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Time-dependent Hartree-Fock theory of charge exchange: Application to He^{2+} + He

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An application of the time-dependent Hartree-Fock (TDHF) theory of charge transfer in atomic collisions is presented. Probabilities for elastic and double symmetric charge exchange are calculated for a fixed laboratory scattering angle and for collision energies from 10 to 70 keV. The TDHF equations are solved using finite difference techniques and propagated in time using the Peaceman-Rachford alternating-direction implicit method. Plots of time-evolved charge densities are presented also.

I. INTRODUCTION

Charge-exchange processes during the collisions of atoms and ions have been studied extensively both theoretically and experimentally. Any of several recent reviews can provide an introduction to the extent of the efforts in this field.[1] Because of the high degree of accuracy which has been achieved in measuring charge-exchange cross sections, the theorist is challenged to devise new and more rigorous computational methods. Theoretical studies of charge exchange between atoms and ions at medium and high energies generally employ basis set expansions (either atomic or molecular) to describe the electronic states of the colliding particles. The nuclei are assumed to follow either straight-line or Coulomb trajectories. These traditional impact-parameter methods require a substantial effort to obtain the relevant coupling matrix elements between the electronic states and require the incorporation of traveling wave-phase factors in order that proper asymptotic scattering states can be defined. This latter requirement, in fact, further complicates the task of calculating the coupling matrix elements. Also in many treatments the truncation of the basis expansion leads to an origin dependence in the couplings.[2] Many efforts have been made to find remedies for these problems.[3] However, by directly integrating the time-dependent Schrödinger equation using either finite difference or finite element techniques for the time evolution of the electronic wave function, the problems with basis set representations are avoided. Time-dependent methods and theories are beginning to be developed by several groups to study atomic-collision processes.[4] In this paper we present results of finite difference calculations to illustrate the time-dependent Hartree-Fock (TDHF) method and to demonstrate its use. The results we present indicate that over a substantial range of collision energies the TDHF solution does yield accurate charge-transfer probabilities. We are encouraged by these results and believe that for some atomic-collision processes this technique is certainly competitive and potentially superior to basis expansion methods used previously.

In the next section we present the TDHF method which has been developed over the past several years for the study of collisions of heavy nuclei and which we have adapted to study atomic-collision phenomena. We present the details of our calculations and the results in the third section. The final section includes our conclusions and a statement of the problems which must be addressed to improve the utility and accuracy of these methods.

THEORY

We are interested in collisions with relatively high velocity (10 – 100-keV laboratory energy) and with small impact parameters. Therefore we can make the following two approximations. First, we assume that the nuclear motion can be approximated by a Coulomb trajectory. At the velocities considered the trajectory differs from a straight line only when the two nuclei are very close together, essentially inside the electronic charge cloud. Second, we assume that the charge density is cylindrically symmetric about an axis [z axis, see Fig. 1(a)] which passes through the target nucleus and is parallel to the line tangent to the scattering trajectory at its point of closest approach. Then the equations governing the evolution of the electronic orbitals depend only on two spatial coordinates r and z ($-\infty < z < \infty$, $0 < r < \infty$), where r measures the perpendicular distance from the z axis. These equations are solved on a two-dimensional finite difference grid. The origin of the coordinate system is fixed at the target nucleus.

The numerical methods we use have been described thoroughly in the nuclear physics literature[5] and therefore are likely to be somewhat unfamiliar. For this reason we repeat the details of the calculations here but emphasize that much of the development has been carried out and presented before.

In this paper we are interested in a two-electron system whose total electronic spin state is a singlet. Therefore, we have no exchange interaction and we can use a single, doubly occupied orbital to describe the wave function for the system. The time-dependent Hartree-Fock equation for the evolution of this single spatial orbital can be written (using atomic units, $e = \hbar = m = 1$) as

