

Physics of surfaces and interfaces

2. Scanning tunneling microscopy and spectroscopy. Theoretical description: Approaches of Bardeen and Tersoff & Hamann

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Outline of current lecture

- * Basic principles of scanning tunneling microscopy and spectroscopy
- * Bardeen's approach for calculation of tunneling current
- * Theory of STM: approach of Tersoff and Hamann

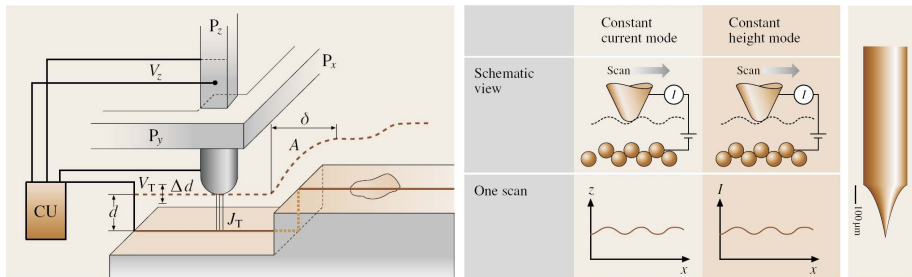
Part I

Basic principles of scanning tunneling microscopy and spectroscopy

Scanning tunneling microscopy (SMT): general scheme

Invention: Binnig & Rohrer (1981), Nobel prize in physics (1986)

This approach is applicable only for conducting samples.



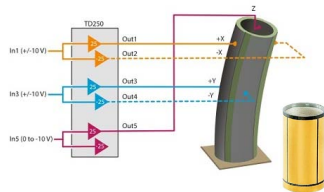
Binnig, Rohrer et al., Phys. Rev. Lett., vol. 49, 57–61 (1982)

Binnig and Rohrer, Surf. Sci. vol. 126, 236–244 (1983)

Chen, *Introduction to scanning tunneling microscopy*. Oxford (1993)

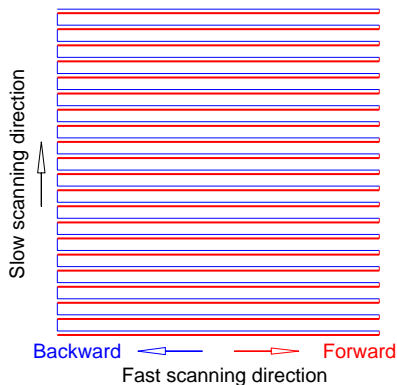
Wiesendanger, *Introduction to scanning probe ...* Cambridge (1994)

Springer Handbook of Nanotechnology (Ed. B. Bhushan, 2010)

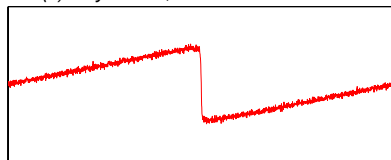


Scanning tunneling microscopy in regime of constant current

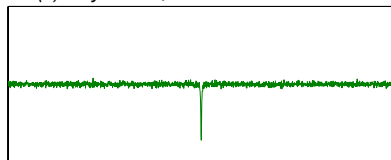
During scanning (i.e. movement of the tip forward-and-backward in the lateral direction), the feedback loop system compares the instant tunneling current I with the set-point value I_0 , defined by an user, and change the distance between the STM tip and the sample surface.



$$z=f(x) @ y=\text{const}, V=\text{const}$$



$$I=f(x) @ y=\text{const}, V=\text{const}$$



Analysis of reconstruction Si(111)7×7

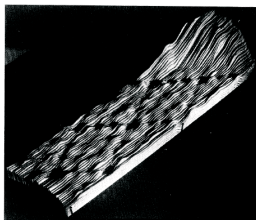
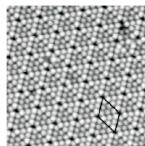
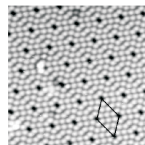
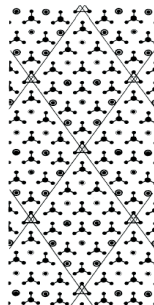
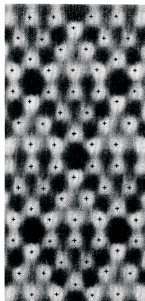
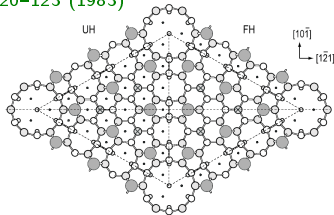


FIG. 1. Relief of two complete 7×7 unit cells, with nine minima and twelve maxima each, taken at 300°C . Heights are enhanced by 55%; the hill at the right grows to a maximal height of 15 \AA . The $[2\bar{1}1]$ direction points from right to left, along the long diagonal.



