu_L = \mu_R = \mu)$

$$f_L(E) = \left(1 + e^{\left(E-(\mu+e\varphi_L)\right)/k_B\Theta}\right)^{-1} = \left(1 + e^{\left((E-e\varphi_L)-\mu\right)/k_B\Theta}\right)^{-1} \equiv f_0(E - e\varphi_L),$$

$$f_R(E) = \left(1 + e^{\left(E-(\mu+e\varphi_R)\right)/k_B\Theta}\right)^{-1} = \left(1 + e^{\left((E-e\varphi_R)-\mu\right)/k_B\Theta}\right)^{-1} \equiv f_0(E - e\varphi_R).$$

3. In order to estimate the number of electronic waves involving in tunneling process in systems with low-transmission barrier, we formally apply periodic boundary conditions $\psi(z) = \psi(z + L_{||})$, which leads to equidistant spectrum of allowed $k-$values

$$k_{||} = \frac{2\pi}{L_{||}}\, n_{||} \quad \text{и} \quad \Delta k_{||} = k_{||}\Big|_n - k_{||}\Big|_{n-1} = \frac{2\pi}{L_{||}},$$

where $L_{||}$ is the length of $L-$electrode, $n_{||}$ is integer.

4. Standard rule for transition from summation to integration along the $\|$−direction

$$\sum_{k_\|} \ldots = \frac{1}{\Delta k_\|} \sum_{k_\|} \Delta k_\| \ldots \simeq \frac{L_\|}{2\pi} \int dk_\| \ldots , \quad \sum_{q_\|} \ldots = \frac{1}{\Delta q_\|} \sum_{q_\|} \Delta q_\| \ldots \simeq \frac{R_\|}{2\pi} \int dq_\| \ldots .$$

The same rule can be applied for $\perp$ −components for the tunnel junctions of large area.

Intermediate result:

$$j = \frac{2eL_\|}{2\pi} \int dk_\| \sum_{\boldsymbol{k}_\perp} \frac{v_{L,\|}}{L_\perp^2 \, L_\|} f_0(E_{\boldsymbol{k}} - e\varphi_L) \left\{1 - f_0(E_{\boldsymbol{k}} - e\varphi_R)\right\} \mathcal{T}_{L\to R} +$$
$$+ \frac{2eR_\|}{2\pi} \int dq_\| \sum_{\boldsymbol{q}_\perp} \frac{v_{R,\|}}{R_\perp^2 \, R_\|} f_0(E_{\boldsymbol{q}} - e\varphi_R) \left\{1 - f_0(E_{\boldsymbol{q}} - e\varphi_L)\right\} \mathcal{T}_{R\to L}.$$

5. For tunneling system uniform in the $\perp$-direction and mirror reflection of electrons from the barrier, $\perp$-components of the wave vectors should be conserved: $\boldsymbol{k}_\perp = \boldsymbol{q}_\perp$. As a result, the energy associated with the motion along the barrier should be conserved: $E_{\boldsymbol{k}_\perp} = E_{\boldsymbol{q}_\perp} = E_\perp$. As a result, the energy associated with the motion along the current should be conserved: $E_{\boldsymbol{k}_\|} = E_{\boldsymbol{q}_\|} = E_\|$. In the other words, we come to a reduced energy conservation law

$$\frac{\hbar^2 k_\|^2}{2m^*} + e\varphi_L = \frac{\hbar^2 q_\|^2}{2m^*} + e\varphi_R.$$

6. For non-magnetic systems the transmission coefficient of the barrier does not depend on the direction of tunneling, therefore $\mathcal{T}_{L\to R} = \mathcal{T}_{R\to L} = \mathcal{T}$. It is clear that the transmission coefficient $\mathcal{T}$ depends only on $E_{\|}$ and voltage bias $U = \varphi_L - \varphi_R$.

7. It is clear that

$$f_0(E - e\varphi_L)\left\{1 - f_0(E - e\varphi_R)\right\} - f_0(E - e\varphi_R)\left\{1 - f_0(E - e\varphi_L)\right\} =$$
$$= f_0(E - e\varphi_L) - f_0(E - e\varphi_R).$$

8. Since $v_{\|} = \hbar^{-1}\,\partial E/\partial k_{\|} = \hbar^{-1}\,dE_{\|}/dk_{\|}$,

$$v_{L,\|}\,dk_{\|} = \frac{dE_{\|}}{\hbar} \quad \text{and} \quad v_{R,\|}\,dq_{\|} = -\frac{dE_{\|}}{\hbar}.$$

9. For planar structure the transverse dimensions of the electrodes should be equal: $L_{\perp} = R_{\perp}$.

Intermediate result:

$$j = \frac{2e}{2\pi\hbar}\int dE_{\|}\sum_{\boldsymbol{k}_{\perp}}\frac{\mathcal{T}(E_{\|})}{L_{\perp}^2}\left\{f_0(E - e\varphi_L) - f_0(E - e\varphi_R)\right\},$$

