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Computation of exchange probability in one-dimensional electron-hydrogen scattering

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We present numerical *ab initio* calculations for a quantum system that is a one-dimensional analog of electron-hydrogen scattering at low energies. This approach allows for an exact treatment of electron correlation. The exchange probability can be computed directly from the full unsymmetrized two-electron wave function. One can thus determine without approximation the relative importance of the direct versus the exchange process. We find that, in this low-energy regime, the exchange probability can be quite high and can exceed the probability of the direct process. We then take into account the exchange probability in a calculation of the single-electron effective potential for the free electron. [S1050-2947(96)03510-X]

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I. INTRODUCTION

When two particles are identical in terms of their dynamical behavior, the identity of each particle is lost, and the two particles can in principle exchange positions with a probability that is given by quantum mechanics. In electron-atom scattering, the incident electron can be captured by the atom, and an atomic electron emitted. The exchange of the two electrons is not a trivial effect since the particles can carry some additional quantum numbers that will determine total transition amplitudes to atomic final states. The physical implications of the effect with respect to atomic collisions have been reviewed extensively by many authors [1].

The importance of exchange for electron-hydrogen scattering was soon realized in early calculations of phase shifts at low energies [2]. Experimental advances created the need for more accurate theoretical estimates of cross sections in later years. The underlying physical mechanism became evident: the longer range of the exchange potential compared to the Hartree potential in Hartree-Fock theories was identified as the cause of larger phase shifts for higher angular momenta in the partial-wave expansion [3]. Corrections to scattering cross sections due to the exchange effect were calculated in the low-energy regime with Hartree-Fock or Thomas-Fermi-Dirac theory for electrons off He [3]. Significant agreement between theory and experiment was found, although some discrepancies still remained. The role of exchange has been investigated also in various atomic and molecular processes, such as low-energy e-H_2 collisions [4].

The exchange effect was included up to second order in the distorted-wave Born series calculations of Madison, Bray, and McCarthy [5]. It was found that this effect was the primary source of disagreement between theory and experiment for intermediate energies (30–200 eV) for elastic scattering, $2s$ and $2p$ excitation. Other perturbation series calculations by Byron, Joachain, and Potvliege [6] contained approximations for higher-order exchange terms for elastic scattering and $2s$ excitation, but not for $2p$ excitation. Further clarification of the role of electron exchange could be made with the recent advances in calculational methods for the e-H scattering problem. We mention the direct, time-independent, numerical approaches of Temkin, Poet, and Wang and Callaway [7], which are based on expansions in two-electron coupled radial functions and strongly depend on appropriate boundary conditions. Also, the recent convergent close-coupling method of Bray and Stelbovics [8] gave very good agreement with experiment.

If initially the incident electron has momentum $\mathbf{k}_1$, and the atom is in its ground state $\phi_1(\mathbf{r}_2)$, then, in the first Born approximation, the direct scattering amplitude for collisional excitation to atomic state n is

$$f_{1n}(\theta,\phi)=-\frac{1}{2\pi}\int d^3r_1\int d^3r_2\,\phi_n^*(\mathbf{r}_2)\times\left(\frac{1}{r_{12}}-\frac{1}{r_1}\right)\phi_1(\mathbf{r}_2)e^{i(\mathbf{k}_1-\mathbf{k}_n)\cdot\mathbf{r}_1}, \tag{1}$$

where the initial and the final wave functions have the asymptotic forms $e^{i\mathbf{k}_1\cdot\mathbf{r}_1}\phi_1(\mathbf{r}_2)$ and $e^{i\mathbf{k}_n\cdot\mathbf{r}_1}\phi_n(\mathbf{r}_2)$, respectively. When exchange is involved, the final wave function is taken as $e^{i\mathbf{k}_n\cdot\mathbf{r}_2}\phi_n(\mathbf{r}_1)$, and the corresponding exchange amplitude becomes

$$g_{1n}(\theta,\phi)=-\frac{1}{2\pi}\int d^3r_1\int d^3r_2\,\phi_n^*(\mathbf{r}_1)\times\left(\frac{1}{r_{12}}-\frac{1}{r_1}\right)\phi_1(\mathbf{r}_2)e^{i(\mathbf{k}_1\cdot\mathbf{r}_1-\mathbf{k}_n\cdot\mathbf{r}_2)}. \tag{2}$$

This is also known as the Born-Oppenheimer approximation as it was obtained first by Oppenheimer [9]. However, in this rather "primitive" description, it is not clear whether the interaction term in Eq. (2) should have $1/r_1$ or $1/r_2$. More complicated analytic expressions in the close-coupling picture are needed.