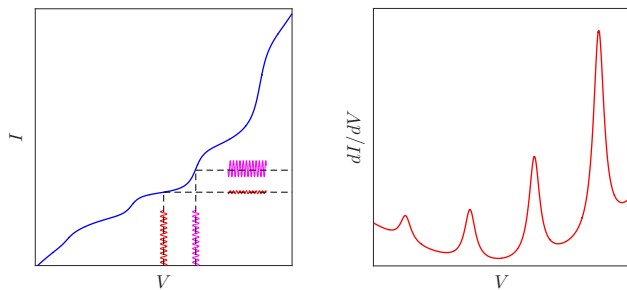
Binnig, Rohrer, Gerber, Weibel, *Phys. Rev. Lett.*, vol. 50, 120–123 (1983)

Oura, Lifshits, Saranin, Zotov, Katayama, *Surface Science: An Introduction*. Springer (2013)



Single-point tunneling spectroscopy

Measurement of local current-voltage ($I - V$) dependence at a fixed position of the STM tip with respect to the sample surface



Modulation technique: $V(t) = V_0 + V_1 \cdot \cos \omega t \implies I(t) = I_0 + I_1 \cdot \cos(\omega t + \gamma)$

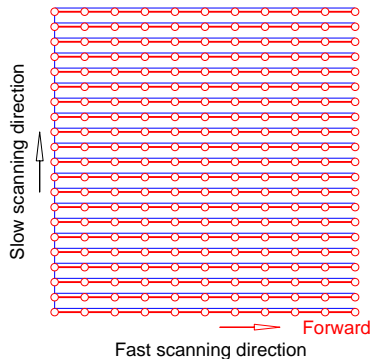
$$I_1 \simeq V_1 \cdot \left(\frac{dI}{dV} \right)_{V_0}$$

Thus, the amplitude of the oscillation of tunneling current measured by a lock-in amplifier is proportional to the differential tunneling conductance dI/dV at given mean bias voltage $V = V_0$.

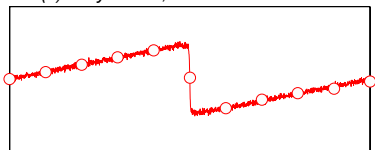
Scanning grid spectroscopy

During scanning process the STM tip periodically stops for the acquiring the local $I - V$ dependences at fixed positions of the STM tip with respect to the sample surface.

Results of measurements: three arrays $z = f(x_n, y_m, V_0)$, $I = f(V, x_n, y_m)$ and $dI/dV = f(V, x_n, y_m)$.

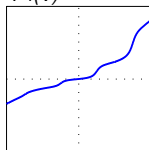


$z=f(x) @ y=\text{const}, V=\text{const}$

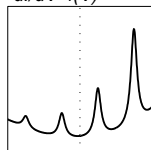


For all points of the grid @ $x, y, z=\text{const}$

$I=f(V)$



$dI/dV=f(V)$

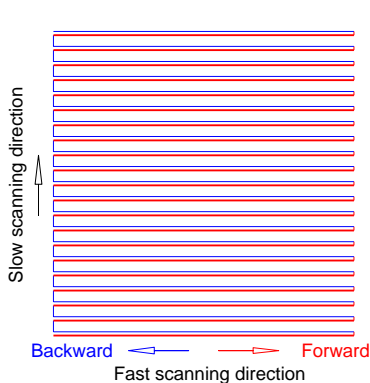


Scanning tunneling microscopy in modulation regime

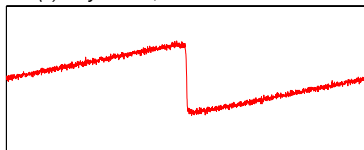
The tip voltage is periodically modulated in time: $V(t) = V_0 + V_1 \cdot \cos \omega t$.

During scanning process the STM tip periodically never stops, while the Control Unit continuously adjust the tip height to keep the tunneling current constant and record the amplitude of the current oscillations, proportional to the local tunneling conductance dI/dV .