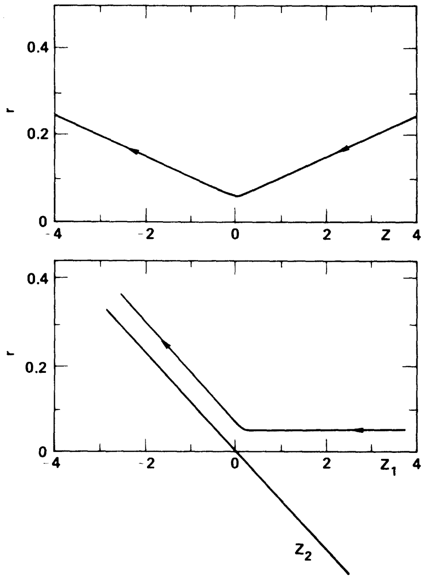

FIG. 1. (a) Coulomb trajectory of scattering nucleus. (b) Axes z_1 and z_2 were used in our modified calculation as described in the text.

$$i\frac{\partial}{\partial t}\phi(\vec{r},t) = h(t)\phi(\vec{r},t)\ , \tag{1}$$

where

$$h(t) = -\tfrac{1}{2}\nabla^2 + \tfrac{1}{2}\int d\vec{r}\,'\frac{\rho(\vec{r}\,',t)}{|\vec{r}-\vec{r}\,'|} - \frac{Z_A}{|\vec{r}-\vec{R}_A(t)|} - \frac{Z_B}{|\vec{r}-\vec{R}_B(t)|}\ . \tag{2}$$

R_A and R_B are the positions, and Z_A and Z_B the charges of the target and scattering nuclei, respectively. The total electronic charge density is given by

$$\rho(\vec{r},t) = 2\,|\phi(\vec{r},t)|^2\ . \tag{3}$$

In Eq. (2) we have shown explictly the time dependencies in the problem.

We write the orbital in cylindrical coordinates as

$$\phi(\vec{r},t) = (2\pi r)^{-1/2} g(r,z,t)e^{i\mu\phi}\ , \tag{4}$$

where μ, the azimuthal quantum number, is zero for cylindrically symmetric states.

We solve Eq. (1) for g_{jk}, the values of the function on the mesh defined by

$$r_j = (j - \tfrac{1}{2})\Delta r,\ \ j = 1,2,\ldots,N_R$$

and

$$z_k = (k - N_z/2)\Delta z,\ \ k = 1,2,\ldots,N_z\ . \tag{5}$$

Then the time-dependent Hartree-Fock equation can be rewritten more conveniently as

$$i\frac{\partial}{\partial t}g_{jk} = (Hg)_{jk} + (Vg)_{jk}\ , \tag{6}$$

where the (Hermitian) horizontal and vertical Hamiltonians are defined by

$$(Hg)_{jk} = -\frac{1}{2(\Delta z)^2}(g_{jk+1} + g_{jk-1} - 2g_{jk}) + \tfrac{1}{2}W_{jk}g_{jk} \tag{7}$$

and

$$(Vg)_{jk} = -\frac{1}{2(\Delta r)^2}(c_j g_{j+1k} + c_{j-1}g_{j-1k} - 2g_{jk}) + \tfrac{1}{2}W_{jk}g_{jk}\ . \tag{8}$$

The coefficients c_j are given by

$$c_j = j/(j^2-\tfrac{1}{4})^{1/2} . \tag{9}$$

Note we use a three-point formula to calculate the kinetic energies in each direction. The potential W in the above equations includes the nuclear attraction terms and the Coulomb term. The Coulomb term presents two significant problems for the numerical integration. First, the term depends on the wave function itself, i.e.,

$$\Phi_c(\vec{r},t) = \tfrac{1}{2}\int d\vec{r}\,' \frac{\rho(\vec{r}\,',t)}{|\vec{r}-\vec{r}\,'|} . \tag{10}$$

This means that ideally the operators H and V should be evaluated at $t_{n+1/2}$ when propagating from t_n to t_{n+1}. This is accomplished approximately by a double-step integration procedure. The first step is to t_{n+1}. We then calculate h at t_n and t_{n+1} to obtain

$$h_{n+1/2} = \tfrac{1}{2}(h_n + h_{n+1}) .$$

Then this Hamiltonian is used for the final propagation step, again from t_n to t_{n+1}.