In our calculations with exact wave functions the previous question can be resolved in a straightforward way. Other uncertainties in formulation or interpretation of scattering calculations, arising from approximations to the exact theory,

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can also be resolved. In this paper the probability amplitudes for both the direct and the exchange processes are computed *ab initio*, and no assumptions are made regarding the form of the amplitudes. In such a computation, instead of using either $1/r_1$ or $1/r_2$, we include both terms with appropriate weights that are time dependent as they evolve during the collision. This picture will become clearer with the computation of the single-electron effective potential in Sec. V. It is the advantage of our *ab initio* approach that there is no need to write expressions for transition amplitudes, since all probabilities are computed directly from the total two-electron wave function.

In Sec. II we present our model and the method of calculation of the exchange probability. In Sec. III we show a simple classical example. The energy dependence of the exchange effect is discussed in Sec. IV. In Sec. V we show how exchange can be taken into account for the calculation of single-electron effective potentials. We summarize our results in Sec. VI.

II. TWO-ELECTRON MODEL AND QUANTITATIVE MEASURE OF EXCHANGE

Our two-electron quantum system [10] consists of two electrons whose spatial coordinates are x_1 and x_2, allowed to move only in one dimension, along the x axis, in the neighborhood of a nucleus of unit positive charge fixed at the origin. It is the one-dimensional analog of the negative hydrogen ion, and by increasing the nuclear charge to 2,3,4,... we would obtain the one-dimensional analogs of He, Li^+,Be^{2+},..., etc. In atomic units ($\hbar=m_e=e=1$) the two-electron Hamiltonian is

$$H=\tfrac{1}{2}p_1^2+\tfrac{1}{2}p_2^2+V(x_1)+V(x_2)-V(x_1-x_2), \tag{3}$$

where both the electron-nucleus attraction and the electron-electron repulsion are described by the nonsingular, soft-core, and asymptotically Coulombic potential:

$$V(x)\equiv-\frac{1}{\sqrt{x^2+1}}. \tag{4}$$

Each electron can move anywhere along the x axis, making the total potential symmetric and parity a good quantum number. The total potential in Eq. (3) and the Hamiltonian H are symmetric under exchange of the spatial coordinates of the two electrons. This property allows for wave functions that are either symmetric or antisymmetric with respect to exchange. The Hamiltonian is also symmetric under spatial reflection of both space coordinates, a property that corresponds to definite parity—the one-dimensional reminder of angular momentum.

It is clear that the two-electron potential retains, in one space dimension, important characteristics of real atomic potentials. Even the soft core of the interaction potential in our model has a ''fundamental'' explanation in the sense that, in a real three-dimensional atom, the two electrons have enough available space to bypass each other.

The hydrogen atom of the target in our two-electron model has been studied extensively in the past. Javanainen, Eberly, and Su [11] introduced the same model potential of Eq. (4) for a single electron and a fixed nucleus in order to study the response of the model hydrogen atom to strong laser fields. The properties of the bare atom, with respect to energy eigenstates and eigenvalues, symmetries, and dipole moments, have been tabulated by Su and Eberly [11]. The ground state is at -0.6703 a.u., the first excited state at -0.2754 a.u., and there is a Rydberg-level scaling rule $E_n=-1/n^2$ for the quantum number n and the energy eigenvalue E_n that is closely followed for higher n's.

For the purpose of solving the Schrödinger equation numerically, the two-electron wave function is represented in space on a two-dimensional grid where each electron's coordinate is discretized as $x_i=(-N/2+i-\frac{1}{2})\Delta x$, with $i=1,2,3,\ldots,N$. Here, $\Delta x=L/N$ is the grid spacing, L the length of the quantization box and N the total number of grid points in the interval $[-L/2,L/2]$. Depending on accuracy requirements L was varied between 100 and 1000 a.u., while Δx was taken in the range 0.10–0.98 a.u. The highest accuracy results have been obtained for $N=1024$ grid points, corresponding to a two-electron wave function of 1024×1024 components.