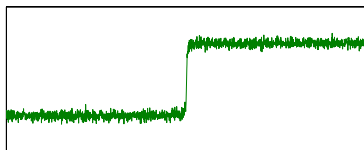
Results of measurements: two arrays $z = f(x, y, V_0)$ and $dI/dV = f(x, y, V_0)$.



$z=f(x) @ y=\text{const}, V=\text{const}$



$dI/dV=f(x) @ y=\text{const}, V=\text{const}$



Part II

Bardeen's approach for calculation of tunneling current

Fermi's golden rule and tunneling current

The rate of quantum transitions (i. e. the number of quantum transition per unit of time) from the initial state i to the final state of discrete spectrum f is essentially constant and it is known to be given by the formula

$$\Gamma_{i \rightarrow f} = \frac{2\pi}{\hbar} |T_{i \rightarrow f}|^2 \delta(E_i - E_f),$$

where $T_{i \rightarrow f}$ is the matrix element of a stationary perturbing Hamiltonian \hat{H}' applied to the system

$$T_{n,m} = \int \Psi_n^*(\mathbf{r}, t) \hat{H}' \Psi_m(\mathbf{r}, t) d\mathbf{r} = e^{-i(E_n - E_m)t/\hbar} \cdot \int \psi_m^*(\mathbf{r}) \hat{H}' \psi_n(\mathbf{r}) d\mathbf{r},$$

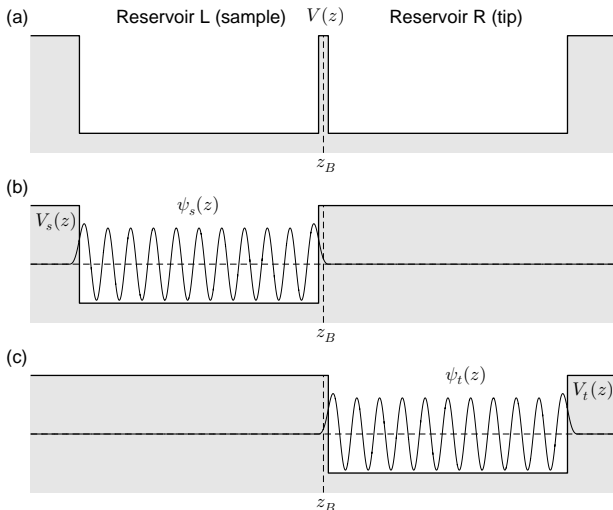
and the delta-function $\delta(E_i - E_f)$ accounts the conservation of energy at quantum transitions.

Recommended methodological notes for educational reading: Emmanuel N. Koukara, *Fermi's Golden Rule*, <http://staff.ustc.edu.cn/~yuanzs/teaching/Fermi-Golden-Rule-No-II.pdf>

Question: How to introduce the tunneling Hamiltonian \hat{H}' in such a way to calculate tunneling current using the Fermi's golden rule $I = e \sum \Gamma_{i,f}$?

Tunneling through low-transmission 1D potential barrier: Bardeen's approach (1)

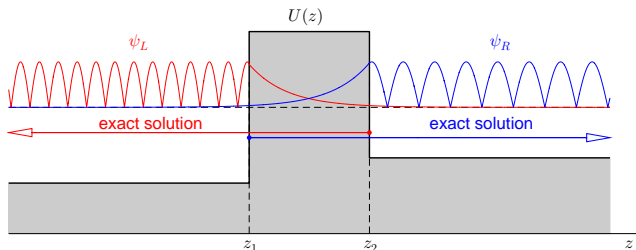
John Bardeen, Nobel prize in physics in 1956 (with Shockley and Brattain for the invention of the transistor) and in 1972 (with Cooper and Schrieffer for microscopic theory of superconductivity)



Tunneling through 1D potential barrier of low-transmission: Bardeen's approach (2)

Bardeen, Phys. Rev. Lett., vol. 6, 57 (1961).

Main idea: the partial wave functions $\psi_{L,n}(z)$ and $\psi_{R,m}(z)$ in a non-interacting system are non-overlapping and thus form the full and orthonormal bases, describing the localization of electrons in the left and right electronic reservoirs, respectively.