Conductance of large-area tunneling junctions

If quantization of transverse modes is not significant ($L_\perp^2 \gg \lambda^2$), we can substitute the summation over $\boldsymbol{k}_\perp$ by the integration over all transverse modes

$$j = \frac{2e}{2\pi\hbar} \int dE_\| \iint \mathcal{T}(E_\|) \left\{ f_0(E - e\varphi_L) - f_0(E - e\varphi_R) \right\} \frac{d^2\, k_\perp}{(2\pi)^2} =$$

$$= \frac{2e}{2\pi\hbar} \int \mathcal{T}(E_\|)\, dE_\| \iint \left\{ f_0(E - e\varphi_L) - f_0(E - e\varphi_R) \right\} \frac{d^2\, k_\perp}{(2\pi)^2}.$$

We introduce the number of electronic modes participating in tunneling process (supply function)

$$\mathcal{N}(E_\|) = \iint \left\{ f_0(E_\| + E_\perp - e\varphi_L) - f_0(E_\| + E_\perp - e\varphi_R) \right\} \frac{d^2\, k_\perp}{(2\pi)^2}.$$

Here we use the obvious relationship $E = E_\| + E_\perp$.

As a result, the density of the tunneling current can be written as follows

$$j = \frac{2e}{2\pi\hbar} \int \mathcal{T}(E_\|) \cdot \mathcal{N}(E_\|) \cdot dE_\|,$$

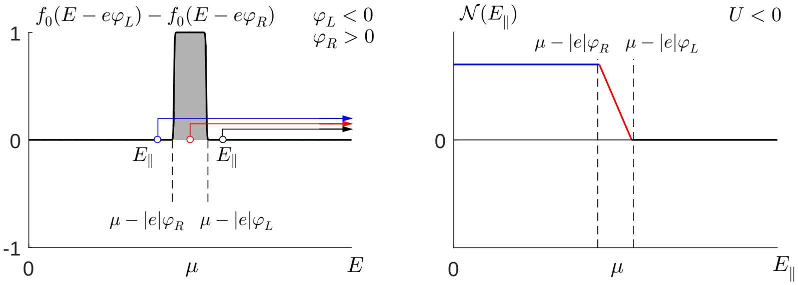
Assume that electrons in the conduction band can be considered as free-electron gas

$$E_\perp = \frac{\hbar^2 k_\perp^2}{2m^*} \implies dE_\perp = \frac{\hbar^2 k_\perp dk_\perp}{m^*} \implies d^2 k_\perp = 2\pi k_\perp dk_\perp = \frac{2\pi m^* dE_\perp}{\hbar^2}.$$

In this model the number of the electronic modes, involving in tunneling process is equal to

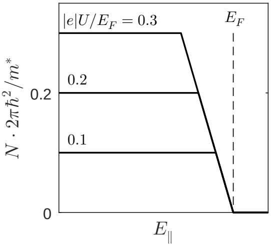
$$\mathcal{N}(E_\parallel) = \iint \left\{ f_0(E_\parallel + E_\perp - e\varphi_L) - f_0(E_\parallel + E_\perp - e\varphi_R) \right\} \frac{2\pi m^* dE_\perp}{(2\pi)^2 \hbar^2} =$$

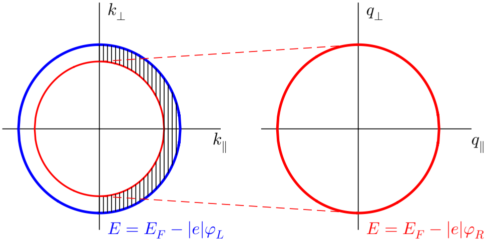
$$= \frac{m^*}{2\pi\hbar^2} \int\limits_{E_\parallel}^{\infty} \left\{ f_0(E' - e\varphi_L) - f_0(E' - e\varphi_R) \right\} dE'.$$



Visual interpretation: cross-sections of Fermi surface*

Electronic states participating in tunneling for the case $U = \varphi_L - \varphi_R < 0$





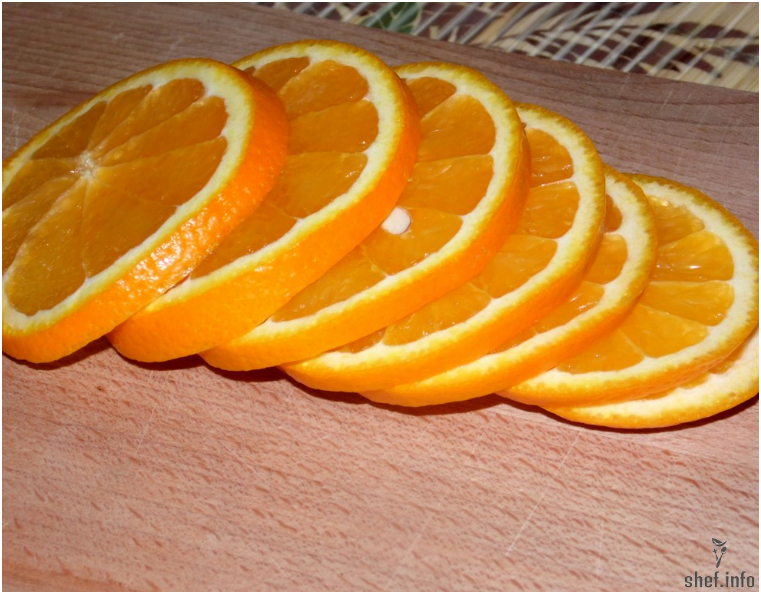
Sectional area of the larger sphere Fermi (provided $0 \le k_\parallel \le k_F$)

