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# On-shell coupled-channel approach to proton-hydrogen collisions without partial-wave expansion

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A fully quantal approach to proton collisions with hydrogen based on the atomic-orbital close-coupling method is presented. The method leads to a system of coupled three-dimensional momentum-space integral equations for the scattering amplitudes. These equations are reduced to two-dimensional ones using an on-shell approximation. Furthermore, by considering the symmetry of the problem, we demonstrate that these can be reduced to just one dimension. The resulting equations are solved without partial-wave expansion. Cross sections for electron transfer in proton collisions with the ground state of atomic hydrogen are calculated and shown to agree well with experiment over a wide energy range.

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## I. INTRODUCTION

The dominant mechanism by which charge exchange in ion-atom collisions takes place can be quite different at varying energies. The theory of this process for a particular energy range is well developed [1]. At very low energies the whole ion-atom system can be considered as a quasimolecule. This feature is successfully exploited in expansion methods utilizing molecular orbitals (MO's). A recent example is the MO method of Krstic and Schults [2]. Methods useful in the intermediate-energy region where the impact velocity is comparable to that of the electron of the target atom include atomic-orbital (AO) close-coupling [3], hyperspherical close-coupling [4], electron-nuclear dynamics (END) formalism [5], and pseudostate methods [6]. At higher energies perturbation methods based on the distorted-wave formalism are widely used [7] which include the continuum distorted wave (CDW) [8], boundary corrected Born [8] approximations, and first- and second-order methods based on the Faddeev-Watson series [9]. The methods based on the Faddeev equations [10,11] potentially span a wider energy range including intermediate and high energies.

Despite the progress in theoretical descriptions of ion-atom collisions mentioned above a single suitable theory to deal with projectile energies ranging from low to high energies has been lacking. To fulfill this gap, the CDW method has been applied at energies as low as 0.1 eV utilizing the impact-parameter model [12]. This makes the method arguably the most general theory of charge exchange in $H^+ + H(1s)$ collisions, spanning the entire nonrelativistic energy regime. However, the CDW method assumes penetration of the projectile into the target and therefore a more detailed justification of the method at such low energies, as well as verification of the validity of the impact-parameter model, may be required. Though being a two-state approach, the underlying theory for this semiclassical impact-parameter method turns out to be complicated and numerical calculations are described as time consuming [12].

The objective of the present paper is to demonstrate that the basic physics [13] of the most fundamental ion-atom process—scattering of a proton on the ground state of a hydrogen atom—can be described by a simple and transparent quantum-mechanical approach in a wide nonrelativistic energy regime. This approach will provide a base on which a fully quantal method will be built that is valid over a broad energy range.

Practically all approaches to ion-atom collisions we mentioned earlier, except the high-energy perturbative ones, use either the partial-wave method or the impact-parameter model in their formalism. The use of the classical impact parameter makes the method semiclassical. This naturally imposes certain limitations on the realm of validity of the method. Estimates based on a number of physical requirements show that the impact parameter model can be used at collision energies of the order of 100 eV per atomic mass unit (amu) or more [1]. The partial-wave expansion is a method of choice for low-energy approaches. The same applies to fully quantal approaches intended to span wider energy ranges which include energies below the limit mentioned above. As the energy increases the number of necessary partial waves can be as high as several thousand. In this work we explore the alternative approach of solving scattering equations directly without recourse to a partial-wave expansion.

Our approach is based on momentum-space integral equations. The momentum-space integral-equation method is widely used in scattering theory. Three-dimensional momentum-space integral equations emerge, for example, in approaches like the close-coupling approach to electron-atom scattering [14] and positronium formation [15] and the Faddeev approach to ion-atom collisions [11]. The standard technique for solving these equations is the use of a partial-wave expansion which transforms them into a sum of one-dimensional equations. With today's computer power, accurate solution of a large set of one-dimensional integral equations is a routine task [14]. However, as mentioned above, for ion-atom collisions where an extremely large number of individual partial waves contribute this technique has clear disadvantages.

