

Implementation of nonseparable exact exchange effects in the first-order nondegenerate adiabatic theory

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We have implemented nonlocal exchange effects rigorously in the first-order nondegenerate adiabatic (FONDA) theory. This implementation requires solving integrodifferential equations that involve double integrals. Separable and model exchange approximations that simplify the inclusion of exchange in the scattering calculations have been previously implemented in the FONDA theory. The discrepancy between the exact exchange FONDA cross sections and the separable and model exchange results suggests that one needs to include exchange rigorously to obtain accurate results over a wide range of energies. Specifically, a difference of up to 30% is observed between the exact and separable exchange FONDA cross sections at near-threshold energies. At higher energies the FONDA results from the rigorous and model exchange implementations disagree by as much as 10%.

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I. INTRODUCTION

The problem of accurately calculating near-threshold inelastic electron-molecule cross sections is becoming increasingly important in such areas as gas discharge devices and pollution control [1,2]. The discrepancy between the existing experimental and theoretical results [3,4] makes this problem even more noticeable [5–8].

Two widely used methods for calculating electron-molecule cross sections are laboratory-frame close coupling (LFCC) [9–11] and adiabatic nuclei (AN) [12–19]. The LFCC method, which takes into account the full interaction between the nuclei and the scattering electron, gives accurate cross sections [20]. In this method the electron-molecule wave function is expanded in complete sets of rotational and vibrational eigenfunctions of the target and angular momentum eigenfunctions of the projectile. In scattering calculations, this expansion has to be truncated to a manageable size and still maintain the desired level of accuracy. This makes the LFCC method not applicable to any but the simplest molecules (e.g., H_2). In the AN theory, one can simplify the LFCC equations via two approximations: (i) separation of target and projectile variables in the system wave function [21]; and (ii) target state degeneracy, i.e., equating the energies of the projectile in the entrance and exit channels. These simplifications makes the AN theory applicable to systems far more complicated than those to which LFCC can be applied [22,23]. The AN method, however, breaks down near the threshold energy range [19].

An alternative method that is much more reliable near threshold and is not as demanding as LFCC was devised by Morrison and Abdolsalami [24,25]. This method,

which is called first-order nondegenerate adiabatic (FONDA), is based on the radial scattering functions of conventional body-frame fixed-nuclei (BF-FN) theory. The target state degeneracy assumption, however, is lifted which makes this method more accurate near threshold energy compared to the AN theory [25–27].

II. THEORY

Irrespective of the method used, three types of interaction will take place between the scattering electron and the target molecule [28,29]. These interactions are static, exchange, and induced polarization. Static and polarization effects in scattering calculations are discussed elsewhere [30–33]. In this paper, we briefly discuss model and separable exchange [34] in the context of the FONDA theory [35] and give a detailed discussion on the rigorous implementation of the exchange effect in this theory.

Treating exchange exactly amounts to explicit consideration of the pairwise interchange of the scattering electron with each of the target electrons. Consequently, the exchange interaction is a nonlocal effect that causes the coupled scattering equations to be of integrodifferential type. Fortunately, the exchange interaction is short range which makes it significant only when the scattering electron is close to the target molecule.

To simplify its inclusion in the scattering calculations, several models have been devised for the exchange effect [36]. One such model, which has been used in the previous FONDA calculations [26], is based on the free-electron-gas (FEG) approximation [37]. In this model potential, we approximate the exchange effect via a local

potential-energy term [36] that can be simply added to the other components of the interaction potential. Making the FEG approximation for the bound orbitals amounts to treating the target electrons as noninteracting fermions [38] occupying a volume V moving in an identical potential field with no mutual forces between them.

The particular model exchange used in our previous calculations treats the ionization potential of the neutral target I as a parameter that is tuned—hence the name tuned free-electron-gas exchange (TFEGE)—to give accurate cross sections and eigenphase sums. The tuning procedure is carried out in the BF-FN formulation within the static-exchange approximation, in which the induced polarization potential is neglected. In this particular implementation, the eigenphase sum in one symmetry at one energy is used from exact exchange calculations to adjust the parameter I so that the corresponding model exchange calculations yield the same value of the eigenphase sum [39].