Following the Bardeen's idea, we consider the *approximate* wave functions for the electrons in the left and right reservoirs (limit of weakly-interacting subsystems)

$$\psi_{L,n} = \begin{cases} \hat{H}\psi_{L,n} = E_{L,n}\psi_{L,n} & \text{при } z \leq z_2; \\ \text{const} \cdot e^{-\kappa_2 z} & \text{при } z > z_2, \end{cases} \quad \psi_{R,n} = \begin{cases} \text{const} \cdot e^{+\kappa_2 z} & \text{при } z \leq z_1; \\ \hat{H}\psi_{R,n} = E_{R,n}\psi_{R,n} & \text{при } z > z_1, \end{cases}$$

where \hat{H} is the exact Hamiltonian of the problem.

Tunneling through 1D potential barrier of low-transmission: Bardeen's approach (3)

We start with the assumption that the electron at initial moment (at $t = 0$) is in the left reservoir in the state, described by one of the localized functions $\psi_{L,n}(z)$. We estimate a probability for this electron to transfer to one of possible electronic states described by the localized wave function $\psi_{R,m}(z)$ in the right reservoir.

We seek for the solution of time-dependent Schrödinger equation in the form of the linear combination of non-perturbed wave functions

$$\Psi(z, t) = c_n(t) \psi_{L,n}(z) e^{-iE_n t/\hbar} + \sum_{m'} d_{m'}(t) \psi_{R,m'}(z) e^{-iE_{m'} t/\hbar},$$

where E_n и E_m are eigenenergies of the initial and final states.

After substitution of the trial function $\Psi(z, t)$ into the non-stationary Schrödinger equation $i\hbar \partial \Psi / \partial t = \hat{H} \Psi$, we get

$$\begin{aligned} i\hbar \dot{c}_n(t) \psi_{L,n}(z) e^{-iE_n t/\hbar} + \sum_{m'} i\hbar \dot{d}_{m'}(t) \psi_{R,m'}(z) e^{-iE_{m'} t/\hbar} = \\ = c_n(t) e^{-iE_n t/\hbar} (\hat{H} - E_n) \psi_{L,n}(z) + \sum_{m'} d_{m'}(t) e^{-iE_{m'} t/\hbar} (\hat{H} - E_{m'}) \psi_{R,m'}(z) \quad (*), \end{aligned}$$

where $\dot{c}_n(t) \equiv dc_n/dt$.

Tunneling through 1D potential barrier of low-transmission: Bardeen's approach (4)

After multiplying the equation (*) at $\psi_{R,m}^*(z)$ and integration over z , we get

$$\sum_{m'} i\hbar \dot{d}_{m'}(t) \langle \psi_{R,m}^*(z) | \psi_{R,m'}(z) \rangle e^{-iE_{m'}t/\hbar} \simeq c_n(t) e^{-iE_n t/\hbar} \langle \psi_{R,m}^*(z) | (\hat{H} - E_n) \psi_{L,n}(z) \rangle.$$

The expression

$$T_{L \rightarrow R} = \langle \psi_{R,m}^*(z) | (\hat{H} - E_n) \psi_{L,n}(z) \rangle$$

can be viewed as a matrix element of quantum transition for the effective Hamiltonian $\hat{H}' = \hat{H} - E_n$ from the initial state $\psi_{L,n}(z)$ (electron in the left box) to the state $\psi_{R,m}(z)$ (electron in the right box).

Provided that $\psi_{R,m}(z)$ are orthonormal functions, we arrive

$$\sum_{m'} i\hbar \dot{d}_{m'}(t) \delta_{m,m'} e^{-iE_{m'}t/\hbar} = i\hbar \dot{d}_m(t) e^{-iE_{m'}t/\hbar} \simeq c_n(t) e^{-iE_n t/\hbar} T_{L \rightarrow R}.$$

This means that the evolution of the coefficients d_m is similar to the expression typical for quantum-mechanical problems

$$i\hbar \dot{d}_m \simeq e^{-i(E_n - E_m)t/\hbar} \cdot T_{L \rightarrow R}.$$

Tunneling through 1D potential barrier of low-transmission: Bardeen's approach (5)

Thus, the matrix element in the Bardeen's problem is equal to

$$\begin{aligned} T_{L \rightarrow R} &= \langle \psi_{R,m}^*(z) | (\hat{H} - E_n) \psi_{L,n}(z) \rangle = \int_{-\infty}^{\infty} \psi_{R,m}^*(z) (\hat{H} - E_n) \psi_{L,n}(z) dz = \\ &= \int_{z_B}^{\infty} \psi_{R,m}^*(z) (\hat{H} - E_n) \psi_{L,n}(z) dz, \end{aligned}$$

where z_B is an arbitrary point inside the tunneling barrier ($z_1 \leq z_B \leq z_2$).