Given an initial wave function $\Phi(x_1,x_2)$, its time evolution is affected by the unitary operator $U(t-t_0)=\exp[-iH(t-t_0)]$ which, for a small time increment Δt, can be decomposed into three operators by ''splitting'' the kinetic energy term $T=p_1^2/2+p_2^2/2$, i.e.,

$$\begin{aligned}U(\Delta t)&=\exp[-i(T+V)\Delta t]\\&=\exp[-iT\Delta t/2]\exp[-iV\Delta t]\exp[-iT\Delta t/2]\\&\quad+O(\Delta t^3).\end{aligned} \tag{5}$$

This symmetric split decomposition is quite advantageous [12]. The action of the kinetic energy operator on the wave function can be performed easily in Fourier space. It is important to note that in contrast to the usual approximations of the second derivative by three- or five-point formulas, the action of the kinetic-energy operator on the spatial grid can be performed exactly here. This allows for much larger spacing Δx than that used in other methods. The middle part of the evolution operator describes the action of the potential energy alone and corresponds to a simple multiplication of the wave function in coordinate space.

In the time domain, a time step of $\Delta t=0.2$ a.u. or bigger is sufficient. Typical program runs consist of up to 40 000 consecutive Fourier transformations for the time evolution, which can be performed quite efficiently on a supercomputer. We have mainly used a Cray-Y MP/C-90 that can perform a fast Fourier transform (FFT) in about 0.56 CPU seconds for a 1024×1024 complex matrix, using very efficient vectorized library routines.

In the case of electron-hydrogen scattering we suppose that the initial total wave function of the two-electron system is a product of the projectile wave packet $\phi_{k_1}(x_1)$ and the atomic ground state $\phi_1(x_2)$. We start with an incident electron represented by a Gaussian wave packet, initially centered at a distance of 100 a.u. on the left of the scattering center, and subsequently propagating to the right, i.e.,

$$\phi_{k_{\mathrm{inc}}}=\frac{1}{(2\pi\sigma^2)^{1/4}}\exp\left[-\frac{(x+100)^2}{4\sigma^2}\right]\exp(ik_{\mathrm{inc}}x), \tag{6}$$

where σ is the spatial width of the Gaussian, taken here to be 30 a.u. The target atom is centered at the origin, and the initial position of the incident wave packet ensures that there is no overlap with the atom before the collision takes place. Our target hydrogen atom is initially in its ground state with $n=1$. As the incident wave packet distorts the atom, passing through the origin, the atomic electron can be excited to higher atomic eigenstates. The final state of the atom, defined at times after the incident wave packet no longer overlaps with the atom, can be described, in general, as a linear combination of the bare atomic eigenstates. If the projectile kinetic energy is less than the first excitation threshold to level $n=2$, the atom returns to its ground state. The scattering is purely elastic. When the projectile energy is high enough to excite the atom to states with $n=2,3,4,...$, not only the atom is left excited after the collision, but the energy of the projectile has changed as well. Since the total energy of the system is conserved (there is no explicit time dependence in the Hamiltonian), the projectile's energy spectrum reflects the state of the target atom.

The time-dependent populations in our case, where two electrons are involved, are actually the same quantities as the probabilities P_n that at least one electron is in the bare atomic eigenstate n. Since the two electrons cannot both be bound in the atom at the same time, we can write

$$P_n(t)=2\int dx_2\left|\int dx_1\phi_n^*(x_1)\psi(x_1,x_2;t)\right|^2. \tag{7}$$

The factor of 2 is due to symmetrization of the initial wave function [10].

For the purpose of detecting exchange [13] the time evolution is calculated without any initial symmetrization of the total wave function, so that the identity of each (distinguishable) electron can be monitored during the collision. Let $\psi(x_1,x_2;t)$ be the total (unsymmetrized) wave function at a time t sufficiently long after the collision. If x_1 is the coordinate of the incident electron and x_2 the coordinate of the initially bound one, the probability that the two electrons have exchanged states is simply

$$P_{\mathrm{ex}}(t)=\sum_n \int dx_2\left|\int dx_1\phi_n^*(x_1)\psi(x_1,x_2;t)\right|^2. \tag{8}$$

We sum over all bound states n in order to include all the possible inelastic channels, except for ionization. We shall see in the following that P_{ex} depends on the energy of the incident electron. In general, the exchange probability becomes negligible for energies high enough that the Born-Oppenheimer approximation of Eq. (2) is valid [1].