The second problem with the Coulomb term is that it is very expensive to evaluate the complete integral in Eq. (10) for *every* point on the grid. Fortunately we can obtain the potential much more efficiently from a differential equation, the Poisson equation,

$$\nabla^2\Phi_c(\vec{r},t) = -4\pi\tfrac{1}{2}\rho(\vec{r},t) . \tag{11}$$

We solve this inhomogeneous differential equation iteratively using an integration technique similar to that described below. We need, however, the potential on the boundaries of the mesh. This is obtained from a moment's expansion of the density about the target nucleus.

We have expressed the Hamiltonian in this particular fashion [Eq. (6)] in order to use the Peaceman-Rachford (PR) method to perform the time integration.[6] If we define $g^{(n)}$ to be the value of the function g at the time $t_n = n\Delta t$, we have according to the PR method

$$g^{(n+1)} = [I + i\tau V]^{-1}[I - i\tau H][I + i\tau H]^{-1}[I - i\tau V]g^{(n)} , \tag{12}$$

where I is the unit operator and $\tau = \Delta t/2\hbar$. It is easy to show that this expression agrees with the expansion of the exact time-evolution operator, $\exp[-i(H+V)\Delta t/\hbar]$, through terms of order $(\Delta t)^2$.

The PR method is a specific example of a class of integrators developed for parabolic equations. This class is called the alternating direction implicit (ADI) methods.[7] They require the solution of two implicit equations which involve tridiagonal sets of equations. The implicit methods have much better stability properties than the explicit difference schemes but they require matrix inversions for their solution. Since the matrices in the ADI method are tridiagonal, their inversions can be achieved very efficiently using Gaussian elimination. Other implicit schemes for equations of this type, for example, the Crank-Nicolson method,[8] require the inversion of banded matrices. The ADI methods involve less computational effort and can be shown to be accurate to the same order in Δt. Predictor-corrector methods also have been used to integrate similar time-dependent equations with stable and accurate results.[9] It is necessary, however, to carry several solutions at previous time steps to accomplish the propagation. This leads to storage problems for functions defined on large grids. Finally, the Taylor expansion of the time-evolution operator, keeping enough terms to preserve the norm and the energy of the wave function has been used.[10] This also has been found to be stable and accurate and may be the optimum method provided the calculation of higher derivatives is much faster than the inversion of tridiagonal matrices. However,the stability properties of this propagation method are not well understood.

Having described the method we have used, we now discuss its application to our particular system. Our initial conditions for this problem consist of a ground-state He atom at the origin of the coordinate system and an incident helium nucleus, He^{2+}. In order to compare our results to existing experimental[11] and theoretical[12,13] data we have chosen the masses of the target and scattering nuclei as 4 and 3 amu, respectively. The initial target state is the lowest eigensolution of the static Hartree-Fock (HF) equation. By introducing a discrete representation of the wave function on a spatial grid we have changed the differential equation to a difference equation. The ground-state solution of the finite difference equations does not equal the ground state of the HF equation except in the limit of an infinitely small grid spacing. So we must determine the ground state of our approximate problem. We do this by integrating the

TDHF equations in imaginary time, $t \rightarrow -it$. Starting with an approximate ground state and requiring the wave function to remain normalized, the "time-" propagated wave function will converge to the ground state.[14] It is easy to see that this is true if we expand our initial guess in terms of the real eigenfunctions ψ_n, and eigenvalues ϵ_n, of the HF equations. The evolving wave function can be written as

$$\psi(t)=\sum_n a_n \psi_n e^{-i\epsilon_n t} . \tag{13}$$

Provided our initial guess is not orthogonal to the ground state, the evolved wave function converges to the desired solution with the excited components dying off exponentially.

The scattering calculations consist of following the time evolution of the electronic wave function through the collision until the nuclei separate to the point where the asymptotic final states may be determined. We calculate the transition probabilities to the final states of interest by projecting the wave function onto the asymptotic eigenfunctions of the system. If we do this as a function of time during the collision, we observe the probabilities approach the asymptotic values although this is not generally true of TDHF equations (see below). When they have become stable, we stop the propagation.

We have found it necessary to make one further approximation due to the finite difference technique used. The singularities in the potential at the two nuclei are modified by allowing the nuclei to have finite size. This is particularly important in the case of the scattering nucleus, the position of which changes constantly relative to the nearby grid points. This would cause severe numerical problems. Although the finite nuclear size reduces the binding energy of the electrons slightly, it does not seem to significantly affect transition probabilities.