$$S_1 = \pi\,(k_F^2 - k_\parallel^2) = \frac{2\pi m^*}{\hbar^2}\left(\frac{\hbar^2 k_F^2}{2m^*} - \frac{\hbar^2 k_\parallel^2}{2m^*}\right) = \frac{2\pi m^*}{\hbar^2}\Big(E_F + e\varphi_L - E_\parallel\Big).$$

Sectional area of the smaller sphere Fermi (provided $0 \le k_\parallel \le k_F'$)

$$S_2 = \pi\,(k_F'^2 - k_\parallel^2) = \frac{2\pi m^*}{\hbar^2}\left(E_F - e\varphi_L + e\varphi_R - \frac{\hbar^2 k_\parallel^2}{2m^*}\right) = \frac{2\pi m^*}{\hbar^2}\Big(E_F + e\varphi_R - E_\parallel\Big).$$

The area of the ring $S_1 - S_2$ for given $E_\parallel$ coincides with the $\mathcal{N}(E_\parallel)$ function!



Appelsine (RU), Apfelsine (DE), Sinaasappel (ND) – apple from China

Tsu-Esaki relationship

We can substitute the functional dependence corresponding to the Fermi-Dirac distributions and obtain

$$\mathcal{N}(E_\parallel) = \frac{m^*}{2\pi\hbar^2}\int\limits_{E_\parallel}^{\infty}\left\{\left(1+e^{-(E_\parallel-\mu-e\varphi_L)/k_B\Theta}\right)^{-1} - \left(1+e^{-(E_\parallel-\mu-e\varphi_R)/k_B\Theta}\right)^{-1}\right\} dE' =$$

$$= \frac{m^*}{2\pi\hbar^2}\cdot k_B\Theta\cdot\left\{\ln\left(1+e^{-(E_\parallel-\mu-e\varphi_L)/k_B\Theta}\right) - \ln\left(1+e^{-(E_\parallel-\mu-e\varphi_R)/k_B\Theta}\right)\right\} =$$

$$= \frac{m^*}{2\pi\hbar^2}\cdot k_B\Theta\cdot\ln\frac{\left(1+e^{-(E_\parallel-\mu-e\varphi_L)/k_B\Theta}\right)}{\left(1+e^{-(E_\parallel-\mu-e\varphi_R)/k_B\Theta}\right)}.$$

Reminder: $\ln a - \ln b = \ln(a/b)$.

Thus, we arrive at Tsu-Esaki relationship, which is valid for all temperatures

$$j = \frac{2e}{2\pi\hbar}\int \mathcal{T}(E_\parallel)\cdot\mathcal{N}(E_\parallel)\cdot dE_\parallel =$$

$$= \frac{2em^*}{(2\pi)^2\hbar^3}\cdot k_B\Theta\cdot\int\limits_0^{\infty}\mathcal{T}(E_\parallel)\ln\frac{\left(1+e^{-(E_\parallel-\mu-e\varphi_L)/k_B\Theta}\right)}{\left(1+e^{-(E_\parallel-\mu-e\varphi_R)/k_B\Theta}\right)}\,dE_\parallel.$$

Conductance of tunnel-junction: limit of low bias and low temperature

Tsu-Esaki relationship can be rewritten in the form

$$j(\mathcal{V}) \simeq \frac{2e}{2\pi\hbar} \int\limits_{\max\{-eU,0\}}^{\infty} \mathcal{T}(E_{\parallel}) \times$$

$$\times \frac{m^*}{2\pi\hbar^2} k_B\Theta \cdot \left\{ \ln\left(1 + e^{-(E_{\parallel} - \mu - e\varphi_L)/k_B\Theta}\right) - \ln\left(1 + e^{-(E_{\parallel} + -\mu - e\varphi_R)/k_B\Theta}\right) \right\} dE_{\parallel}.$$

It is clear at the low temperature ($\Theta \to 0$) the following asymptotic expression are valid

$$\ln\left(1 + e^{-(E_{\parallel} - \mu - e\varphi_L)/k_B\Theta}\right) \simeq \frac{1}{k_B\Theta} \cdot \begin{cases} 0 & \text{at } E_{\parallel} \geq \mu - |e|\varphi_L, \\ -(E_{\parallel} - \mu - e\varphi_L) & \text{at } E_{\parallel} < \mu - |e|\varphi_L; \end{cases}$$

and

$$\ln\left(1 + e^{-(E_{\parallel} - \mu - e\varphi_R)/k_B\Theta}\right) \simeq \frac{1}{k_B\Theta} \cdot \begin{cases} 0 & \text{at } E_{\parallel} \geq \mu - |e|\varphi_R, \\ -(E_{\parallel} - \mu - e\varphi_R) & \text{at } E_{\parallel} < \mu - |e|\varphi_R. \end{cases}$$