III. EXAMPLE WITH FREE ELECTRONS AND THE CLASSICAL PICTURE OF EXCHANGE

Before we proceed with the quantum-mechanical exchange effect it would be useful to explore a classical analog, namely, a zero impact-parameter collision between two identical hard spheres. We know that when one of the two spheres is incident upon another, which is initially at rest in some laboratory frame, the incident sphere takes the place of the standing one after the collision, while the initially standing one moves with the velocity that the incident one had before the collision. This is due to the conservation of both momentum and kinetic energy. Although the two conservation laws give two solutions of the problem, one with complete exchange and one with no effect at all, only the former one is physically acceptable in the case of hard spheres. Given zero impact parameter, the spheres must interact and cannot avoid each other, so that only full exchange can occur. If the spheres are not assumed to be ''hard'' so that they can pass through each other (but we still have a purely elastic collision with conservation of kinetic energy), then both solutions are acceptable in the framework of the conservation laws.

In quantum mechanics one can simulate classical collisions with the scattering of wave packets that represent particles. The quantum-mechanical packets should behave classically if they have negligible probability of passing through each other, and one can make their mutual potential barriers much higher than their kinetic energies to ensure this. In that case, complete exchange of the two packets is expected to happen. In Fig. 1(a) we show the joint two-electron probability distributions in the form of contour plots in four time frames during the collision of the two free electrons.

The time sequence is from top to bottom. The plots are made in the two-dimensional plane of the two-electron coordinates, x_1 (vertical) and x_2 (horizontal). In the figure we see a two-dimensional Gaussian distribution that moves in the positive x_1 direction towards the center, and then turns right towards the positive x_2 axis. The probability distribution for electron x_2, initially centered at the origin of the x_2 axis, is moving along the positive x_2 axis after the collision, while at the same time the probability distribution for electron x_1, initially moving in the positive x_1 direction, remains centered at the origin of the x_1 axis. This is exactly the quantum realization of classical hard-sphere exchange scattering.

If the kinetic energies of the two wave packets are higher than their mutual potential barriers, then they both become transparent with finite probabilities of reflection and transmission through each other. This effect is clearly shown in Fig. 1(b). We see that the wave packet initially incident toward the positive x_1 direction continues to travel in the same direction after the collision, although some small part of it is exchanged and moves in the positive x_2 direction. The two electrons have almost completely passed through each other and the exchange scattering appears to be a ''small'' effect.

In our studies here, the kinetic energy of the incident electron is always less than the potential barrier of the other electron. For the soft-core Coulombic potential of Eq. (4), the maximum height of the barrier is 1 a.u. of energy, which is higher than the ionization potential of 0.67 a.u. that serves as the upper bound of the energy range of the projectile in our studies. The two electrons, therefore, can completely exchange states during the collision, if no potential from the atomic nucleus is present. However, it is exactly the presence of the nucleus that lowers the total ''effective'' potential barrier that the incoming electron experiences during its collision with the atomic electron, allowing for finite direct and exchange probabilities. In Sec. IV we will see how these probabilities depend on the incident electron energy.