This expression can be written in a symmetric form

$$T_{L \rightarrow R} = \int_{z_B}^{\infty} \left\{ \psi_{R,m}^*(z) (\hat{H} - E_n) \psi_{L,n}(z) - \psi_{L,n}(z) (\hat{H} - E_m) \psi_{R,m}^*(z) \right\} dz.$$

Taking into account the conservation of the energy at tunneling process ($E_n = E_m$) and after integration by parts, we get a simple expression for the matrix element

$$T_{L \rightarrow R} = -\frac{\hbar^2}{2m^*} \left\{ \psi_{L,n} \frac{d}{dz} \psi_{R,m}^* - \psi_{R,m}^* \frac{d}{dz} \psi_{L,n} \right\}_{z=z_B}$$

Tunneling through 1D potential barrier of low-transmission: Bardeen's approach (6)

The matrix elements for the direct and reverse tunneling processes in 1D case are equal to

$$T_{L \rightarrow R} = -\frac{\hbar^2}{2m^*} \left\{ \psi_{L,n} \frac{d}{dz} \psi_{R,m}^* - \psi_{R,m}^* \frac{d}{dz} \psi_{L,n} \right\}_{z=z_B}$$
$$T_{R \rightarrow L} = -\frac{\hbar^2}{2m^*} \left\{ \psi_{R,m} \frac{d}{dz} \psi_{L,n}^* - \psi_{L,n}^* \frac{d}{dz} \psi_{R,m} \right\}_{z=z_B},$$

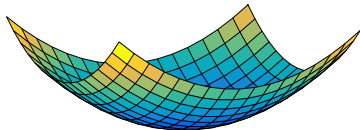
where z_B is the arbitrary point inside the tunneling barrier.

These expressions look like probability flux in quantum mechanics (up to numerical coefficient)

$$j = \frac{i\hbar}{2m^*} \left\{ \psi \frac{d\psi^*}{dz} - \psi^* \frac{d\psi}{dz} \right\}.$$

Generalization for three-dimensional case:

$$T_{L \rightarrow R} = -\frac{\hbar^2}{2m^*} \iint_S \left\{ \psi_{L,n} \nabla \psi_{R,m}^* - \psi_{R,m}^* \nabla \psi_{L,n} \right\}_n \cdot d\mathbf{S},$$



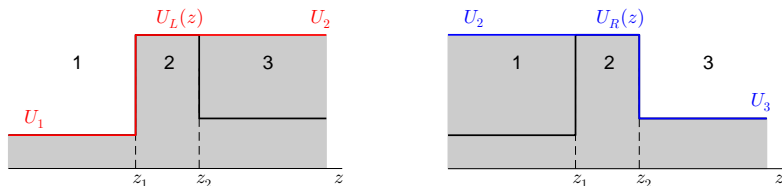
where S is an arbitrary surface inside the barrier, \mathbf{n} is the normal vector.

Homework for inspired students: estimate of the transmission coefficient of 1D square barrier

A model potential has the following form

$$U(z) = \begin{cases} U_1 & \text{at } z < z_1, \\ U_2 & \text{at } z_1 < z < z_2, \\ U_3 & \text{at } z > z_2 \end{cases}$$

The auxiliary potentials for the 'left' and 'right' problems, which can be considered separately



It is possible to demonstrate that the transmission coefficient (do not mix it with the matrix element) are equal to

$$\mathcal{T} = \frac{16k_1\kappa_2^2k_3}{(k_1^2 + \kappa_2^2)(\kappa_2^2 + k_3^2)} e^{-2\kappa_2(z_2 - z_1)}.$$

It perfectly coincides with the exact answer for the transmission coefficient in the limit of low-transmission barrier ($\kappa_2(z_2 - z_1) \rightarrow \infty$).

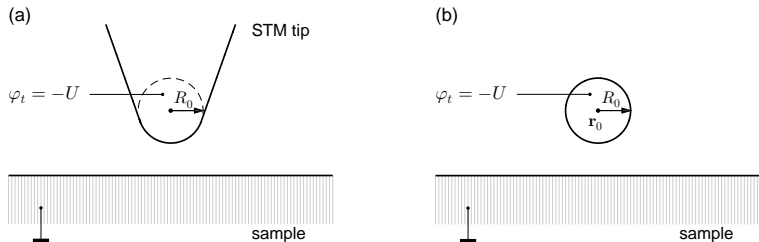
Part III

Theory of STM: approach of Tersoff and Hamann

Problem of Tersoff and Hamann (1)

Tersoff and Hamann, Phys. Rev. Lett. vol. 50, 1998 (1983)

We consider tunneling effect between metallic semi-space with flat surface (at $z < 0$) and metallic tip with an apex of spherical shape of the radius R . For sake of simplicity we assume that the Fermi energies and the work functions are equal: $E_F^{(s)} = E_F^{(t)} = E_F$ and $W_s = W_t = W$.

