Exchange-assisted tunneling in the classical limit

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Abstract - The exchange interaction and correlations may produce a power law decay instead of the usual exponential decrease of the wave function under potential barrier. The exchange-assisted tunneling vanishes in the classical limit, however, the dependence on the Planck constant \( \hbar \) is different from that for a conventional single-particle tunneling.

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Introduction. – The Hartree-Fock method usually provides a very good zero approximation for many-body problems. Comparisons with “exact” solutions in light atoms show that the corrections to the Hartree-Fock results typically are not very large and may be taken into account using many-body perturbation theory methods (see, e.g., ref. [1] and references therein).

In the Hartree-Fock equations the exchange interaction is described by the non-local (integration) operator \( K(r) \), and the well-known theorems proven for the Schroedinger equation with a local potential \( U(r) \) are violated if we add the exchange term (or any other non-local operator). The Hartree-Fock equation for a fermion (e.g., bound atomic electron) at orbital \( \Psi_b(r) \) has the following form:

\[
-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} \Psi_b(r) + (U(r) - E) \Psi_b(r) = K(r),
\]

(1)

\[
K(r) = \sum_q \Psi_q(r) \int \Psi_q(r') \frac{e^2}{|r - r'|} \Psi_b(r') dr'.
\]

(2)

Here the summation runs over all occupied orbitals \( \Psi_q(r) \) with the same spin projection as \( \Psi(r) \). The range of \( K(r) \) is determined by the range of the highest orbitals \( \Psi_q(r) \) which stay outside the integral in eq. (2). If \( \Psi_q(r) \) belongs to continuum (like an electron state in a conducting band in a crystal), the range is infinite. In this case the range of the bound electron solution of eq. (1) (e.g., atomic 1s orbital) is also infinite since \( \Psi_b(r) \) cannot vanish if the right-hand side of eq. (1) is not zero.

According to [2,3] (see also [4–6]) the exchange can produce a power law decay instead of the usual exponential decrease in a classically forbidden region. For inner orbitals inside molecules decay is \( r^{-2} \) [2], for macroscopic systems \( \cos(k_f r)r^{-\nu} \), where \( k_f \) is the Fermi momentum and \( \nu = 3 \) for 1D, \( \nu = 3.5 \) for 2D and \( \nu = 4 \) for 3D crystal [2,3]. Correlation corrections within the perturbation theory approach do not change these conclusions [3,4]. Slow decay increases the spin-spin interaction between localized spins in solids and the under-barrier tunneling amplitudes. According to Amusia ref. [7], the exchange interaction may increase the probability of ionization of inner atomic electrons by an external electric field by many orders of magnitude. Amusia claimed that this enhancement may explain experimentally observed enhancement of multielectron ionization by a strong laser field, see, e.g., refs. [8,9] (a different enhancement mechanism, an “atomic antenna”, was suggested by Kuchiev [10] and rediscovered by Corkum [11]).

In this paper we want to consider the problem in the classical limit \( \hbar \to 0 \). In the case of a single-particle problem a wave function under the potential barrier is exponentially small, \( \Psi \sim \exp(-\int |p|dr/\hbar) \), i.e. the probability of the tunneling tends to the classical result (zero) very fast, it contains \( \exp(-1/\hbar) \). Here \( |p| = \sqrt{2m(U(r) - E)} \) is the semiclassical under-barrier momentum. At first glance, one may say that the exchange interaction does not exist in the classical physics, therefore, the probability of the exchange-assisted tunneling should also rapidly vanish. Moreover, any effects of identity of particles (Fermi and Bose statistics) should vanish when the wavelength \( \lambda = \hbar/p \) tends to zero. However, the answer may be not as simple as it looks. For example, let us consider a two-electron problem.

A homogeneous electric field is applied to a hydrogen atom where the electron energy is \( E_b \). If the field is not too strong, the probability of the tunneling to the state
of the same energy $E_b$ in continuum outside the atom is practically zero.