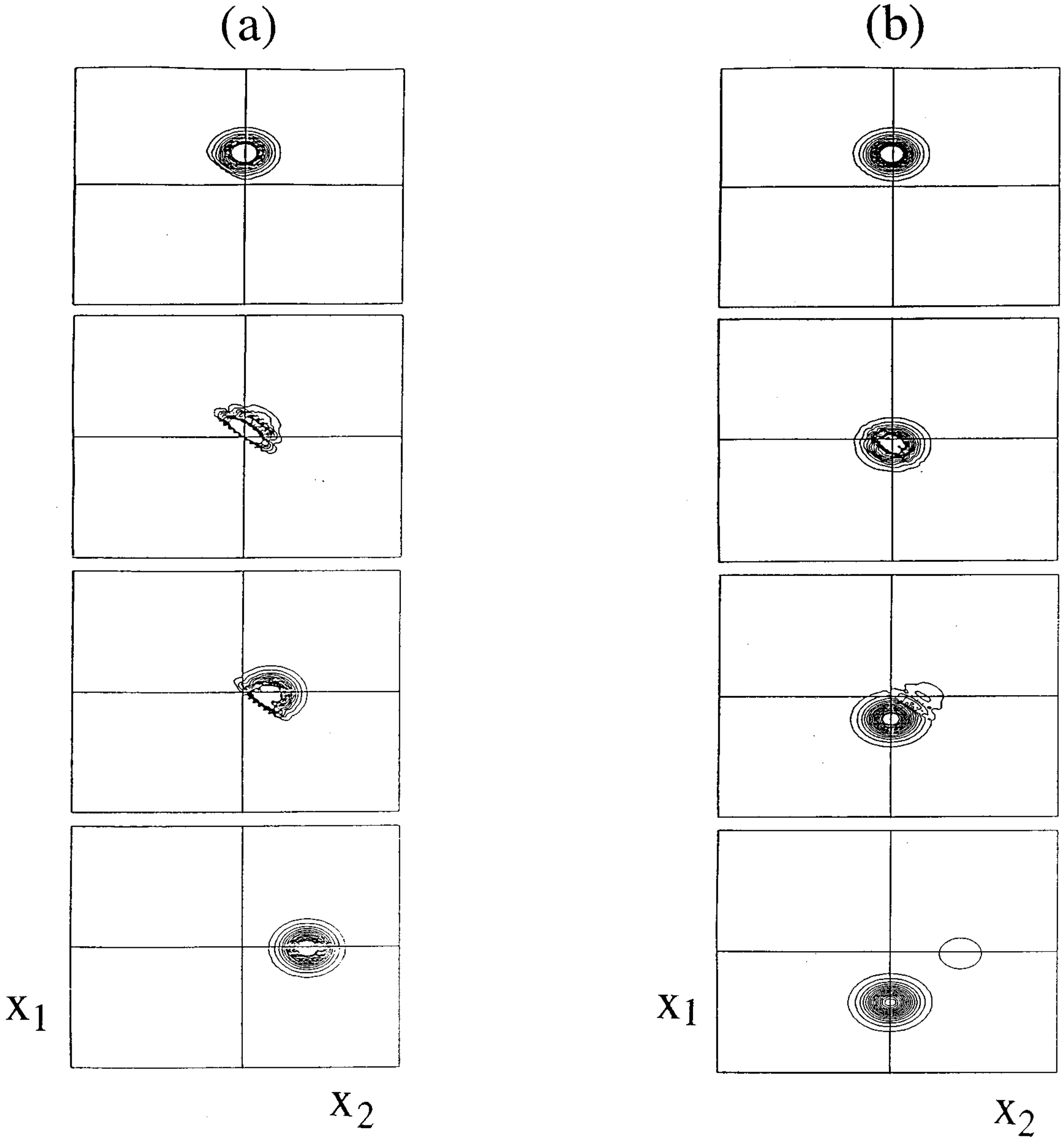

FIG. 1. (a) The joint two-electron probability distribution $|\psi(x_1,x_2)|^2$ in four subsequent time frames (top to bottom) during the collision. The two electrons are free particles. One of them is initially at rest with its probability distribution centered at the origin along the x_2 axis (horizontal). The other electron is incident toward the positive x_1 axis (vertical). The kinetic energy in the rest frame is 0.3 a.u. After the collision the two electrons are fully exchanged. (b) Same as (a), but with kinetic energy slightly higher than 1, the maximum height of the mutual potential barriers. There is only a very small amount of exchange probability after the collision.

IV. ENERGY DEPENDENCE AND THRESHOLD BEHAVIOR

The most interesting feature of the exchange probability P_{ex} of Eq. (8) is its energy dependence. It is well known that it decreases rapidly with increasing energy, since in the Born-Oppenheimer formula (2) the exponential function oscillates very rapidly for high energies so that the net effect of the interference between the atomic and the free-electron wave function is zero [14]. This interference effect does not occur in the direct amplitude of formula (1) since the position variables in the atomic and the free-electron wave functions are integrated separately. This conclusion for high energies is valid since formula (2) is also valid in the high-energy regime.

However, since there is no reliable approximation of the scattering amplitudes in the low-energy regime, one cannot estimate the importance of the exchange effect in that regime in a straightforward way. In this work we compute the probability of exchange for a range of energies. In Fig. 2 we show the total probability of exchange as a function of energy. We notice a quite broad and high maximum of 0.57 at an energy of 0.14 a.u. It becomes, therefore, higher than the probability of the direct process $1-0.57=0.43$. The exchange probability tends to zero for very low energies, since the reflection coefficient approaches 1 for attractive potentials when the incident energy tends to zero. On the right-hand side of the maximum the exchange probability decreases with energy, and eventually it should tend to zero as expected from the