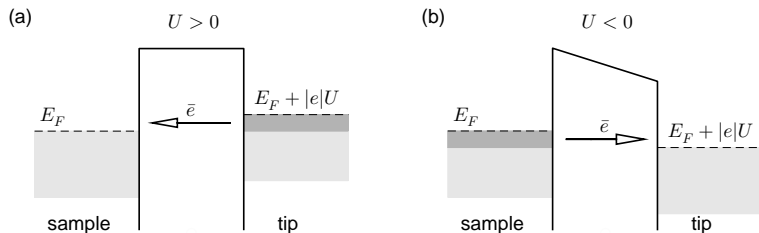


Here U is the potential of the sample with respect to a tip ($\varphi_s = 0$ and $\varphi_t = -U$).

Let $T_{s \rightarrow t}$ be the matrix element, corresponding to the transition of the electron from one of possible states in the sample with wave function ψ_s and energy E_s to one of possible states in the tip with wave function ψ_t and energy E_t .

Problem of Tersoff and Hamann (2)

Band diagram of tunneling contact



If $\varphi_t = -U > 0$, then the electrochemical potential of tip

$$\mu' = E_F + e\varphi_t = E_F + |e|U$$

is larger than that for the sample ($\mu' = E_F$). As a result, tunneling current is associated mainly with quantum transitions from the electronic states in the tip to the *empty* electronic states of the sample.

If $\varphi_t = -U < 0$, then the electrochemical potential of tip is smaller than that for the sample. As a result, tunneling current is associated mainly with quantum transitions from the *filled* electronic states in the sample to the tip.

Problem of Tersoff and Hamann (3)

The rate of the quantum transitions according to the Fermi's golden rule at equal to

$$\Gamma_{s \rightarrow t} = \frac{2\pi}{\hbar} |T_{s \rightarrow t}|^2 \delta(E_s - E_t).$$

Full tunneling current, associated with all possible transitions between the electronic states in the sample and the tip is equal to

$$\begin{aligned} I &= \sum_s \sum_t e \Gamma_{s \rightarrow t} \left\{ f_0(E_s - e\varphi_s) - f_0(E_t - e\varphi_t) \right\} = \\ &= -\frac{2\pi|e|}{\hbar} \sum_s \sum_t |T_{s \rightarrow t}|^2 \left\{ f_0(E_s) - f_0(E_t - |e|U) \right\} \delta(E_s - E_t), \end{aligned}$$

where $\varphi_s = 0$ и $\varphi_t = -U$ are the electrical potentials of the sample and the tip; the difference $\{f_0(E_s) - f_0(E_t - |e|U)\}$ accounts the disbalance between the occupied states in the sample and empty states in the tip at $U > 0$, and

$$f_0(E) = \left(1 + e^{(E-E_F)/k_B\Theta} \right)^{-1}$$

is the equilibrium Fermi-Dirac statistical distribution for particles with half-integer spin, and Θ is the absolute temperature.

Problem of Tersoff and Hamann (4)

We introduce the differential conductance dI/dU of the tunneling contact

$$\frac{dI}{dU} = -\frac{2\pi|e|}{\hbar} \sum_s \sum_t |T_{s \rightarrow t}|^2 \left(-\frac{d}{dU} f_0(E_t - |e|U) \right) \delta(E_s - E_t).$$

It is obvious, that at $k_B\Theta \ll E_F$ and $k_B\Theta \ll |eU|$ (Θ is the absolute temperature)

$$\begin{aligned} \frac{d}{dU} f_0(E_t - |e|U) &= \frac{|e|}{k_B\Theta} \frac{e^{(E_t - |e|U - E_F)/k_B\Theta}}{(1 + e^{(E_t - |e|U - E_F)/k_B\Theta})^2} = \\ &= \frac{|e|}{4k_B\Theta} ch^{-2} \left(\frac{E_t - |e|U - E_F}{2k_B\Theta} \right) \simeq |e| \delta(E_t - (E_F + |e|U)). \end{aligned}$$

Thus, at low temperatures the differential tunneling conductance is equal to

$$\frac{dI}{dU} = \frac{2\pi|e|^2}{\hbar} \sum_s \sum_t |T_{s \rightarrow t}|^2 \delta(E_s - (E_F + |e|U)) \delta(E_t - (E_F + |e|U)).$$

For further simplification one should consider the analytical expression for the matrix element $T_{s \rightarrow t}$.