CALCULATIONS AND RESULTS

We have calculated the time evolution of the electronic wave function during the collision of a helium nucleus with a ground-state helium atom. We determined transition probabilities for the two processes,

$$^3\mathrm{He}^{2+}+{}^4\mathrm{He}(1s^2)\xrightarrow{P_0}{}^3\mathrm{He}^{2+}+{}^4\mathrm{He}(1s^2) \tag{14a}$$

and

$$^3\mathrm{He}^{2+}+{}^4\mathrm{He}(1s^2)\xrightarrow{P_2}{}^3\mathrm{He}(1s^2)+{}^4\mathrm{He}^{2+} \tag{14b}$$

for a fixed laboratory scattering angle and a range of collision energies. The elastic P_0 and double charge transfer P_2 probabilities are compared with experimental results of Keever and Everhart (KE) and with theoretical results of Harel and Salin[12] (HS) and of Lopez *et al.*[13] (LMPRY).

The integration parameters used in these calculations are collected in Table I. The incident particle was approximately 4 Å from the target when the integration was begun and was a similar distance away when the asymptotic analysis was completed. The results were insensitive to an increase of this distance. We used an integration time step of 1–4 Å/c with the value chosen so that 600–700 integration steps were required for each collision. The spatial grid contained 20 720 points. Each calculation required approximately 12 min on the CRAY-1 computer. The nuclear radius used in the reported calculations is 0.06 Å. We also performed calculations with half as many grid points in each direction with twice the time step, and with the nuclear size twice as large. We found the answers shifted by, at most, a few percent for any of these changes. Doubling the size of the nucleus shifted the peak positions by approximately 20% of their widths at half maximum and their heights were changed by 20 to 30%. Of course, when the peaks shift, the results at a particular energy can change quite dramatically. However, the overall qualitative agreement remains good.

As discussed above we generated our initial state by integrating the TDHF equations in imaginary time. We used a single Gaussian with an exponential parameter of two for our initial guess and converged to the ground state in about 30 iterations. We obtained a ground-state energy of −77.7598 eV compared to the restricted Hartree-Fock (RHF) limit of −77.8692 eV.[15] Errors in this number are

TABLE I. Integration parameters.

Δr	0.06 Å
Δz	0.06 Å
N_r	80
N_z	259
Δt	1–4 Å/c
p_r (nuclear radius)	0.06 Å
b (impact parameter)	0.009–0.063 Å
n_t (number of time steps)	600–700

due to both the finite size of the nucleus and the finite difference approximation. The result for twice the grid spacing and for a nucleus with twice the diameter is -75.5550 eV.

Having obtained our initial wave function, we follow its time evolution through the collision with the scattering nucleus by repeated evaluation of the propagation equation [Eq. (12)]. The time-dependent position of the scattering nucleus is determined by a Coulomb trajectory. For the energies considered, the trajectory, to a good approximation, consists of two straight line segments joined at the point of closest approach between the two nuclei. The angle between the line segments is chosen to be consistent with a laboratory scattering angle of 3°. The actual Coulomb trajectory deviates from the two straight lines only when the nuclei are very close together and well inside the electronic charge cloud. Obviously, the field due to the scattering nucleus is not cylindrically symmetric in our coordinate system except for the case of a head-on collision. In order that our assumption of cylindrical symmetry be accurate, we are restricted to considering only small impact parameters and small scattering angles. (If this impact parameter is too small, the consequent large scattering angle negates our assumption.) In the axial symmetric approximation the potential due to the scattering nucleus [the last term in Eq. (2)] is given by

$$\int_0^{2\pi} \frac{d\phi}{|\vec{R}-\vec{r}|} = \int_0^{2\pi} \frac{d\phi}{[(Z-z)^2+(b-r\cos\phi)^2+(r\sin\phi)^2]^{1/2}}$$
$$=\pi[2/(a+c)^{1/2}+c/(a+c)^{3/2}+\cdots], \qquad (15)$$

where $a+c=(Z-z)^2+(r+b)^2$, $c=2rb$, and Z and b are the coordinates of the scattering nucleus. For small values of b it was sufficient to keep the first two terms in the above expansion to obtain stable results.