If $\varphi_L > \varphi_R$, then the band structure of the left electrode is shifted *down* relative to the band diagram of the right electrode, so the resulting electron flow is negative and comes from the right electron in the left one. It corresponds to *positive* tunneling current density ($e = -|e|$). To estimate the current density, it is necessary to consider three energy intervals

$$j \simeq -\frac{2|e|}{2\pi\hbar}\int \mathcal{T}(E_\parallel)\cdot\frac{m^*}{2\pi\hbar^2}\cdot\left\{\begin{array}{ll} 0 & \text{at } E_\parallel > \mu - |e|\varphi_R \\ -(\mu + e\varphi_R - E_\parallel) & \text{at } \mu - |e|\varphi_L < E_\parallel < \mu - |e|\varphi_R \\ -|e|(\varphi_L - \varphi_R) & \text{at } E_\parallel < \mu - |e|\varphi_L \end{array}\right\}\cdot dE_\parallel$$

Let us put for definiteness $\varphi_L = U$ и $\varphi_R = 0$, then

$$j \simeq \frac{2|e|}{2\pi\hbar}\,\frac{m^*}{2\pi\hbar^2}\int \mathcal{T}(E_\parallel)\cdot\left\{\begin{array}{ll} 0 & \text{at } E_\parallel > \mu \\ (\mu - E_\parallel) & \text{at } \mu - |e|U < E_\parallel < \mu \\ |e|U & \text{at } E_\parallel < \mu - |e|U \end{array}\right\}\cdot dE_\parallel$$

or

$$j \simeq \frac{2|e|}{2\pi\hbar}\cdot\frac{m^*}{2\pi\hbar^2}\cdot|e|U\int\limits_0^{\max\{\mu-|e|U,0\}}\mathcal{T}(E_\parallel)\,dE_\parallel +$$

$$+\frac{2|e|}{2\pi\hbar}\cdot\frac{m^*}{2\pi\hbar^2}\int\limits_{\max\{\mu-|e|U,0\}}^{\mu}\mathcal{T}(E_\parallel)\cdot(\mu - E_\parallel)\,dE_\parallel.$$

Taking into account the symmetry between the emitter and the collector, we can write the expression valid for an arbitrary sign of U

$$j \simeq sign\, U \cdot \left\{ \frac{|e|^2 m^*}{2\pi^2\hbar^3}\ |U| \int\limits_0^{\max\{\mu-|eU|,0\}} \mathcal{T}(E_\parallel)\ dE_\parallel + \right.$$
$$\left. + \frac{|e| m^*}{2\pi^2\hbar^3} \int\limits_{\max\{\mu-|eU|,0\}}^{\mu} \mathcal{T}(E_\parallel)\cdot(\mu - E_\parallel)\ dE_\parallel \right\}.$$

At $|U| \to 0$ the second term is a value of a higher-order smallness and can be omitted.

At $|eU| \ll \mu$ one can get a universal linear dependence of the tunneling current $I = j \cdot S$ on applied voltage U (here S is the area on tunneling junction). The conductance of the tunnel junction is equal to

$$G \equiv \frac{I}{U} = S \cdot \frac{|e|^2 m^*}{2\pi^2\hbar^3} \int\limits_0^{\mu} \mathcal{T}(E_\parallel)\, dE_\parallel,$$

We can use the expression for low-transmission square barrier (see lecture 1) and get

$$\mathcal{T}(E_\parallel) = \frac{16\, k_1\, \varkappa^2\, k_3}{(k_1^2 + \varkappa^2)(\varkappa^2 + k_3^2)}\ e^{-2\varkappa w} \quad \Longrightarrow \quad G \simeq S \cdot \frac{e^2}{4\pi^2\hbar}\, \mathcal{T}(\mu)\, \frac{\varkappa(\mu)}{w},$$

Cold electron emission

Cold electron emission or field emission is the process of emission of electrons from a solid under the action of an electric field, in contrast to thermoelectron emission, occurring at high temperatures. The regime of cold field emission is essentially the process of tunneling in a strong electric field.

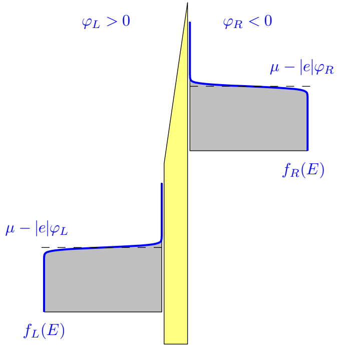
We assume for definiteness $\varphi_L = U > 0$ и $\varphi_R = 0$.

Trapezoidal potential barrier
$V(z) = -|e|U + \mu + W + |e|U\,z/w$ for $0 \le z \le w$, where w is the width of the barrier, W is work function.

Under the condition $|eU| > \mu + W$ the trapezoidal barrier can be viewed as a triangular one.