Recently we solved the three-dimensional momentum-space Lippmann-Schwinger equations for an electron-hydrogen scattering model directly, without the partial-wave expansion [16]. The results reproduced those obtained with the partial-wave method indicating that direct solution of the three-dimensional integral equations for scattering can be a reliable alternative to the partial-wave expansion method. Here we extend this method to ion-atom collisions. We use atomic units except where otherwise specified.

## II. MOMENTUM-SPACE INTEGRAL-EQUATION FORMALISM

Consider the scattering of a proton on a hydrogen atom in the ground state. There could be direct scattering of the proton or the proton may leave the reaction zone, having captured the electron of the atom. In the AO close-coupling approach to the problem the total scattering wave function is expanded in terms of asymptotic channel functions with unknown coefficients. After substituting the expansion into the Schrödinger equation for the scattering wave function and using the Bubnov-Galerkin principle [17] one obtains a system of integro-differential equations for the coefficients. Following [18] this system can be transformed into a set of coupled effective two-body (Lippmann-Schwinger-type) momentum-space integral equations for transition amplitudes $T_{\beta\alpha}$:

$$T_{\beta\alpha}(\boldsymbol{q}_\beta,\boldsymbol{q}_\alpha) = V_{\beta\alpha}(\boldsymbol{q}_\beta,\boldsymbol{q}_\alpha) + \sum_{\nu=\alpha,\beta}\int d\boldsymbol{q}_\nu \frac{V_{\beta\nu}(\boldsymbol{q}_\beta,\boldsymbol{q}_\nu)T_{\nu\alpha}(\boldsymbol{q}_\nu,\boldsymbol{q}_\alpha)}{(q_\alpha^2/2M - q_\nu^2/2M + i0)}, \quad (1)$$

where $\boldsymbol{q}_\nu$ is the momentum of a freely traveling proton relative to the c.m. of the hydrogen atom in channel $\nu$, $M = m(m+1)/(2m+1)$ is the reduced mass of the two fragments, and $m$ is the mass of the proton. The effective potentials are given by

$$V_{\beta\alpha}(\boldsymbol{q}_\beta,\boldsymbol{q}_\alpha) = \langle \boldsymbol{q}_\beta|\langle\psi_\beta|\vec{H} - E|\psi_\alpha\rangle|\boldsymbol{q}_\alpha\rangle, \quad (2)$$

where $\psi_\nu$ is the ground-state wave function of hydrogen atom in channel $\nu$, $H=H_0+v$ is the total three-body Hamiltonian, $H_0$ is the three-free-particle Hamiltonian, $E$ is the total energy, $v=v_\alpha+v_\beta+v_\gamma$ is the full interaction, and $v_i$ is the interaction between particles of pair $i$, $i=\alpha,\beta,\gamma$, with $v_\gamma$ denoting the interaction in the proton-proton pair. Here we use the arrow on the differential Hamiltonian operator to indicate the direction in which it acts. In cases where there is a residual Coulomb potential in reaction channels (for example, scattering of multiply charged ions on atoms or ion-ion collisions) the plane waves in Eq. (2) should be replaced by corresponding Coulomb functions; however, this does not change the general definition given in Eq. (2) [19,20]. In the particular on-shell case, acting with the Hamiltonian operator on the bra state we have

$$V_{\beta\alpha}(\boldsymbol{q}_\beta,\boldsymbol{q}_\alpha) = \langle \boldsymbol{q}_\beta|\langle\psi_\beta|v - v_\alpha|\psi_\alpha\rangle|\boldsymbol{q}_\alpha\rangle. \quad (3)$$

Calculation of the effective potential for direct scattering $V_{\alpha\alpha}(\boldsymbol{q}'_\alpha,\boldsymbol{q}_\alpha)$ is straightforward. The effective potential for rearrangement $V_{\beta\alpha}(\boldsymbol{q}_\beta,\boldsymbol{q}_\alpha)$ in the on-shell case is given by a sum of the two terms evaluated by Oppenheimer [21], Brinkman and Kramers [22], and Jackson and Schiff [23].

