Field-emission current from quantum system

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Abstract. A universal semiclassical approach is developed to calculate an emission current from a quantum system (atom, ion, metal cluster, metal surface, graphene ribbon, etc.) in a stationary electric field. The same expression is in use for a spherical emitter (atom, negative ion, metal cluster) and a plane metal surface. It is shown the results agree with those of other methods.

1. Introduction
The interest in the field-emission from a quantum system has quickened because of a new nano-dimension objects (metal cluster, graphene, nanotubes and so on) appearance, the geometry of the systems being various. The semiclassical approach is used to calculate the emission current from the spherical atom and ion [1]. In the paper we attempt to construct an universal field-emission current expression [2] for a various emitter geometry and to verify it by solving the well-known problems and comparing the results with those of other methods.

It’s assumed that the emitter electron with an energy $E_{em}$ is tunneling through a wide barrier

$$l \gg h/\sqrt{2mE_{em}}$$

2. Semiclassical approach
Semiclassical expression for the tunneling current is derived using the semiclassical 3D wave function [3]

$$\Psi(r) = \Psi_0(r_0) \left| \frac{p_0(r_0)}{p(r)} \right|^{1/2} \exp \left( \frac{i}{\hbar} S(r_0, r) - \frac{1}{2} \int_{r_0}^{r} dl \text{div} \mathbf{e} \right)$$

Here the points $r_0$ and $r$ belong to the same trajectory of the particle motion with the boundary conditions $r = r_0, p = p_0(r_0)$, $dl$ is an arc element along the trajectory, $p(r) = \nabla S(r)$ is a momentum, $S(r_0, r) = \int_{r_0}^{r} dl \text{p}$ is a classical action, $\mathbf{e} = p/p$ is an unit momentum vector, $p(r) = \sqrt{2m(E - U(r))}$ is an absolute value of the momentum vector, $E$ and $U(r)$ are the electron total and potential energies. Generally there is a sum of a few waves in the right part of Eq.(2). In the case $\Psi_0$ is the partial wave function, which phase gradient is equal to the initial momentum vector $p_0(r_0)$.

The corresponding current

$$j(r) = \frac{1}{m} \mathbf{e}(r)|p_0(r_0)||\Psi_0(r_0)|^2 \exp \left( \int_{r_0}^{r} dl \text{div} \mathbf{e} \right)$$

satisfies a continuity equation $\text{div} j = 0$ in the classical permitted region.
The tunneling probability in a unit time is equal to \( w = \int_{\Sigma} ds \mathbf{j}(r) \). Here \( \Sigma \) is the surface that embraces the barrier region. Every point \( r \) of the surface \( \Sigma \) has the initial point \( r_0 \) along the same trajectory. Whole of these points forms a surface \( \Sigma_0 \) which we set inside the barrier region far away from the inner barrier surface to use the WKB approximation of an electron wave function. The surface \( \Sigma_0 \) is also assumed to be far from the outer barrier surface to minimize the outer field effect. To satisfy these demands one needs a wide barrier that agrees with the condition Eq.(1).

In this case the action in Eq.(2) is equal to \( S(r_0, r) = i \text{Im} S(r_0, r_{ex}) + S(r_{ex}, r) \) with \( r_{ex} \) being the barrier exit point. Here the imaginary unit is connected with an absolute value of the momentum vector. The current vector is then given by

\[
\mathbf{j}(r) = \frac{1}{m} e(r) |\mathbf{p}_0(r_0)||\Psi_0(r_0)|^2 \exp \left( \int_{r_0}^{r} dl \text{div} \mathbf{e} - \frac{2}{\hbar} \text{Im} S(r_0, r_{ex}) \right). \tag{4}
\]

The current Eq.(4) outside the barrier satisfies a continuity equation too. It is evident from the equations \( dr_0/dl = dr_{ex}/dl = 0 \) for the same trajectory.

One can prove that the Eq.(4) describes a permanent quantity when the point \( r \) being into the barrier region and the magnitude \( \text{Im} S(r_0, r_{ex}) \) relating to the points \( r_0, r_{ex} \) as before. It is because of the same trajectory connects the points \( r_0, r, r_{ex} \) with each other regardless of their order. The Eq.(4) in this case doesn’t of course coincide with a true current.

Using the conservation of the quantity Eq.(4) one can replace the surface \( \Sigma \) to superpose the whole of these points forms a surface \( \Sigma_0 \). The action in Eq.(2) is equal to

\[
I = 2e \sum_{em} w_{em} f(E_{em}) = 2e \sum_{em} f(E_{em}) \int_{\Sigma_0} ds \mathbf{j}(r_0) \exp \left( -\frac{2}{\hbar} \text{Im} S(r_0, r_{ex}) \right). \tag{5}
\]

with the Fermi distribution function \( f(E) = (1 + e^{(E-\mu)/T})^{-1} \), where \( \mu \) is a chemical potential. Here \( \mathbf{j}(r_0) \) looks like the field-free current \( \mathbf{j}(r_0) = e(r_0)|\mathbf{p}_0(r_0)||\Psi_0(r_0)|^2/m_e \).