The expression for the tunneling current (see page 17)

$$j \simeq sign\,U \cdot \frac{|e|m^*}{2\pi^2\hbar^3} \int\limits_0^{\mu} \mathcal{T}(E_\parallel)(\mu - E_\parallel)\, dE_\parallel .$$



The transmission coefficient of the triangular barrier can be estimated by means of the WKB theory

$$\mathcal{T}(E_{\parallel}) = \exp\left\{-\frac{2}{\hbar}\int\limits_{a}^{b} \big|p(z)\big|\, dz\right\} =$$

$$= \exp\left\{-\frac{2\sqrt{2m^*}}{\hbar}\,\frac{w}{|e|U}\int\limits_{a}^{b}\sqrt{-|eU| + \mu + W + z' - E_{\parallel}}\, dz'\right\} =$$

$$= \exp\left\{-\frac{4}{3}\,\frac{\sqrt{2m^*}}{\hbar}\,\frac{w}{|eU|}\,\left(\mu + W - E_{\parallel}\right)^{3/2}\right\},$$

where $a = 0$ and $b = w\cdot(\mu + W - E_{\parallel})/|eU|$ are classical turning points for $U < 0$ and $a = w - w\cdot(\mu + W - E_{\parallel})/|eU|$ and $b = w$ are classical turning points for $U > 0$.

Let us assume that the work function and, accordingly, the height of the potential barrier for electrons are sufficiently large, which allows us to consider the limit $\mu - E_{\parallel} \ll W$

$$\left(\mu + W - E_{\parallel}\right)^{3/2} \simeq W^{3/2}\left(1 + \frac{3}{2}\,\frac{(\mu - E_{\parallel})}{W}\right) \simeq W^{3/2} + \frac{3}{2}\,W^{1/2}\,(\mu - E_{\parallel}),$$

$$\mathcal{T}(E_{\parallel}, U) = \exp\left\{-\frac{4}{3}\,\frac{\sqrt{2m^*}\,w}{\hbar|eU|}\,W^{3/2}\right\}\,\exp\left\{-\frac{2\sqrt{2m^*W}\,w}{\hbar|eU|}\,\left(\mu - E_{\parallel}\right)\right\}.$$

We introduce a dimensionless parameter $B = 2\sqrt{2m^* W_0}\mu w/(\hbar|eU|)$ and rewrite the expression for the current density as follows

$$j = sign U \cdot \frac{|e|m^*}{2\pi^2\hbar^3} \int\limits_0^{\mu} (\mu - E_{\|})\, \mathcal{T}(E_{\|})\, dE_{\|} =$$

$$= sign U \cdot \frac{|e|m^*}{2\pi^2\hbar^3} \exp\left\{-\frac{4}{3}\frac{\sqrt{2m^*}\,w}{\hbar|eU|}W^{3/2}\right\}\mu^2 \int\limits_0^1 (1-E)\, e^{-B\,(1-E)}\, dE.$$

Taking into account the following standard integral

$$\int\limits_0^1 (1-E)\, e^{-B\,(1-E)}\, dE = \frac{1}{B^2} - e^{-B}\frac{(1+B)}{B^2} \simeq \begin{cases} 1/2 - B/3, & B < 1; \\ 1/B^2, & B \gg 1, \end{cases}$$

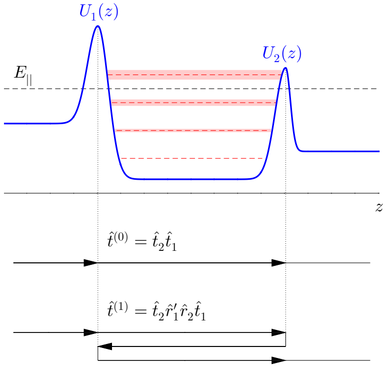
for $B \gtrsim 1$ we come to the Fowler–Nordheim relationship (1926), which describes non-linear dependence of the tunneling current on the bias voltage U

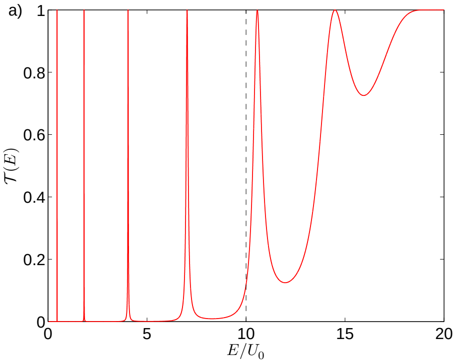
$$j \simeq sign\, U \times \frac{|e|}{16\pi^2\hbar W}\frac{|eU|^2}{w^2} \exp\left(-\frac{4}{3}\frac{\sqrt{2m^*}\,w}{\hbar|eU|}W^{3/2}\right).$$

Fowler–Nordheim plot is the dependence $\ln I$ on U, allowing us to estimate work function

$$\ln I \simeq const + \ln|U|^2 - \frac{4}{3}\frac{\sqrt{2m^*}\,w}{\hbar|eU|}W^{3/2}.$$