At this stage conventional approaches use expansion of $V_{\beta\alpha}(\boldsymbol{q}_\beta,\boldsymbol{q}_\alpha)$ and $T_{\beta\alpha}(\boldsymbol{q}_\beta,\boldsymbol{q}_\alpha)$ into partial waves. However, for applicability of our approach across the entire energy range of interest we do not do this. We solve Eq. (1) in an on-shell approximation. A simple classical estimate shows that in proton-hydrogen collisions neglecting off-shell effects should be reasonably accurate. Since the probability that the electron, while being transferred, changes the energy of the incident proton is of order $1/m$, one may expect that off-shell effects are also about $1/m$ in order of magnitude.

For the purpose of practical calculations it is convenient to make the following transformation: $\boldsymbol{q}_\beta \to -\boldsymbol{q}_\beta$. This allows one to introduce a combined amplitude $T(\boldsymbol{q}',\boldsymbol{q}) = \{T_{\alpha\alpha}(\boldsymbol{q}',\boldsymbol{q}), T_{\beta\alpha}(\boldsymbol{q}',\boldsymbol{q})\}$ and effective potential $V(\boldsymbol{q}',\boldsymbol{q}) = \{V_{\alpha\alpha}(\boldsymbol{q}',\boldsymbol{q}), V_{\beta\alpha}(\boldsymbol{q}',\boldsymbol{q})\}$. We use the spherical coordinate system $\boldsymbol{q}=\{q,\theta,\varphi\}$. For simplicity we put the $z$ axis along the incident momentum and use the compact notation $T(q,\theta',\varphi') \equiv T(q,\theta',\varphi';q,0,0)$. Then using the Cauchy formulas for the singular integral in Eq. (1) and neglecting the principal-value part we have the two-dimensional integral equation

$$T(q,\theta',\varphi') = V(q,\theta',\varphi';q,0,0) - i\pi q\int_0^\pi d\theta'' \sin\theta'' \int_0^{2\pi} d\varphi'' \times V(q,\theta',\varphi';q,\theta'',\varphi'')T(q,\theta'',\varphi''). \quad (4)$$

We see that in the on-shell approximation our close-coupling method coincides with that of Chaudhuri *et al.* [24] based on a similar approximation [18] to the Alt-Grassberger-Sandhas form [25] of the Faddeev equations. However, Alt *et al.* [11] suggest that the results of Chaudhuri *et al.* [24] are too low (by as much as a factor of 2 at 1 keV) at the lower energies. Hence, the true potential of the on-shell approach has not yet been assessed.

In solving Eq. (4) we use an important conclusion established recently in [16]. By solving a three-dimensional integral equation for scattering amplitude $T(q,\theta,\varphi)$ in electron-hydrogen collisions using a three-dimensional quadrature we have explicitly shown that the result (when it has converged and is correct) did not depend on the variable $\varphi$. We can take advantage of this fact to substantially reduce the complexity of the problem. Since $T(q,\theta,\varphi)$ does not depend on the variable $\varphi$, we can simply set $\varphi=0$. Then from Eq. (4) we have

$$T(q,\theta',0) = V(q,\theta',0;q,0,0) - i\pi q\int_0^\pi d\theta'' \sin\theta'' K(q,\theta',\theta'')T(q,\theta'',0), \quad (5)$$

where

$$K(q,\theta',\theta'') = \int_0^{2\pi} d\varphi'' V(q,\theta',0;q,\theta'',\varphi''). \quad (6)$$

We have verified that solutions of Eqs. (4) and (5) do in fact yield the same results, though the latter required much less computation due to effectively being one dimensional. The reason that Eq. (5) can be used is that, in addition to $T(q,\theta,\varphi)$ being independent of $\varphi$, the effective potential $V(\boldsymbol{q}';\boldsymbol{q}'')$ entering Eq. (4) depends only on $q$ and $\boldsymbol{q}'\cdot\boldsymbol{q}''$. Since $\boldsymbol{q}'\cdot\boldsymbol{q}''=q^2[\cos\theta'\cos\theta''+\sin\theta'\sin\theta''\cos(\varphi'-\varphi'')]$, we