Wave functions of electrons near the sample and the tip (1)

Reminder: the matrix element of tunneling transition is equal to

$$T_{s \rightarrow t} = -\frac{\hbar^2}{2m^*} \left\{ \psi_s(\mathbf{r}) \frac{\partial}{\partial n} \psi_t^*(\mathbf{r}) - \psi_t^*(\mathbf{r}) \frac{\partial}{\partial n} \psi_s(\mathbf{r}) \right\}_{\text{inside barrier}},$$

therefore we need to know the non-perturbed wave functions $\psi_s(\mathbf{r})$ and $\psi_t(\mathbf{r})$ inside the tunneling barrier.

Stationary wave functions of electrons in the sample $\psi_s(\mathbf{r})$ and near the tip $\psi_t(\mathbf{r})$ meet 3D stationary Schrödinger equation

$$-\frac{\hbar^2}{2m} \Delta \psi(\mathbf{r}) + V(\mathbf{r}) \psi(\mathbf{r}) = E \psi(\mathbf{r}), \quad (*)$$

where $V(\mathbf{r})$ is the potential energy, equal to $E_F + W$ outside the sample and the tip.

At low temperatures the main flux of particles is associated with electrons of the highest energy: $E_t \simeq E_F$ and $E_s \simeq E_F$, since the transmission of the tunneling barrier for such electrons is minimal. As a result, the Schrödinger equation (*) for $E_t \simeq E_F$ and $E_s \simeq E_F$ is reduced to the following form

$$\Delta \psi_s(\mathbf{r}) - \varkappa^2 \psi_s(\mathbf{r}) = 0 \quad \text{и} \quad \Delta \psi_t(\mathbf{r}) - \varkappa^2 \psi_t(\mathbf{r}) = 0,$$

where $\varkappa = \sqrt{2m_0 W} / \hbar$ is the inverse radius of the localization of both wave functions.

Wave functions of electrons near the sample and the tip (2)

The wave functions $\psi_t(\mathbf{r})$ outside the tip ($\rho > R_0$) meet the equation

$$\Delta\psi_t(\mathbf{r}) - \kappa^2\psi_t(\mathbf{r}) = 0 \quad \text{or}$$
$$\frac{1}{\rho^2} \frac{\partial}{\partial \rho} \left(\rho^2 \frac{\partial \psi_t}{\partial \rho} \right) + \frac{1}{\rho^2} \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi_t}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 \psi_t}{\partial \varphi^2} \right] - \kappa^2 \psi_t = 0,$$

where (ρ, θ, φ) is the spherical coordinate system with the origin at the center of curvature of the tip.

The wave function of electrons $\psi_t(\mathbf{r})$ near the metallic sphere can be expanded into a series of spherical functions

$$\psi_t(\rho, \theta, \varphi) = \sum_{\ell, m} C_{\ell, m} R_{\ell}(\kappa\rho) Y_{\ell, m}(\theta, \varphi),$$

where $C_{\ell m}$ are coefficients; ℓ is the quantum number characterizing orbital momentum; and m is the magnetic quantum number characterizing a projection of the orbital momentum at the z -axis.

For the radial part of the wave function of the electron near the tip we get the equation

$$\frac{1}{\rho^2} \frac{d}{d\rho} \left(\rho^2 \frac{d}{d\rho} R_{\ell}(\kappa\rho) \right) - \frac{\ell(\ell+1)}{\rho^2} R_{\ell}(\kappa\rho) + \kappa^2 R_{\ell}(\kappa\rho) = 0.$$

Effect of s -orbital to the tunneling conductance (1)

The first term in the expansion, corresponding to the s -state and $\ell = 0$, gives us

$$\psi_t^{(s)}(x, y, z) = C \frac{e^{-\varkappa|r-r_0|}}{\varkappa|r-r_0|},$$

where \mathbf{r}_0 is the radius-vector from the origin to the center of the spherical apex. We assume that the constant C makes the wave function normalized with respect to available volume.