Reminder: resonant tunneling in a double-barrier structure



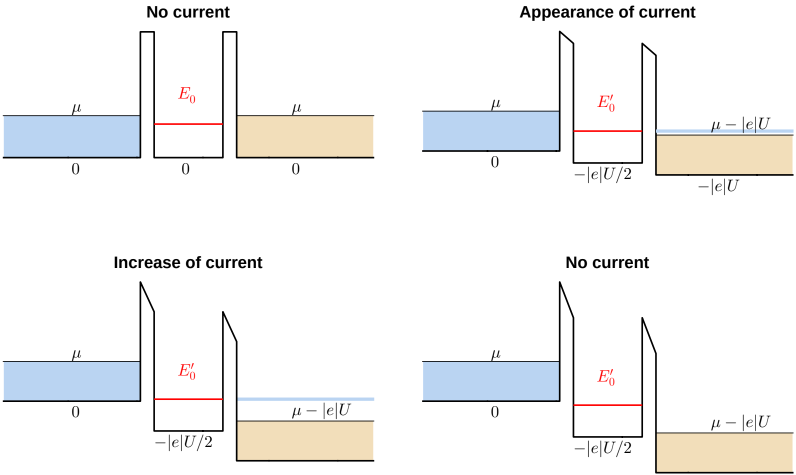


$$t = \frac{t_1 t_2}{1 - r_1' r_2} \quad \text{and} \quad \mathcal{T} = \left|\frac{t_1 t_2}{1 - r_1' r_2}\right|^2 = \frac{\mathcal{T}_1 \mathcal{T}_2}{1 + \mathcal{R}_1\mathcal{R}_2 - 2\sqrt{\mathcal{R}_1\mathcal{R}_2}\cos\left(\arg r_1' + \arg r_2\right)},$$

where $\mathcal{R}_{1,2}$ and $\mathcal{T}_{1,2}$ are coefficients of reflection and transmission through the first and second barriers, correspondingly.

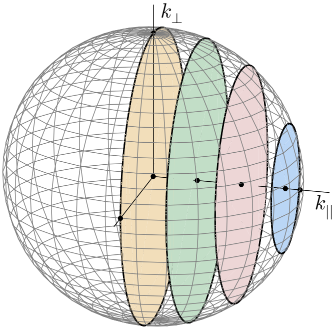
Quantum-size effects in tunneling: resonant-tunneling diode

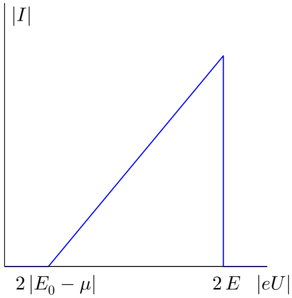
In order to study quantum-size effects in tunneling, we consider double-barrier structure with a single localized level with the energy $E_0 < \mu$:



Criteria for appearance and disappearance of the current:
$E_0 - |e|U/2 > \mu - |e|U$ и $E_0 - |e|U/2 < 0$.

Current-voltage dependence: qualitative arguments





Necessary condition for resonant tunneling in double-barrier structure

$$E_{||} = \frac{\hbar^2 k_{||}^2}{2m^*} = E_0 - \frac{|e|U}{2} \quad \Longrightarrow \quad k_{||} = \frac{\sqrt{2m^*\,(E_0 - |e|U/2)}}{\hbar}$$

Sectional area of Fermi sphere of the radius $k = \sqrt{k_F^2 - k_{||}^2}$ determines the number of resonant electrons

$$S = \pi k^2 = \pi\,\frac{2m^*}{\hbar}\,\left(\mu - E_0 + \frac{|e|U}{2}\right) \quad \text{for} \quad 2|E_0 - \mu| < |eU| < 2E_0.$$

Current-voltage dependence: numerical arguments

Energy spectrum of quasi-two-dimensional gas: $E = \hbar^2 \boldsymbol{k}_\perp^2/2m^* + E_0$.

We use Tsu-Esaki formula to calculate the density of tunneling current in planar structure at low temperatures

$$j \simeq \frac{2e}{2\pi\hbar} \int\limits_{\max\{e(\varphi_R-\varphi_L),0\}}^{\infty} \mathcal{T}(E_\parallel) \cdot \frac{m^*}{2\pi\hbar^2} \cdot k_B\Theta \cdot \ln\left\{\frac{1+e^{-(E_\parallel-\mu-e\varphi_L)/k_B\Theta}}{1+e^{-(E_\parallel-\mu-e\varphi_R]/k_B\Theta}}\right\} dE_\parallel =$$

$$= \frac{em^*}{2\pi^2\hbar^3} \int\limits_0^{\mu} \mathcal{T}(E_\parallel) \cdot (\mu - E_\parallel)\, dE_\parallel .$$

For definiteness we assume $\varphi_L = 0$ and $\varphi_R = U$. The transmission coefficient for double-barrier structure is equal to

$$\mathcal{T}(E_\parallel) \simeq T_{max} \cdot \frac{\Gamma^2}{\Big[E_\parallel - (E_0 - |e|U/2)\Big]^2 + \Gamma^2},$$

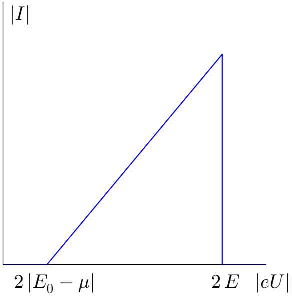
where $\Gamma = \hbar/\tau$ is the linewidth (see lecture 2), τ is the life time of the quasistationary localized state, T_{max} is the maximal transmission of the double-barrier structure, depending on partial transmissions of the left and right barrier.