4. Tunneling probability from a spherical system

Let us calculate the tunneling probability from the electron bound \( E, l, m \)-state in a radial symmetric system in an outer electric field \( \mathbf{F}(z) \parallel z \) axis \((\mathbf{F}(z) = F(z)\mathbf{k})\) within the semiclassical theory Eq.(5). We have no need to know a specific view of the inner field. One assumes only that the outer field is small in comparison with the inner field inside and nearby the emitter.

It is evident that only a little surface environment of \( z \) axis gives a main contribution to the integral in the Eq.(5), that is a region of small angles \( \theta \ll 1 \). One can prove that in this case the WKB approximation of the angular part of the wave function \( \Psi_0(r) = R_{El}(r)Y_{lm}(\theta, \varphi) \) is right for the small values \( l, m \) too and write

\[
Y_{lm}(\theta, \varphi) = A_{lm} e^{im\varphi}, \quad |A_{lm}| = \frac{1}{2|m||m|! \sqrt{2l + 1}} \frac{(l + |m|)!}{4\pi (l - |m|)!}.
\]

Furthermore the small values \( \theta \) mean approximately \( \mathbf{j}(r_0) \parallel r_0 \).

Let us divide action in the Eq.(5) into two parts

\[
S(r_0, r_{exit}) = \int_{r_0}^{r} dl \mathbf{p} = \int_{z_0}^{z_{exit}} dz p_z + \int_{r_{exit \perp}}^{r_0 \perp} dr \perp p_\perp, \tag{6}
\]

where

\[
p_z = \sqrt{p^2(r) - p_\perp^2}, \quad dr \perp = \frac{1}{m_e} p_\perp dt, \quad p_\perp = p \sin \theta.
\]
Because of assumed smallness of the inner field in the barrier region \( \mathbf{p}_\perp \approx \mathbf{p}_{0\perp} \). So the second term in the Eq.(6) is equal to the value \( p^2_{0\perp} \tau_E(F) \), where

\[
\tau_E(F) = \int_{z_0}^{z_{\text{ex}}} \frac{dz}{|p_z(\theta = 0)|} \tag{7}
\]
is the time of the motion between the points \( z_0 \) and \( z_{\text{ex}} \) that is equal to the time of the motion between the points \( \mathbf{r}_{0\perp} \) and \( \mathbf{r}_{\text{ex}\perp} \).

After accounting for a small value \( p_{0\perp} = p_0 \theta \) in the Eq.(6) we have the following expressions for the action

\[
S(\mathbf{r}_0, \mathbf{r}_{\text{ex}}) = i\sigma_E(F) + i\frac{|p_0|^2 \tau_E(F)}{2} \theta^2, \tag{8}
\]

\[
\sigma_E(F) = \int_{z_0}^{z_{\text{ex}}} dz |p_\perp(\theta = 0)|. 
\]

Here the quantities \( \sigma_E(F) \), \( \tau_E(F) \) depend on the particle energy \( E \) and outer field \( F \).

After integration over \( \theta \) the tunneling probability is given by

\[
w(E; l, m) = \pi r_0^2 R_{\text{El}}^2(\mathbf{r}_0) |m|! |A_{lm}|^2 \frac{p_{0\perp}}{m_e} \times \exp(-2\sigma_E(F)/\hbar) \left( \frac{p_{0\perp}^2 \tau_E(F)/\hbar}{|p_{0\perp}^2 \tau_E(F)/\hbar|^{m+1}} \right) \tag{9}
\]

If the sum of fields in the point \( \mathbf{r}_0 \) are small one can write

\[
|p_{0\perp}(\mathbf{r}_0)| \approx p_E = \sqrt{2m_e|E|}.
\]

Let us use the common expression Eq.(9) to calculate the ionization probability of the atom or negative ion by the uniform electric field \( F \). An asymptotic form of the radial function is then given by

\[
R_{\text{El}}(\mathbf{r}_0) = C_{\text{El}} p_{\perp}^{3/2}(p_E r_0/\hbar)^{\lambda-1} \exp(-p_E r_0/\hbar). \tag{10}
\]