It should be emphasized that the wave function $\psi_t^{(s)}(x, y, z)$ can be written via the Green function $G(\mathbf{r} - \mathbf{r}_0)$

$$\psi_t^{(s)}(x, y, z) = \frac{4\pi C}{\varkappa} G(\mathbf{r} - \mathbf{r}_0) \quad \text{and} \quad G(\mathbf{r} - \mathbf{r}_0) = \frac{e^{-\varkappa|r-r_0|}}{4\pi|r-r_0|}.$$

where $G(\mathbf{r} - \mathbf{r}_0)$ is the singular solution of the Schrödinger (Helmholtz-like) equation

$$-\Delta G(\mathbf{r} - \mathbf{r}_0) + \varkappa^2 G(\mathbf{r} - \mathbf{r}_0) = \delta(\mathbf{r} - \mathbf{r}_0).$$

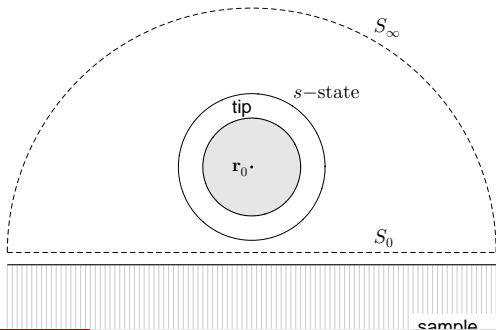
Reminder: the second Green theorem is

$$\oint_S \left\{ u \frac{\partial v}{\partial n} - v \frac{\partial u}{\partial n} \right\} dS = \int_V \{ u \Delta v - v \Delta u \} dV.$$

Effect of s -orbital to the tunneling conductance (2)

We consider a surface S_0 lying between the sample and the tip and a surface of infinite radius S_∞ . Since both ψ_s and ψ_t are exponentially decay at the increase of the distance from the corresponding surfaces, the surface integral over to S_∞ is equal to zero

$$\begin{aligned} T_{s \rightarrow t}^{(s)} &= -\frac{\hbar^2}{2m^*} \int_{S_0 + S_\infty} \left\{ \psi_t^{(s)} \frac{\partial \psi_s}{\partial n} - \psi_s \frac{\partial \psi_t^{(s)}}{\partial n} \right\} dS = \\ &= -\frac{\hbar^2}{2m} \iiint_{z>0} \left\{ \psi_t^{(s)} \nabla^2 \psi_s - \psi_s \nabla^2 \psi_t^{(s)} \right\} dV. \end{aligned}$$



Effect of s -orbital to the tunneling conductance (3)

Taking into account that $\nabla^2\psi_s = \varkappa^2\psi_s$, $\nabla^2\psi_t^{(s)} = \varkappa^2\psi_t^{(s)} - 4\pi C\varkappa^{-1}\delta(\mathbf{r} - \mathbf{r}_0)$, and $\psi_t^{(s)*} = \psi_t^{(s)}$, we come to the important result

$$\begin{aligned} T_{s \rightarrow t}^{(s)} &= -\frac{\hbar^2}{2m^*} \int_{z>0} \left\{ \psi_t^{(s)} \varkappa^2 \psi_s - \psi_s \varkappa^2 \psi_t^{(s)} + \psi_s \frac{4\pi C}{\varkappa} \delta(\mathbf{r} - \mathbf{r}_0) \right\} dV = \\ &= -\frac{\hbar^2}{2m^*} \int_{z>0} \psi_s(\mathbf{r}) \frac{4\pi C}{\varkappa} \delta(\mathbf{r} - \mathbf{r}_0) dV = -\frac{\hbar^2}{2m^*} \frac{4\pi C}{\varkappa} \cdot \psi_s(\mathbf{r}_0). \end{aligned}$$

Intermediate conclusion: the matrix element of the tunneling transition is proportional to the wave function of the electron of the sample in the center of the tip provided that the dominant contribution is associated with the s -wave orbitals of the electrons near the tip apex.

As a result, the square of the absolute value of the matrix element is proportional to the probability to detect the electron of the sample in the center of the tip

$$\left| T_{s \rightarrow t}^{(s)} \right|^2 = \left(\frac{\hbar^2}{2m^*} \right)^2 \left(\frac{4\pi}{\varkappa} \right)^2 |C|^2 \cdot |\psi_s(\mathbf{r}_0)|^2.$$