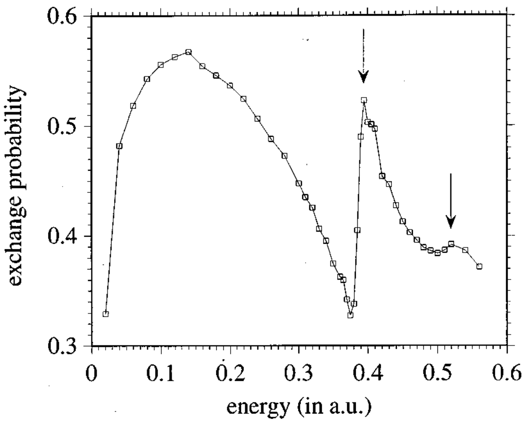

FIG. 2. The total probability of exchange after the collision as a function of the incident electron energy. The quantity that is plotted is the value of $P_{\rm ex}$ of Eq. (5) at sufficiently long times t after the collision.

Born-Oppenheimer approximation for the behavior of the exchange scattering amplitude at high energies [14]. The only interruption of the monotonic decrease comes from the atomic excitation resonance at 0.39 a.u., between the ground and the first excited state. Also, the resonance at 0.52 a.u. for the $n=3$ excited state is clearly visible. No other resonances are seen as the total exchange probability decreases drastically to very low values near the ionization threshold.

In Figs. 3(a) and 3(b) we show the portion of exchange probability in the reflection and transmission probabilities, respectively. The total reflection and transmission coefficients are shown in Fig. 4. We see that, qualitatively, they are not very different from the corresponding coefficients for an attractive square well potential.

In Fig. 3(b) the probability of exchange in transmission seems to be higher than the probability of the direct process in the low-energy regime of 0.05–0.25 a.u. A maximum of the exchange and a minimum of the direct probability can be observed at the atomic excitation resonance of 0.39 a.u. For higher energies, beyond the atomic resonances, the direct process dominates.

Finally, we notice the remarkable effect that can be seen clearly in Fig. 3(a), namely, for reflection the direct and the exchange processes are almost equally probable for a wide range of energies above 0.05 a.u. In order to understand qualitatively why this occurs, let us picture the hydrogen atom in one dimension as consisting of a nucleus fixed at the origin and an electron standing ‘‘at rest’’ with equal probabilities on either side of the nucleus. When an incident electron coming from the left is scattered by this system, it can be exchanged with the atomic electron and partially reflected by the nucleus. No reflection from the collision with the standing electron can occur because of the conservation of momentum and kinetic energy in analogy to the classical problem discussed in Sec. III. Two *equally probable* processes contribute to reflection: (a) The incident electron encounters the atomic electron first, before the nucleus, and it completely exchanges positions with it. The outgoing electron can now be reflected by the potential of the nucleus with probability R. In this process the finally reflected electron is not the same as the initially incident one, but it is exchanged with the initially atomic one. (b) The incident electron encounters the nucleus first and is reflected with probability R. The finally reflected electron is the same as the initially incident one.

We have assumed that the atomic electron's probability distribution is not significantly affected by the polarization effects induced to the atom by the incident electron. However, for very low energies (here, below 0.04 a.u.) polarization effects become important, and the atomic electron's probability distribution is significantly moved to one side of

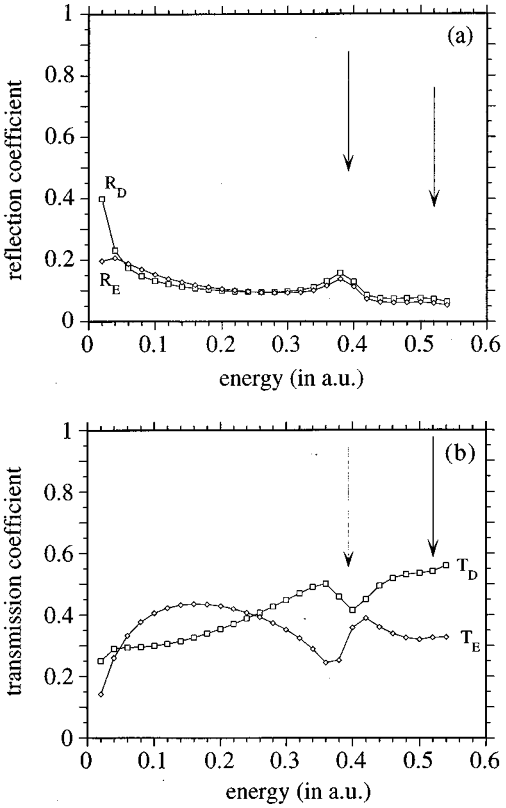

FIG. 3. (a) Reflection coefficient due to direct (R_D) and exchange process (R_E) as a function of energy. (b) Transmission coefficient due to direct (T_D) and exchange process (T_E) as a function of incident energy.