Finally, we report calculations using two different procedures. The first of these simply uses the Coulomb trajectory for the ${}^3\mathrm{He}^{2+}$-${}^4\mathrm{He}^{2+}$ system with an impact parameter chosen so that in the laboratory reference frame the scattering angle is 3°. To allow for the recoil of the target nucleus the scattering angle in our coordinate system is 5.25°. At the largest separations, the trajectory reaches distances >0.2 Å from the z axis. We were concerned that the electrons transferred to the scattering nucleus would see an attraction significantly different from the true interaction due to the corrections given in Eq. (15). Therefore, we performed a second series of calculations using, for the first half of the collision, the z axis of our coordinate system which is labeled z_1 in Fig. 1 and then shifting to the z axis labeled by z_2 for the second half. We noted in our earlier calculations that at the distance of closest approach the charge density collapses around the two nuclei which, for the small impact parameters considered, must appear to the electrons to be a Be nucleus. Thus we change coordinate systems in the middle of the calculations and assume the compact wave function is unaltered by the shift. Throughout the collision the distance of the scattering nucleus from the axis is approximately equal to the impact parameter. By tilting the axes this way during the collision we assume that we obtain a more accurate representation of the charge-exchange states asymptotically. The results are, in fact, better.

KE measured[11] the direct scattering and two-electron capture probabilities at a scattering angle of 3° for collision energies from 3 to 100 keV. They did not distinguish ground and excited product states. We have calculated probabilities only for elastic P_0 and double charge exchange into the ground state P_2. We presume these are the dominant contributions to the probabilities reported by KE. We show the comparison of our two calculations with the experimental results in Fig. 2. The results of two earlier theoretical efforts which utilize molecular basis set expansions to approximate the electronic wave functions are shown also. The earliest of these by LMPRY, employed a three-term molecular state expansion and Coulomb trajectories for the nuclei.[12] Their results for double charge transfer agree qualitatively with experiment. HS expand the wave function in a linear combination of symmetrized products of one electron, diatomic molecular orbitals.[13] They use the impact-parameter method (rectilinear trajectories) and include 12 molecular states in their expansion. They