Using model exchange, the laboratory-frame FONDA (LF-FONDA) K matrix becomes [26]

$$K_{j_l, j_{l_0}'}^J = -\frac{2}{(k_j k_0)^{1/2}} \sum_{\Lambda} A_{j\Lambda}^J \left[\sum_{\lambda l'} g_{\lambda}(l'; \Lambda) I_{l'\lambda}^{\Lambda}(l l_0; k_j) \right] \times A_{j_0\Lambda}^{j_0 l_0}, \quad (1)$$

where the radial integral is

$$I_{l'\lambda}^{\Lambda}(l l_0; k_j) = \int_0^{\infty} \hat{j}_l(k_j r) v_{\lambda}(r) W_{l_0}^{\Lambda}(r, k_0) dr, \quad (2)$$

and

$$K_{l' j_l, l' j_{l_0}'}^{JM} = \frac{-2}{(k_j k_0)^{1/2}} \sum_{\Lambda} A_{j\Lambda}^J \left[\sum_{l'\lambda} g_{\lambda}(l'; \Lambda) I_{l'\lambda}^{\Lambda}(l l_0; k_j) \right] + \left[\sum_{l'} \int_0^{\infty} \hat{j}_l(k_j r_1) \int_0^{\infty} K_{l'l'}^b(r_1, r_2) W_{l_0}^{\Lambda}(r_2, k_0) dr_1 dr_2 \right] A_{j_0\Lambda}^{j_0 l_0}, \quad (5)$$

where

$$K_{l'l'}^b(r_1, r_2) = r_1 r_2 \int Y_l^{\Lambda*}(\hat{r}_1) K(\bar{r}_1, \bar{r}_2) Y_{l'}^{\Lambda}(\hat{r}_2) d\hat{r}_1 d\hat{r}_2 \quad (6)$$

is the BF-FN exchange kernel and $K(\bar{r}_1, \bar{r}_2)$ is given by

$$K(\bar{r}_1, \bar{r}_2) = \sum_{n=1}^{N_{\text{occ}}} \frac{\phi_n(\bar{r}_1)}{|\bar{r}_1 - \bar{r}_2|} \phi_n^*(\bar{r}_2). \quad (7)$$

In these equations, $Y_l^{\Lambda}(\hat{r}_1)$ are the spherical harmonics with $\phi_n(\bar{r})$ representing the molecular orbitals, and the sum in Eq. (7) runs over all occupied target orbitals. The radial wave functions $W_{l_0}^{\Lambda}(r, k_0)$ can be found by solving the BF-FN radial equations [34]

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k_0^2 \right] W_{l_0}^{\Lambda}(r, k_0) = 2 \sum_{l'} V_{ll'}^{\Lambda}(r) W_{l_0}^{\Lambda}(r, k_0) + \int_0^{\infty} K_{l'l'}^b(r, r_1) W_{l_0}^{\Lambda}(r_1, k_0) dr_1. \quad (8)$$

$$g_{\lambda}(l'; \Lambda) = \left[\frac{2l'+1}{2l+1} \right]^{1/2} C(l'\lambda l; \Lambda 0) C(l'\lambda l; 00). \quad (3)$$

Here, $W_{l_0}^{\Lambda}(r, k_0)$ represents the BF-FN radial wave function and $v_{\lambda}(r)$ is the expansion coefficient of the interaction potential in terms of Legendre polynomials, with $A_{j\Lambda}^J$, $\hat{j}_l(k_j r)$, and $C(l'\lambda l; \Lambda 0)$ being the frame transformation matrix, Ricatti Bessel function, and Clebsch Gordan coefficients, respectively. In these equations, k_0^2 and k_j^2 represent the initial and final energy of the scattering electron. It should be noted that in (1) the rigid-rotor approximation is made; i.e., the vibrational motion of the target molecule is ignored. The radial wave function is obtained by solving the following coupled radial equation:

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k_0^2 \right] W_{l_0}^{\Lambda}(r, k_0) = 2 \sum_{l'} V_{ll'}^{\Lambda}(r) W_{l_0}^{\Lambda}(r, k_0), \quad (4)$$

which is the standard BF-FN radial equation. Here, l corresponds to the orbital angular momentum of the scattering electron, l_0 designates a particular linearly independent solution, and Λ represents the projection of the orbital angular momentum of the scattering electron on the internuclear axis.

It is advantageous to present the appropriate equations for exact exchange FONDA theory before discussing separable exchange in the context of this theory. With exchange treated exactly, within the static-exchange approximation [40,41], the LF-FONDA K matrix is given by [26]

Note that the first and second terms on the right-hand side of Eqs. (5) and (8) represent the static-polarization and the exchange effects, respectively. Now, we can discuss the FONDA theory assuming separable exchange.