Then another electron with energy $E_c$ (above the barrier) hits the atomic electron, loses energy $E_c - E_b$ and occupies the state with energy $E_b$ (equal to the energy of the bound electron) in continuum outside the atom.

The lost energy $E_c - E_b$ is transferred to the bound electron which gets enough energy ($E_c$) to pass the barrier. Both electrons are free and have the same energies $E_b$ and $E_c$.

This process imitates the “tunneling” of a particle with the energy $E_b$ (for non-identical particles one more collision with the reverse energy exchange is needed to imitate the “tunneling”). This picture looks like a purely classical one. Therefore, it is not obvious why the exchange-assisted tunneling must vanish for $h \to 0$.

A related question: if this effect vanishes, is the law exponential (similar to the vanishing of the single-particle tunneling), or does it vanish less rapidly?

**Two-well potential.** – To answer these questions it is instructive to consider a simple model with a minimal number of discrete states involved (to avoid interference of different contributions during summation and integration over spectrum which may change the law of $h$ dependence; this happens for the dependence on distance $r$ [3]).

We start from a model of resonance tunneling from one potential well to another potential well. The case of symmetric double-well potential has been solved, e.g., in the textbook [12]. There are two levels corresponding to the symmetric (ground state) and antisymmetric wave functions. The tunneling produces the splitting of these levels, $E_{\pm} = E_1 \mp t_1$ where $t_1 \sim \exp(-\int |p|dr/h)$ is the tunneling amplitude, and the integral is taken between the classical turning points.

If the first potential well (“$L$”) is slightly deeper than the second potential well (“$R$”), the ground-state wave function may be represented as $\psi_g = \psi_{1L} + B_{11}\psi_{1R}$, where $B_{11} \sim t_1/(E_{1L} - E_{1R})$. Here we assume that the distance to other levels is large, $t_1 \ll (E_{1L} - E_{1R})$ and the probability of the particle in the ground state to be in the well $R$ is exponentially small (proportional to the squared tunneling amplitude, $B_{11}^2 \sim t_1^2/(E_{1L} - E_{1R})^2$).

Now we add a second particle (identical fermion or boson) to a higher state $2$ which has energy close to the top of the barrier. We can present its wave function as $\psi_2 = A_2\psi_{2L} + B_2\psi_{2R}$, where the coefficient $B_2$ is not necessarily small. In this case the probability of the particle in the ground orbital to be in the potential well $R$ is no longer proportional to the exponentially small parameter $t_1^2$. Indeed, the following two-step process takes place.

**Step 1:** the second particle tunnels from the potential well $L$ (orbital $\psi_{1L}$) to the potential well $R$ (orbital $\psi_{2R}$).

**Step 2:** two-body process $2R, 1L \to 1R, 2L$ due to a nondiagonal Coulomb exchange interaction which transfers the first particle from orbital $1L$ to the orbital $2L$ and the second particle from $2R$ to $1R$.

As a result of these two steps, we have no change in the occupation of the state 2 and transfer of a particle from the ground state $1L$ to $1R$. This gives the amplitude for the ground state particle to be in the well “$R$”:

$$B_{G1} \sim \frac{G(2, 1L; 1R, 2)}{E_{1L} - E_{1R}},$$

where

$$G(2, 1L; 1R, 2) = \int \psi_2(r)\overline{\psi_{1L}(r)} \frac{e^{-2}}{|r - r'|} \psi_1(r')\overline{\psi_2(r')}drdr$$

is the Coulomb exchange integral. Note that the potential wells here may have one, two or three dimensions.

This result may also be derived from the Hartree-Fock equations (1), (2) for the orbital $\Psi_g = \psi_1 = \psi_{1L} + \delta\psi_1$, by projecting it to the orbital $\psi_{1R}$. Note that the contribution of the direct term in the Coulomb interaction between the particles 1 and 2 is included into the mean-field potential $U(r)$.