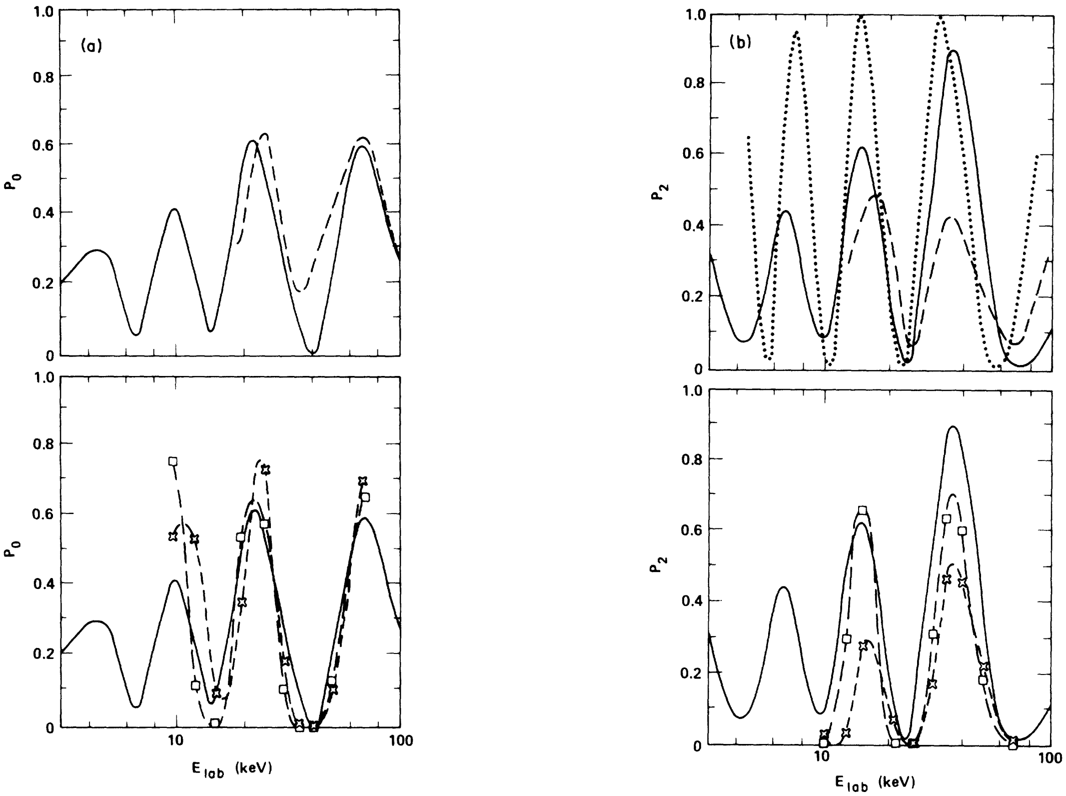

FIG. 2. Probabilities P_n for n electron capture for collision energies in keV and at a laboratory scattering angle of 3°. Experiment —— (KE); theory · · · · (LMPRY), — — — (HS), ——×—— (present), ——□—— (present, modified). × and □ indicate calculated points.

find that at the collision energies they considered (>20 keV) the symmetric double charge exchange [reaction (14b)] completely dominates the two-electron transfer probability. The agreement with experiment of our TDHF results is at least as good as the results of the elaborate calculations of HS.

One of the more interesting products of time-dependent calculations is the actual evolution of the wave function during the collision. We show in Figs. 3 and 4 density plots of the wave function at particular instants in time. The scattering nucleus initially lies to the right of the target atom and moves to the left past the stationary target nucleus during the collision. In Fig. 3 the collision results in a large probability for double charge exchange and in Fig. 4 the elastic channel is the most probable. This can be seen from the larger charge density around either the scattering or the target nucleus in the final state in each figure. Note that in both cases the charge density at the midpoint of the collision collapses significantly, then expands quite rapidly. Owing to the crude treatment of the wave function at the edges of the grid, there appears at later times in the calculations some pieces of wave function which correspond to ionized electrons being reflected by the boundary. Note that these pieces correspond to a very small fraction of the total wave function. These contours are lower by several orders of magnitude from the peak densities.

Finally, since we can project our wave function at any time onto asymptotic eigenfunctions, we can consider the adequacy of an atomic basis expansion in representing the electronic state. In Fig. 5 we show the projections of the TDHF wave function onto the two final states [represented by reactions (14a) and (14b)] as a function of time at energy $E=35$ keV. Note the oscillatory behavior of the transfer probability near the midpoint of the collision. The wave function for the charge-exchange state is constructed by multiplying ground-state wave function, centered at the projectile, by the plane wave factor e^{ikz}, where k is the wave number of an electron moving with the local velocity of the scattering nucleus. We can see from Fig. 5 that the sum of the two probabilities is less than 1 indi-

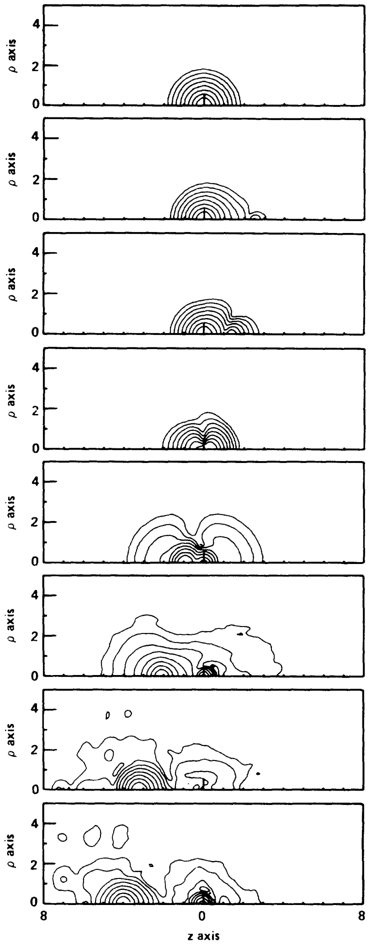

FIG. 3. Charge-density plots at various times during the collision. The radial coordinate is ρ. Note large transfer of probability at later times (P_2, large). Contours separated by $\sqrt{10}$. $E_{\mathrm{lab}}=35$ keV.