The variables \bar{r}_1 and \bar{r}_2 in (7) can be decoupled, resulting in the breakdown of the double integral in (5) into the product of two integrals by using the separable representation of the exchange kernel [26]. To this end, we expand the exchange kernel $K(\bar{r}_1, \bar{r}_2)$ in terms of an orthonormal basis set $\{X^i(\bar{r})\}$. Making this expansion on both \bar{r}_1 and \bar{r}_2 , we get

$$K(\bar{r}_1, \bar{r}_2) = \sum_{jk} X^j(\bar{r}_1) K_{jk} [X^k(\bar{r}_2)]^*, \quad (9)$$

where

$$K_{jk} = \int \int [X^j(\bar{r}_1)]^* K(\bar{r}_1, \bar{r}_2) X^k(\bar{r}_2) d\bar{r}_1 d\bar{r}_2. \quad (10)$$

The angular dependence in Eq. (9) can be removed by expanding the basis functions in terms of spherical harmonics as

$$X^j(\hat{r}) = \sum_l X_{lm}^j(r) Y_l^m(\hat{r}). \quad (11)$$

Substituting (11) into (9) and integrating over the angular variables, we obtain [26]

$$K_{ll'}^b(r_1, r_2) = \sum_{jk} X_{lm}^j(r_1) K_{jk} [X_{l'm}^k(r_2)]^* \\ = \mathbf{X}_{lm}(r_1) \mathbf{K} [\mathbf{X}_{l'm}(r_2)]^\dagger. \quad (12)$$

In (12), $\mathbf{X}_{lm}(r_1)$ and \mathbf{K} represent a row matrix containing the elements $X_{lm}^j(r_1)$ and a full matrix containing the elements K_{jk} , respectively. The double sum in Eq. (12) can be simplified to a single sum if the matrix \mathbf{K} is replaced by its diagonal form. Hence we can introduce a unitary transformation \mathbf{U} such that

$$\mathbf{U}^\dagger \mathbf{K} \mathbf{U} = \mathbf{E}, \quad (13)$$

where

$$E_{jk} = e_j \delta_{jk}, \quad (14)$$

with $\{e_j\}$ being the eigenvalues of \mathbf{K} . Substituting (13) into (12) and introducing

$$\bar{\mathbf{X}}_{lm}(r_1) = \mathbf{X}_{lm}(r_1) \mathbf{U}, \quad (15)$$

we obtain

$$K_{ll'}^b(r_1, r_2) = \sum_j \bar{X}_{lm}^j(r_1) e_j [\bar{X}_{l'm}^j(r_2)]^* \\ = \bar{\mathbf{X}}_{lm}(r_1) \mathbf{E} [\bar{\mathbf{X}}_{l'm}(r_2)]^\dagger. \quad (16)$$

Using (16) and (5), we can write the LF-FONDA K matrix as [26]

$$K_{jl,j'l'}^{JM} = \frac{-2}{(k_j k_0)^{1/2}} \sum_\Lambda A_{j\Lambda}^{Jl} \left[\left[\sum_{l'\lambda} g_\lambda(l'l'; \Lambda) I_{l'\lambda}^\Lambda(l_0; k_j) \right] + \sum_{l'} \sum_j e_j M_m^j(l, k_j) N_{l'm}^{j\Lambda}(l_0, k_j) \right] A_{j_0\Lambda}^{Jl_0}. \quad (17)$$

Here

$$M_m^j(l, k_j) = \int_0^\infty \hat{j}_l(k_j r_1) \bar{X}_{lm}^j(r_1) dr_1, \quad (18)$$

and

$$N_{l'm}^{j\Lambda}(l_0, k_j) = \int_0^\infty W_{l_0}^\Lambda(r_2, k_0) [\bar{X}_{l'm}^j(r_2)]^* dr_2. \quad (19)$$

In our previous FONDA calculations of the electron- H_2 cross sections assuming separable exchange, we used the occupied and unoccupied (virtual) orbitals of H_2 as the basis for the expansion of the exchange kernel. These orbitals were expanded in terms of a Gaussian basis set containing 35 functions of s , p_x , p_y , and p_z type [26]. Now, we discuss the implementation of the exact (rigorous) exchange in the FONDA theory.

