Exchange interaction radically changes behavior of a quantum particle in a classically forbidden region: simple model

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Exchange interaction strongly influences the long-range behavior of localized electron orbitals and quantum tunneling amplitudes. In the Hartree-Fock approximation the exchange produces a power-law decay instead of the usual exponential decrease at large distances. To show that this effect is real (i.e. not a result of the approximation) we consider a simple model where different effects may be accurately analyzed. Applications include huge enhancement of inner electron ionization by a static electric field or laser field considered in Ref. [1].

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I. INTRODUCTION

One of the first famous results of Quantum Mechanics was that a particle may tunnel through a potential barrier. The tunneling amplitude is exponentially small in the classical limit. This result may be incorrect if we take into account the exchange interaction and correlation effects. In the Hartree-Fock equations the exchange interaction is described by the non-local (integranoperator), 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). According to [2] (see also [3, 4, 5]) the exchange can produce a power-law decay instead of the usual exponential decrease at large distances. For inner orbitals inside molecules decay is $r^{-2}$, for macroscopic systems $\cos(k_r r)r^{-\nu}$, where $k_r$ is the Fermi momentum and $\nu = 3$ for 1D, $\nu = 3.5$ for 2D and $\nu = 4$ for 3D crystal. Slow decay increases the spin-spin interaction between localized spins in solids and the under-barrier tunneling amplitudes.

A very interesting manifestation of this phenomenon has been suggested by Amusia in Ref. [1]. He showed that the exchange interaction may increase probability of ionization of inner atomic electrons by an external electric field by many orders of magnitude (in one of the examples the enhancement factor was $10^{100}$). Amusia claimed that this enhancement may explain experimentally observed enhancement of multi-electron ionization by a strong laser field, see e.g. Ref. [6] (a different explanation, an “atomic antenna” mechanism, was suggested by Kuchiev [7] and rediscovered by Corkum [8]).

All theoretical results [1, 2, 3, 4, 5] mentioned above have been obtained in the Hartree-Fock approximation. Naturally, one may ask a question: is this enhancement real or is it just an artefact of an approximate solution? Indeed, the Hartree-Fock method ignores correlation effects which sometimes play a very important role. An estimate of the correlation effects have been done in Ref. [2]. The conclusion is that if the correlation corrections may be treated using perturbation theory, their long-range effect is less significant than that of the exchange. However, it is important to consider a simple model where different effects can be accurately analyzed and check if the enhancement of the quantum tunneling by the exchange interaction really takes place.

Let us consider 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 [9]. 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, $|p| = \sqrt{2m(U(r) - E_1)}$ is the semiclassical under-barrier momentum and the integral is taken between the classical turning points.

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

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 $\psi_2 = A_2\psi_{2a} + B_2\psi_{2b}$ 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 b 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 a (orbital $\psi_{2a}$) to the potential well b (orbital $\psi_{2b}$).

Step 2: two-body process $2b, 1a \rightarrow 1b, 2a$ due to a non-diagonal Coulomb exchange interaction which transfers the first particle from orbital 1a to the orbital 2a and the second particle from 2b to 1b.

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 1a to 1b. This gives the amplitude for the ground state particle to be in the well “b”:

$$B_{1a} \sim \frac{G(2, 1a; 1b, 2)}{E_{1a} - E_{1b}}, \quad (1)$$
where
\[ G(2, 1a; 1b, 2) = \int \psi_2(r)^\dagger \psi_{1a}(r) \frac{e^2}{|r - r'|} \psi_{1b}(r') \psi_2(r') dr' dr \]
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 equation for the orbital \( \psi_1 = \psi_{1a} + \delta \psi_1 \),
\[ -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} \psi_1(r) + (U(r) - E_1) \psi_1(r) = K(r), \]
by projecting it to the orbital \( \psi_{1b} \). Here
\[ K(r) = \psi_2(r) \int \psi_2(r')^\dagger \frac{e^2}{|r - r'|} \psi_1(r') dr' \]
is the exchange term. 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 (2) gives us dependence of the amplitude \( B_{G1} \) on the distance \( |a - b| \) between the wells a and b. If the distance \( |a - b| \gg r_1 \) where \( r_1 \) is the size of the orbital 1a, we can expand 1/|r - r'| near |r - r'| = |a - b|. Integral with the first term 1/|a - b| of this expansion vanishes due to the orthogonality of the wave functions \( \psi_{1a}(r) \) and \( \psi_2(r) \). Therefore, the expansion starts from 1/|a - b|^2.

Now we may discuss a contribution of the correlation effects. They correspond to higher orders in the perturbation theory in the Coulomb interaction integrals G, so they decay with distance faster than 1/|a - b|^2.

Similarly, the enhancement of the tunneling takes place for the ionization of an inner atomic electron by an external electric field. We just need to make the length of the potential well “b” infinitely large, so the orbitals 1b and 2b will be in the continuum.

It is instructive to compare the exchange enhancement mechanism with the atomic antenna mechanism [6, 7]. In the antenna mechanism an external electron is ionized by a strong laser field, oscillates in this field and accumulates energy. Then this electron collides with the parent ion and ionizes it. In the exchange mechanism the external electron plays a passive role, it does not change its initial energy. Then this electron collides with the parent ion in a strong laser field, oscillates in this field and accumulates energy for the ionization of an inner atomic electron by an external electric field. We just need to make the length of the potential well “b” infinitely large, so the orbitals 1b and 2b will be in the continuum.

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We should check if the exchange enhancement survives in the case of a stronger Coulomb interaction. Consider the two-well problem with a very large Coulomb repulsion between two particles. A minimum of the Coulomb energy is achieved when the particles are in different wells, in state \( \psi_{1a} \psi_{2b} \) or \( \psi_{1b} \psi_{2a} \). Mixing between these states may be produced by the non-diagonal exchange interaction \( G(2b, 1a; 1b, 2a) \), i.e. it does not require any tunneling at all. Two other states \( \psi_{1a} \psi_{2a} \) and \( \psi_{1b} \psi_{2b} \) are separated from the lower states by the large Coulomb energy \( Q = Q_{aa} - Q_{ab} \) where \( Q_{aa} \) and \( Q_{ab} \) are the Coulomb energies for the particles in the same well and different wells correspondingly. Mixing between the states \( \psi_{1a} \psi_{2a} \) and \( \psi_{1b} \psi_{2b} \) may be achieved in 3 steps.

Step 1: tunneling of particle from 2a to 2b with creation of an intermediate state \( \psi_{1a} \psi_{2b} \) separated by the energy interval Q.

Step 2: the non-diagonal exchange interaction \( G(2b, 1a; 1b, 2a) \) transfers \( \psi_{1a} \psi_{2b} \) to \( \psi_{1b} \psi_{2a} \). At this step we have mixing of the single-particle states 1a and 1b, \( B_{G1} \sim t_2 G(2b, 1a; 1b, 2a)/Q^2 \).

Step 3: the tunneling from 2a to 2b.

We see again that we do not need the exponentially small tunneling amplitude \( t_1 \), i.e. the exchange enhancement works. The only suppression we have here is due to the large Coulomb matrix element Q in the denominator of the mixing amplitude \( t_{eff} \sim t_2 G^2(2b, 1a; 1b, 2a)/Q^2 \).

(Note that a similar suppression due to a large value of Q transforms a half-filled conducting band in solids into the Mott insulator. This transition influences the exchange power tail for a localised electron in solids - see discussion in [2]).

Similar results may be obtained for an attraction between the particles. This may be a model for a tunneling of an inner electron through a Josephson junction.

Thus, the exponential enhancement of the tunneling due to the exchange interaction really exists.

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