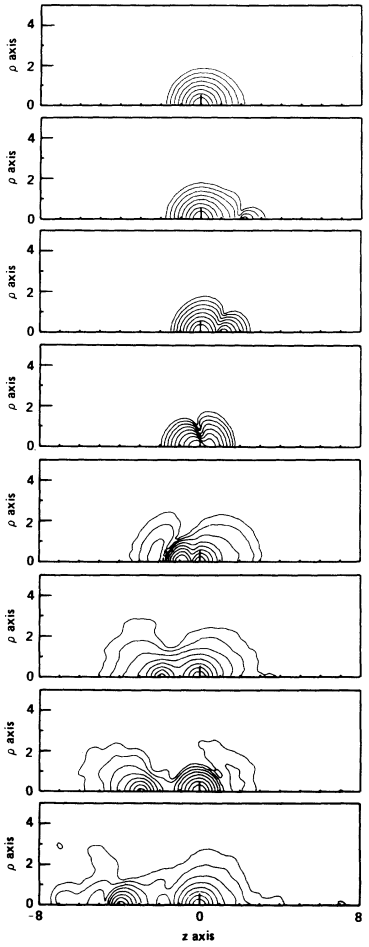

FIG. 4. Charge-density plots (P_0, large). $E_{\mathrm{lab}}=20$ keV.

cating that, as one would expect, a two-state expansion is inadequate for this case. In fact, if the two-state basis were sufficient, the sum of the probabilities would be larger than 1 due to the nonorthogonality of the states.

CONCLUSIONS

We have shown that it is feasible to calculate reasonably accurate charge-transfer probabilities over a substantial range of collision energies for systems with more than one electron using the TDHF method. Our results compare well with the existing experimental data, reproducing the peak heights and positions somewhat better than the previous molecular basis set calculations. In principle, we would also project our final wave functions onto single charge-exchange final states and onto excited states. The excited states, of course, cannot be generated by the imaginary time propagation technique if they are not the lowest state of a given symmetry. The major limitation on our

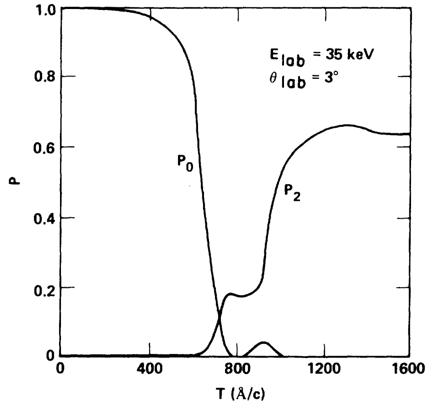

FIG. 5. Time-dependent projections onto atomic (asymptotic) states.

present method is the small range of impact parameters which can be treated accurately. We are currently extending the method to solve the TDHF equations in the rotating coordinate system whose *z* axis follows the internuclear axis throughout the collision. In this case there is coupling between states with different projections of electronic orbital angular momentum along this axis due to Coriolis forces. Fortunately, for electrons, the number of such angular momentum states which are important is limited so that it is feasible to generate complete cross sections.

One of the remaining problems in these calculations is to find a way to determine the ionization probabilities. Since in ionic systems and even in neutral systems there exists an infinite number of bound states, we cannot determine the ionization fraction by projecting out the bound contributions.[9a] A second major need is to find a prescription for projecting wave functions of systems with more than three electrons onto Hartree-Fock final states. Owing to the nonlinearity of the HF equations, the transition amplitudes obtained by projecting the TDHF wave function onto a set of final states oscillate in time even asymptotically.[16] Possible remedies for this problem have been suggested but not thoroughly tested.[4(b),4(c),17] If these two problems can be solved, it would seem possible to use TDHF calculations for atomic collisions over the entire range of energies which are too high for molecular basis expansions to be feasible and too low for the atomic expansions to be practical.