TABLE I. Elastic scattering and electron capture cross sections for $H^+$ collisions with $H(1s)$ in units of $\pi a_0^2$ [$a(\pm b)$ stands for $a \times 10^{\pm b}$].

| Energy (keV) | Elastic scattering |  | Electron capture |  |
|---|---|---|---|---|
|  | Ref. [24] | Present | Ref. [24] | Present |
| 1.0(−3) |  | 2.280(+2) |  | 3.946(+1) |
| 4.0(−3) |  | 1.782(+2) |  | 3.633(+1) |
| 1.0(−2) |  | 1.484(+2) |  | 3.410(+1) |
| 4.0(−2) |  | 1.064(+2) |  | 3.092(+1) |
| 1.0(−1) |  | 8.098(+1) |  | 2.883(+1) |
| 4.0(−1) |  | 4.626(+1) |  | 2.539(+1) |
| 1.0 | 1.686(+1) | 2.682(+1) | 1.191(+1) | 2.216(+1) |
| 2.0 | 1.132(+1) | 1.530(+1) | 1.015(+1) | 1.848(+1) |
| 5.0 | 5.653 | 5.843 | 7.345 | 1.177(+1) |
| 1.0(+1) | 2.835 | 2.645 | 4.869 | 6.550 |
| 1.5(+1) | 1.824 | 1.754 | 3.405 | 4.087 |
| 2.0(+1) | 1.357 | 1.365 | 2.451 | 2.730 |
| 3.0(+1) | 9.550(−1) | 1.003 | 1.350 | 1.382 |
| 5.0(+1) | 6.990(−1) | 7.020(−1) | 4.890(−1) | 4.716(−1) |
| 1.0(+2) | 4.170(−1) | 4.220(−1) | 7.340(−2) | 6.942(−2) |
| 2.0(+2) | 2.380(−1) | 2.397(−1) | 6.020(−3) | 5.769(−3) |
| 4.0(+2) | 1.290(−1) | 1.301(−1) | 2.890(−4) | 2.825(−4) |
| 8.0(+2) | 6.700(−2) | 6.845(−2) | 9.300(−6) | 9.180(−6) |
| 1.0(+3) | 5.500(−2) | 5.539(−2) | 2.880(−6) | 2.855(−6) |
| 2.0(+3) | 2.800(−2) | 2.838(−2) | 6.630(−8) | 6.588(−8) |

see that $V(\boldsymbol{q}';\boldsymbol{q}'')$ is a periodic function of $\varphi'-\varphi''$. This shows that if the variable $\varphi''$ runs over the full period, the value of $\varphi'$ is irrelevant. Thus, in our approach we have in fact a one-dimensional integral equation with no singularities which we solve using the standard Gauss-Legendre quadrature.

## III. RESULTS

We have calculated total electron capture and elastic scattering cross sections for $H^+$ collisions with $H(1s)$ in a wide range of energy of the incident proton spanning from 1 eV to a few MeV in the laboratory frame. We considered the two protons as distinguishable particles. Therefore, we start from the impact energy of 1 eV, above which indistinguishablity effects can be neglected. Table I shows our cross sections in comparison with those of Chaudhuri *et al.* [24], confirming the expectations of Alt *et al.* [11]. We are confident that our results are correct as we checked them using semiclassical calculations at energies where the impact-parameter model is reliable.

Figure 1 shows our results for electron-capture cross sections in comparison with other calculations and experimental data [26–34]. Despite the simplicity of the present approach the agreement between our results and the experimental data is very good over a wide range of energy. The present electron-capture cross sections underestimate the data in the 10−100-keV region. This is not surprising since at present our approach is a simple two-state one. At these energies the contribution from the excited states of hydrogen and the ionization channel reach their maxima and become significant. Also shown in this figure is the elastic scattering cross section. In Fig. 2 we present a more detailed comparison of our results with those obtained in rigorous low-energy methods which require considerable computation, whereas our calculations take only a few minutes on a standard desktop PC.