For particular case of two symmetric and low-transmission barriers ($\Gamma = \hbar/\tau \to 0$ and $T_{max} \to 1$), the Lorentz shape of the dependence $\mathcal{T}(E_{\|})$ can be roughly considered as a narrow rectangle of unit height and width $2\hbar/\tau \to 0$ (in order to keep the integral transmission), positioned at $E_{\|} = E_0 - |e|U/2$, or even as delta-function (formally).

Using mean value theorem for definite integrals, we get

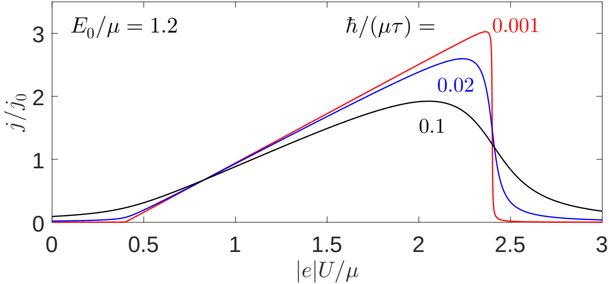
$$j = \frac{em^*}{2\pi^2\hbar^3} \int\limits_0^{\mu} \mathcal{T}(E_{\|})\,(\mu - E_{\|})\,dE_{\|} =$$

$$= \frac{em^*}{2\pi^2\hbar^3} \int\limits_0^{\mu} \frac{2\hbar}{\tau}\,\delta\left(E_{\|} - \left(E_0 - \frac{|e|U}{2}\right)\right)(\mu - E_{\|})\,dE_{\|} = -\frac{e^2 m^*}{2\pi^2\hbar^2\tau}\left\{U - \frac{2(E_0-\mu)}{|e|}\right\}.$$



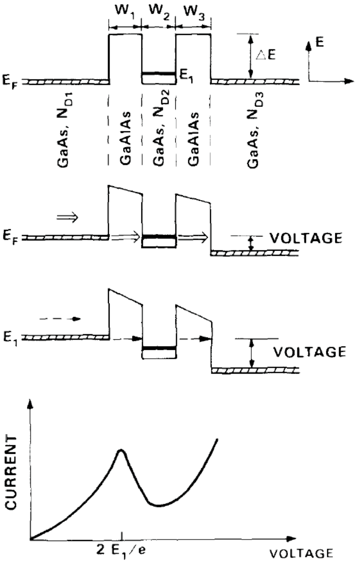
In general case for finite τ one can get the following expression

$$j = \frac{em^*}{2\pi^2\hbar^2\tau}\left\{\left(\mu - E_0 - \frac{eU}{2}\right)\left(\text{arctg}\,\frac{(\mu - E_0 - eU/2)}{\hbar/\tau} + \text{arctg}\,\frac{(E_0 + eU/2)}{\hbar/\tau}\right) - \right.$$
$$\left. - \frac{\hbar}{2\tau}\ln\frac{(\mu - E_0 - eU/2)^2 + \hbar^2/\tau^2}{(E_0 + eU/2)^2 + \hbar^2/\tau^2}\right\}.$$



The voltage interval with negative differential resistance dI/dU points to that such double-barrier structure can be a source of electromagnetic radiation (in THz range).

Resonant tunneling in semiconductor heterostructures



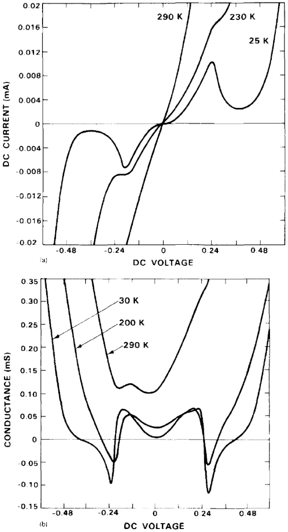
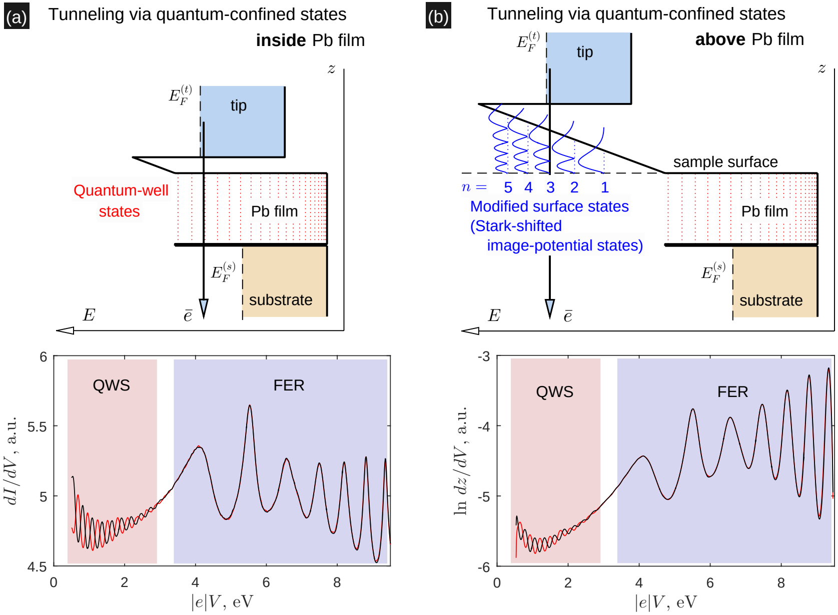