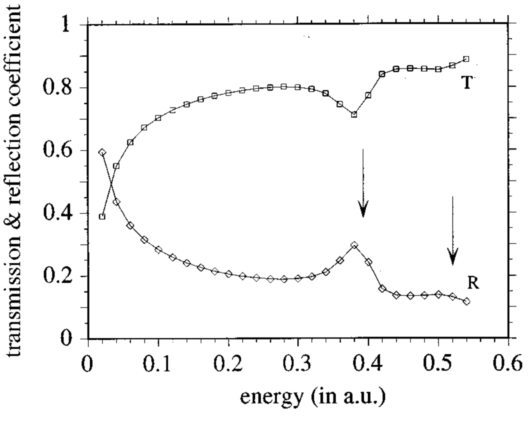

FIG. 4. Total reflection (R) and transmission (T) coefficients as functions of the incident electron energy.

the nucleus, opposite to the side of the approaching incident electron. In that case, process (b) can happen with higher probability than process (a), leading to lower exchange probability in total reflection. This is evidently in agreement with Fig. 3(a) for energies below 0.04 a.u.

V. ELECTRON EXCHANGE AND SINGLE-ELECTRON EFFECTIVE POTENTIALS

The total potential energy that a system of two electrons with coordinates x_1 and x_2 experiences in the field of a nucleus is

$$V_{\text{tot}}(x_1,x_2)=V(x_1)+V(x_2)-V(x_1-x_2), \qquad (9)$$

where $V(x_1)$ and $V(x_2)$ are the attractive potentials from the nucleus, and $-V(x_1-x_2)$ is the repulsive electron-electron interaction potential. The expectation value of the force that the electron with coordinate x_1 experiences is [13]

$$\begin{aligned}\langle F(x_1;t)\rangle &= \left\langle -\frac{\partial}{\partial x_1} V_{\text{tot}}(x_1,\tilde{x}_2)\right\rangle \\ &= \int d\tilde{x}_1 \int d\tilde{x}_2 \psi^*(\tilde{x}_1,\tilde{x}_2;t) \\ &\quad \times \left[-\frac{\partial V(x_1)}{\partial x_1}+\frac{\partial V(x_1-\tilde{x}_2)}{\partial x_1}\right]\psi(\tilde{x}_1,\tilde{x}_2;t).\end{aligned} \qquad (10)$$

The single-electron effective potential (SEEP) that corresponds to this force is set equal to zero at infinity (the boundary of our quantization box is at $-L/2$), and we define

$$V_{\text{eff}}(x_1;t)=-\int_{-L/2}^{x_1} dx_1' \langle F(x_1';t)\rangle,$$

which finally becomes

$$V_{\text{eff}}(x_1;t)=V(x_1)-\int d\tilde{x}_2 P(\tilde{x}_2;t)V(x_1-\tilde{x}_2), \qquad (11)$$

where we have set all terms of $V_{\text{tot}}(x_1,x_2)$ in Eq. (9) equal to zero at the boundary of the quantization box. We have also defined the time-dependent single-electron probability density as

$$P(\tilde{x}_2;t)=\int d\tilde{x}_1 |\psi(\tilde{x}_1,\tilde{x}_2;t)|^2. \qquad (12)$$

We derived formula (11) in a straightforward way without taking into account the exchange effect. However, we have already seen that the probability of the two electrons exchanging their coordinates is quite high and it can even exceed the probability of the direct process. Therefore, our computation of the single-electron effective potential is incomplete, since each electron does not have a distinct role (projectile or target) during the total interaction time in a collision. Corrections have to be made so that the effective potential for the initially incident electron is the same as the potential for the finally outgoing electron, regardless of whether or not exchange has occurred. This problem goes beyond the traditional theoretical treatment of effective potentials. A brief discussion is given by Goldberger and Watson [15].