Equation (4) gives us dependence of the amplitude $B_{G1}$ on the distance $l$ between the wells $L$ and $R$. If the distance $l \gg r_1$ where $r_1$ is the size of the orbital $1L$, we can expand $1/|r - r'|$ near $|r - r'| = l$. Integral with the first term $1/l$ of this expansion vanishes due to the orthogonality of the wave functions $\psi_1(r)$ and $\psi_2(r)$. Therefore, the expansion starts from $1/l^2$. The correlation effects correspond to higher orders in the perturbation theory in the Coulomb interaction integrals $G$, so they decay with distance faster than $1/l^2$.

**Classical limit.** – Now consider the classical limit $h \to 0$. The exchange term in the Hartree-Fock equations (1), (2) seems to extend to a large distance (under the barrier) if we consider the exchange interaction of an under-barrier particle ($\Psi_g = \psi_1$) with an above-barrier one ($\Psi_q = \psi_2$). The second term (the first non-vanishing term) in the multipole expansion of $K(r)$ gives us $\psi_2(r)/r^2$ decay in the under-barrier area in the right-hand side of eq. (1). Contrary to the single-particle tunneling amplitude ($t_1 \sim \exp(-\int |p|dr/h)$) this dependence does not contain $h$.

How the classical limit may be reached in this case? The $h$ dependence actually comes from the coefficient in front of $\psi_2(r)/r^2$ which is given by the integral in $K(r)$.

The answer here depends on what kind of states we consider.

1. Two semi-classical states, one below the barrier, another above the barrier. In this case we have integral between two rapidly oscillating functions in $K(r)$ in eq. (2), $\sim \int (dr/|r - r'|)\cos(\int p_1(r)dr/h) \times \cos(\int p_2(r')dr'/h)$. The integrals of this type are considered in the textbook [12] in the chapter about matrix elements between semiclassical states. Such integrals are exponentially small at $h \to 0$ (they contain $\exp(-1/h)$), therefore, the coefficient before $\psi_2(r)$ in $K(r)$ in eq. (2) in the right-hand side of eq. (1) (and the exchange-induced $\delta\psi_1$) vanishes.
2. Wave function of the first particle, $\psi_1$, is essentially a quantum state, a ground state or a low-energy state. Here the result depends on the properties of the potential $U(r)$. If this potential is smooth near the minimum, we may use the oscillator wave functions to describe the low-energy states. The exchange integral in this case contains product of the oscillator function and the rapidly oscillating semiclassical wave function, $\sim \exp(-\xi^2/2)\exp(ipx/\hbar) = \exp(-(\xi - \xi_0)^2/2)\exp(-p^2/(2m\omega\hbar))$, where $\xi = x\sqrt{m\omega/\hbar}$. The exchange integral is exponentially small again (see the last exponent).

3. A singular attractive potential (a model of a diatomic molecule). In this case the size of the lowest states so rapidly tends to zero at $\hbar \to 0$ that there are no oscillations inside. Consider, for example, a Coulomb ground state where the size is given by the Bohr radius $a_B = h^2/(me^2)$. At $r < a_B$ the product $(p/\hbar)r < 1$, i.e. there are no oscillations. Therefore, $K(r)$ has no exponential suppression for $\hbar \to 0$. However, the size of the ground state ($\sim a_B$) tends to zero and the binding energy ($\sim e^2/a_B$) to infinity, so this case actually has no classical limit.

Conclusion. – We see that the exchange-assisted tunneling vanishes in the classical limit (it still may be exponentially enhanced in comparison with the single-particle tunneling). The process considered is different from the classical “ionization by collision” case where we do not fix final energy of each particle (provided the total final energy is equal to the initial energy, $E_{1f} + E_{2f} = E_{1i} + E_{2i}$), the energy exchange depends on the initial conditions. In the exchange-assisted tunneling the spectrum of particle energies in the final state is exactly the same as in the initial state ($E_{1f} = E_{2i}$, $E_{2f} = E_{1i}$), therefore, we, in fact, have imposed an additional constraint. For classical processes this event has zero phase volume (zero probability).

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