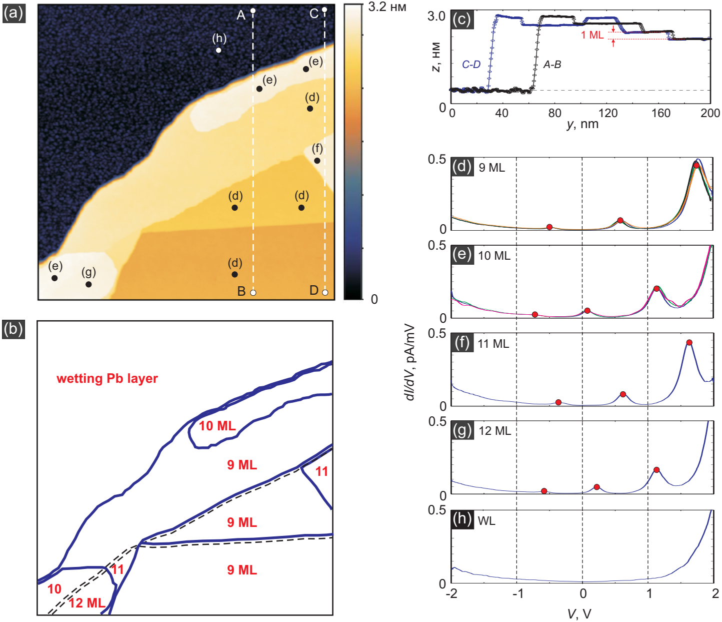
FIG. 2. (a) Current-voltage and (b) conductance (dI/dV)-voltage curves at three temperatures. Notice that resonant tunneling features can be seen even at room temperature.

Sollner, Goodhue, Tannenwald, Parker and Peck, Appl. Phys. Lett., vol. 43, 588-590 (1983)

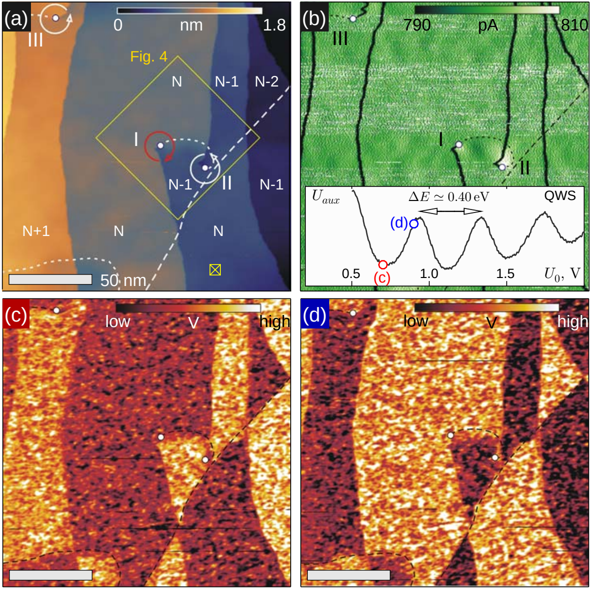
Resonant tunneling in metallic thin films



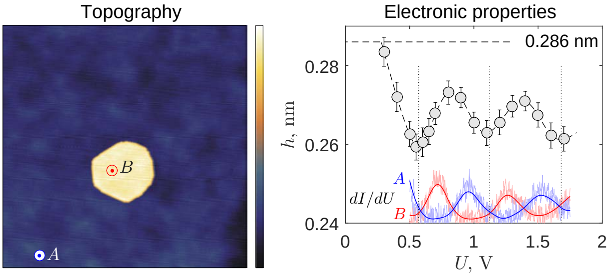
Tunneling interferometry for thin Pb(111) films



Visualization of subsurface defects in thin Pb(111) films



Oscillations of visible height of monatomic Pb(111) step



A. Yu. Aladyshkin, Oscillatory bias dependence of the visible height of the monatomic Pb(111) steps: consequence of the quantum-size effect in thin metallic films // Journal of Physical Chemistry C, vol. 127 (27), pp. 13295–13301 (2023)