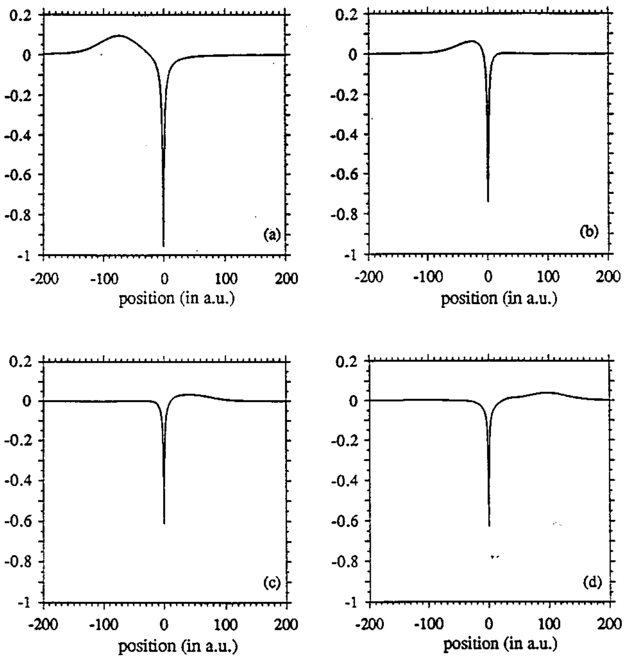

FIG. 5. The time-dependent single-electron effective potential for the bound electron of the atomic target. The energy of the incident electron is 0.44 a.u. Formula (11) has been used instead of Eq. (8). The position in the horizontal axis is in a.u. The times for the (a), (b), (c), and (d) figures are 4, 8, 12, and 16 cycles, respectively [1 cycle$=2\pi/(E_2-E_1)=15$ a.u., for the lowest two hydrogenic energy eigenstates]. The center of the wave packet passes the origin after seven cycles from the moment that the packet is at the initial position ($x=-100$ a.u.).

In order to correct for the exchange effect we rewrite formula (11) taking into account the probabilities $P_{\text{ex}}(t)$ of exchange and $P_{\text{di}}(t)=1-P_{\text{ex}}(t)$ of direct process. Therefore, we write

$$\begin{aligned}V_{\text{eff}}(x_1;t) &= [1-P_{\text{ex}}(t)]\left[V(x_1)-\int d\tilde{x}_2 P(\tilde{x}_2;t)V(x_1-\tilde{x}_2)\right] \\ &\quad + P_{\text{ex}}(t)\left[V(x_1)-\int d\tilde{x}_1 P(\tilde{x}_1;t)V(x_1-\tilde{x}_1)\right].\end{aligned} \qquad (13)$$

If one uses the notation $P(\tilde{x}_1;t)\equiv P_1(x;t)$ and $P(\tilde{x}_2;t)\equiv P_2(x;t)$ for the probability distributions of electrons 1 and 2, respectively, then Eq. (13) is simplified to

$$\begin{aligned}V_{\text{eff}}(x_1;t) &= V(x_1)-\int dx[P_{\text{di}}(t)P_2(x;t) \\ &\quad + P_{\text{ex}}(t)P_1(x;t)]V(x_1-x).\end{aligned} \qquad (14)$$

Figure 5 shows the SEEP for the case when the incident electron energy is 0.44 a.u., with the use of the improved formula (14). The asymmetries are due to the partial reflection of the incident electron.

Of course, if the wave function is properly symmetrized, then $P_1(x;t)=P_2(x;t)$, and formula (14) reduces to Eq. (11). Therefore, Eq. (11) is correct for particles that are assumed to be identical.

Finally, we mention that it has already become obvious how important the time dependence is for the treatment of exchange effects. Traditional scattering theory is designed to ignore the detailed processes inside the interaction region and considers only states at long times before and after the collision, with boundary conditions playing an important role.

VI. SUMMARY

We have presented numerical *ab initio* calculations for a one-dimensional two-electron model quantum system of electron-hydrogen scattering. This approach has allowed for an exact treatment of the electron correlation. We dealt with phenomena that dominate scattering in low energies, where correlation effects become very important as the incident electron has sufficient time to ‘‘see’’ and perturb the state of the bound electron of the target. The exchange probability was computed directly from the two-electron wave function. We found that, in this low-energy regime, the exchange probability can be quite high and can even exceed the probability of the direct process. We then took into account the exchange probability in the calculation of the single-electron effective potential for the free electron. Our one-dimensional model system is evidently well suited to describe exchange, and it permits a fully time-dependent treatment of scattering. This is in contrast, of course, to the time-independent treatment provided by the traditional scattering theories based on asymptotic initial and final states.

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