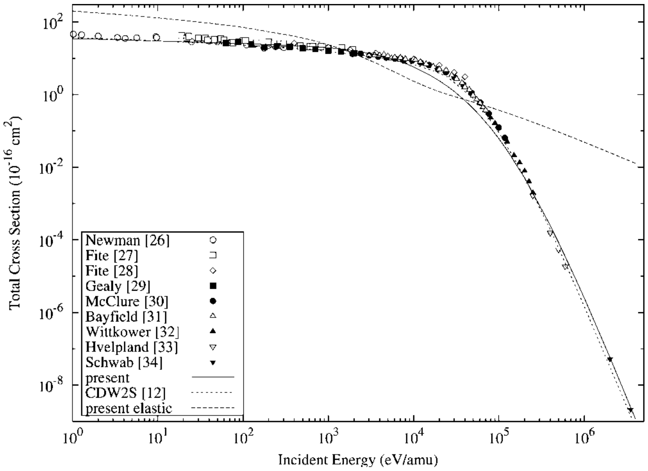

FIG. 1. Electron-capture cross sections for $H^+$ collisions with $H(1s)$. The symbols indicate experimental points while the lines show the calculations. Present results for elastic scattering are also given.

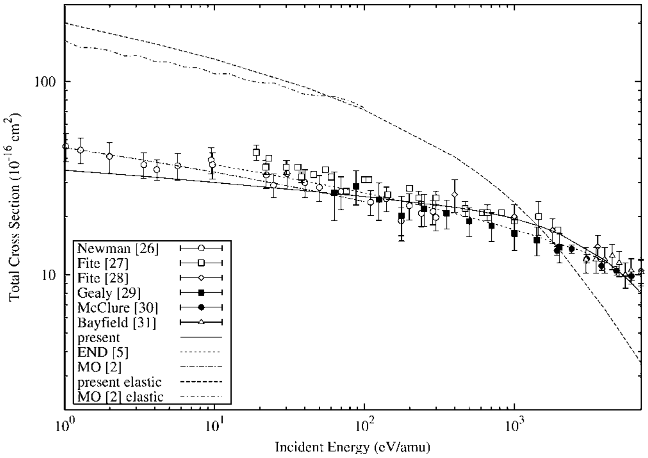

FIG. 2. Electron-capture cross sections for $H^+$ collisions with H(1*s*). The symbols indicate experimental points while the lines show the calculations. Present results and those of Krstic and Schultz [2] for elastic scattering are also given.

Figures 1 and 2 also include data [26] for electron capture in $H^+ + D$ collisions since at energies above 1 eV the isotopic effects are negligible. In fact, the present results are equally valid for all $A^+ + B$ systems, where $A, B = \mathrm{H, D, T}$.

## IV. CONCLUSION

Summarizing, in this paper we have presented a simple fully quantum-mechanical approach to proton-hydrogen collisions based on the atomic-orbital close-coupling method. The method leads to a system of coupled three-dimensional momentum-space integral equations for the scattering amplitudes. These equations have been reduced to two-dimensional ones using the on-shell approximation. The resulting equations have been solved directly without partial-wave expansion. Cross sections for electron transfer in proton collisions with the ground-state hydrogen have been calculated and shown to agree well with experiment over a wide energy range. One of the main results of the present paper is given by Eqs. (5) and (6), where by considering the symmetry properties of the problem, we showed that the resulting two-dimensional integral equations can be further reduced to just one-dimensional ones. We emphasize that this result is independent of the on-shell approximation and can be applied generally.

The on-shell approximation used in the present work does not include quantum effects like the role of virtual transitions. These can only be determined by solving the integral equations emerging in the present approach without approximation. Thus, steps in further developing this promising method would be the removal of the on-shell approximation and adding more atomic orbitals to the expansion. In addition, the lower limit of validity of the method can be shifted to sub-eV energies by taking into account the indistinguishability of the protons. A distinctive feature of the method is that it ultimately allows one to include the ionization channel in a convenient way using a square-integrable pseudobasis. The results show that the expansion method based on fully quantal formulation of the atomic-orbital close-coupling method can be a suitable base on which a more rigorous wide-energy method can be built.

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