Here \( C_{\text{El}} \) is a numeral coefficient, \( \lambda = m_e \alpha/(\hbar p_E) \), \( U(r \to \infty) = -\alpha/r \). For the short-range potential (negative ion) \( \alpha = 0 \). The condition Eq.(1) holds true under \( \hbar m_e F \ll p_{\perp}^2 \). As a result of the integration in Eqs.(7),(8) and substitution into Eq.(9) we easily get a well-known expression [1] (in the atomic units)

\[
w(E; l, m) = |C_{\text{El}}|^{3/2} \left( \frac{2m_e}{\hbar} \right)^{l+1} \left( \frac{l+|m|}{l-|m|} \right)! \exp \left( \frac{2p_{\perp}^2}{p_{\perp}^2} \right)^{2\lambda-|m|-1} \left( \frac{2p_{\perp}^2}{p_E} \right) \times \exp \left( \frac{2p_{\perp}^2}{3F} \right) \tag{10}\]

5. Field-emission current from a metal planar surface

The Bardeen transfer Hamiltonian (BTH) method [4] and jellium model have been used in the paper [5] to calculate the field-emission current from a metal surface at the temperature \( T = 0 \). Let us derive the corresponding expression within the semiclassical approach Eq.(5) and compare the results.

Assuming that the jellium surface normal and the electron emission direction are along the \( z \) axis \( (\mathbf{F}(z) \parallel z \text{ axis}) \), the wave function \( \Psi_0(\mathbf{r}) \) can be written as

\[
\Psi_0(\mathbf{r}) = \psi_n(z) e^{i\mathbf{k}_\perp \cdot \mathbf{r}_\perp},
\]

where \( \mathbf{r}_\perp, \mathbf{k}_\perp \) are the vectors normal to \( z \) direction. The eigenvalues \( E \) may be written as

\[
E_n(k_\perp) = \varepsilon_n + \frac{\hbar^2}{2m_e} k^2_\perp.
\]
Here ε_n are a “normal” energy spectrum. In this case a surface Σ_0 in Eq.(5) is the plane z = z_0.

Let us calculate the current through the cross-sectional area σ of this plane

\[ I = 2e \sigma \sum_n \int \frac{dk}{4\pi^2} \theta(E_F - E_n(k)) \ j_n(z_0) \ \exp \left( -\frac{2}{\hbar} \text{Im} S_n[z_0, z_{ex}] \right) \]  

(11)

The integration over k is expressed as \( (E_F - \varepsilon_n)/(2\pi\hbar^2) \).

Using the semiclassical asymptotic form for \( \psi_n(z) \) in the barrier region we have a following expression for the current at point \( z_0 \)

\[ j_n(z_0) = \frac{|C_n|^2}{4m_e} \ \exp \left( -\frac{2}{\hbar} \text{Im} S_n[z_n, z_0] \right), \]

where \( z_n \) is the inner turning point.

The expression for the field-emission current density \( J = I/\sigma \) is then given by the same equation as in the paper [5]

\[ J = \frac{e}{4\pi\hbar^2} \sum_n (E_F - \varepsilon_n)|C_n|^2 \times \exp \left( -\frac{2}{\hbar} \int_{z_n}^{z_{ex}} dz' |p_n(z')| \right), \ |p_n(z)| = \sqrt{2m(\varepsilon_n - U(z))}. \]  

(12)

6. About effective potential in the barrier region One needs to know an effective potential \( U(\mathbf{r}) \) in the barrier region to calculate an action \( S(r_0, r_e) \) in Eq.(5). If an emitter is considered to be a conducting system (that is right for a metal surface in the section 5, for a metal cluster when using Eq.(9) and so on) it is necessary to account for an image potential in addition to the sum of inner and outer potentials. Let us cite here some image potentials for a various emitter geometry [6].

The classical image potentials at a distance \( z \) of the conductive sphere of radii \( R \) and metal surface are correspondingly given by \( U_{sph}(z) = -eR/(2z^2 - R^2) \), \( U_{surf}(z) = -e/4z \). The interaction energy of the charge \( e \) with the conductive half plane \( z = 0, \ x < 0 \), that may be a model of a wide graphene ribbon, is equal to

\[ U_{h-pd}(x, z) = \frac{e^2}{4\pi} \left[ \frac{1}{\sqrt{x^2 + z^2}} + \frac{1}{z} \arcsin \frac{z}{\sqrt{x^2 + z^2}} \right]. \]  

(13)

Here \( x \) is the distance of the ribbon edge and \( z \) is the perpendicular distance from the ribbon plane.

7. Conclusion We have developed the common semiclassical approach to calculate the field-emission current from quantum systems with a various geometry provided that a barrier is wide and the outer field doesn’t distort the eigenstates of the emitter. The method requires the knowledge of the free-field emitter electron energy spectrum and WKB wave functions on some surface in the barrier region and effective potential in the region between this surface and barrier exit surface.

We have solved two known problems to verify the method.

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