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[1] (a) J. B. Delos, Rev. Mod. Phys. 53, 287 (1981); (b) B. C. Garrett and D. G. Truhlar, in *Modern Theoretical Chemistry: Advances and Perspectives*, edited by D. Henderson (Academic, New York, 1980), Vol. 6; (c) E. W. McDaniel, M. R. Flannery, H. W. Ellis, F. L. Eisele, W. Pope, and T. G. Roberts, *Compilation of Data Relevant to Rare-Gas and Rare-Gas Monohalide Excimer Lasers* (U. S. Army Missile Research and Development Command, Redstone Arsenal, Alabama, 1977), Vol. I Technical Report No. H-78-1; (d) *Structure and Collisions of Ions and Atoms, Topics in Current Physics*, edited by I. A. Sellin (Springer, New York, 1978), Vol. 5; (e) C. F. Barnett, J. A. Ray, E. Ricci, I. Wilker, E. W. McDaniel, E. W. Thomas, and H. G. Gilbody, Controlled Fusion Atomic Data Center, Oak Ridge National Laboratory, Oak Ridge, Tennessee, Report No. ORNL5206 (unpublished).

[2] (a) D. R. Bates and R. McCarroll, Proc. R. Soc. London, Ser. A 245, 175 (1958); (b) C. F. Melius and W. A. Goddard III, Phys. Rev. A 10, 1541 (1974); (c) J. Vaaben and K. Taulbjerg, J. Phys. B 14, 1815 (1981).

[3] (a) T. G. Schmalz, E. B. Stechel, and J. C. Light, J. Chem. Phys. 70, 5660 (1979); (b) J. B. Delos, Phys. Rev. A 23, 2301 (1981).

[4] (a) V. Maruhn-Rezwani, N. Grun, and W. Scheid, Phys. Rev. Lett. 43, 512 (1979); (b) K. R. Sandhya Devi and S E Koonin, *ibid.* 47, 27 (1981); (c) M. Horbatsch and R. M. Dreizler, Z. Phys. A 300, 119 (1981); (d) C. Bottcher (unpublished).

[5] A. K. Kermin and S. E. Koonin, Ann. Phys. (N.Y.) 100, 332 (1976); (b) P. Bonche, S. Koonin, and J. W. Negele, Phys. Rev. C 13, 1226 (1976); (c) S. E. Koonin, K. T. R. Davies, V. Maruhn-Rezwani, H. Feldmeier, S. J. Krieger, and J. W. Negele, *ibid.* 15, 1359 (1977); (d) H. Flocard, S. E. Koonin, M. S. Weiss, *ibid.* 17, 1682 (1978); (e) K. R. Sandhya Devi, M. R. Strayer, and J. M. Irvine, J. Phys. G 4, L97 (1978).

[6] D. W. Peaceman and H. H. Rachford, J. Soc. Indust. Appl. Math. 3, 28 (1955).

[7] (a) R. Varga, *Matrix Iterative Analysis* (Prentice Hall, Englewood Cliffs, N.J., 1962); (b) A. R. Mitchell, *Computational Methods in Partial Differential Equations* (Wiley, London, 1969).

[8] E. A. McCullough, Jr. and R. E. Wyatt, J. Chem. Phys. 54, 3578 (1971); see also Ref. 7(a), p. 262.

[9] (a) K. C. Kulander, J. Chem. Phys. 69, 5064 (1978); (b) K. R. Sandhya Devi and M. R. Strayer, Phys. Lett. 77B, 135 (1978).

[10] H. Flocard and M. S. Weiss, Phys. Lett. (in press); see also Ref. 5(d).

[11] W. C. Keever and E. Everhart, Phys. Rev. 150, 43 (1966)

[12] C. Harel and A. Salin, J. Phys. B 13, 785 (1980).

[13] V. Lopez, A. Macias, R. D. Piacentini, A. Riera, and M. Yanez, J. Phys. B 11, 2889 (1978).

[14] K. T. R. Davies, H. Flocard, S. Krieger, and M. S. Weiss, Nucl. Phys. A342, 111 (1980).

[15] H. F. Schaefer III, *The Electronic Structure of Atoms and Molecules* (Addision-Wesley, Reading, Mass., 1972), p. 88.

[16] J. J. Griffin, P. C. Lichtner, and M. Dworzecka, Phys. Rev. C 21, 1351 (1980).

[17] Y. Alhassid and S. E. Koonin, Phys. Rev. C 23, 1590 (1981); see also Refs. 4(b) and 4(c).