The BF-FN radial wave functions can be found by solving Eq. (8) using the linear-algebraic (LA) method [34]. This method uses a Gaussian quadrature to convert

the integrals in this equation into sums. As a result, the set of coupled equations is converted into a set of linear algebraic equations which can easily be solved. Next, we find the FONDA K matrix by transforming Eq. (5) into a form suitable for the LA method. To simplify the analysis, we break the FONDA K matrix into its static-polarization and exchange components as follows:

$$K_{jl,j'l'}^J = K_{jl,j'l'}^J(\text{static} + \text{polarization}) + K_{jl,j'l'}^J(\text{exchange}), \quad (20)$$

where $K_{jl,j'l'}^J(\text{static} + \text{polarization})$ and $K_{jl,j'l'}^J(\text{exchange})$ represent the first and second terms in (5), respectively. As far as the static-polarization part is concerned, we can easily use a Gaussian quadrature to transform the radial integral (2) into a sum. For the exchange part, however, we can write

$$K_{jl,j'l'}^J(\text{exchange}) = - \frac{2}{(k_j k_0)^{1/2}} \sum_\Lambda A_{j\Lambda}^{Jl} \left[\sum_{l' \alpha\beta} \sum_j j_l(k_j r_\alpha) K_{ll'}^b(r_\alpha, r_\beta) W_{l_0}^\Lambda(r_\beta, k_0) \omega_\alpha \omega_\beta \right] A_{j_0\Lambda}^{Jl_0}, \quad (21)$$

where r_α and ω_α are a set of points and weights for a given quadrature. This equation can be written as

$$K_{jl,j'l'}^J(\text{exchange}) = - \frac{2}{(k_j k_0)^{1/2}} \sum_\Lambda A_{j\Lambda}^{Jl} \left[\sum_{l' \beta} \sum_\beta W_{l_0}^\Lambda(r_\beta, k_0) \omega_\beta X_{ll'}(r_\beta) \right] A_{j_0\Lambda}^{Jl_0}, \quad (22)$$

where

$$X_{ll'}(r_\beta) = \sum_\alpha \hat{j}_l(k_j r_\alpha) K_{ll'}^b(r_\alpha, r_\beta) \omega_\alpha. \quad (23)$$

The exchange kernel in (23) can be expressed as [34]

$$K_{ll'}^b(r_\alpha, r_\beta) = \sum_{i=1}^N \sum_{l''l'''\lambda} g_\lambda(l'l''l'''\lambda) |mm_i\rangle \phi_{l''m_i}^i(r_\alpha) \phi_{l'm_i}^i(r_\beta) \\ \times (r_\beta) \frac{r_{<}^\lambda}{r_{>}^{\lambda+1}}, \quad (24)$$

where $g_\lambda(l'l''l'''\lambda | mm_i)$ is a product of four vector-coupling coefficients [42] and $r_{<}$ ($r_{>}$) the minimum (maximum) of r_α and r_β . Substituting (24) into (23) and splitting the g_λ factor, we get [34,42]

$$X_{ll'}(r_\beta) = \sum_{i=1}^{N_{\text{occ}}} \sum_{\mu=-|m_i|}^{|m_i|} \phi_{l''m_i}^i(r_\beta) C_a^{l'''\mu}(l'\lambda | m\mu - m) \\ \times Y_{l\mu}^\lambda(r_\beta), \quad (25)$$

where

$$Y_{i\mu}^{\lambda}(r_{\beta}) = \sum_{l''} C_a^{l''\mu}(l_{\lambda} | -m m + \mu) \mathcal{Y}_{\lambda}^{l''l}(r_{\beta}), \quad (26)$$

and

$$\mathcal{Y}_{\lambda}^{l''l}(r_{\beta}) = \sum_{\alpha} \omega_{\alpha} \phi_{l''m_i}^{i,m_i}(r_{\alpha}) \frac{r_{\alpha}^{\lambda}}{r_{\alpha}^{\lambda+1}} \hat{j}_l(k_j r_{\alpha}). \quad (27)$$

In Eq. (25) the sum over projections of the symmetry of the bound orbitals m_i is explicitly shown. Equation (27) can be divided into two sums; one for $1 < \alpha < \beta$ and one for $\beta < \alpha < N_p$, where N_p is the number of points used in the Gaussian quadrature. This equation then becomes

$$\mathcal{Y}_{\lambda}^{l''l}(r_{\beta}) = r_{\beta}^{-\lambda-1} \gamma_{\lambda}^1 + r_{\beta}^{\lambda} \bar{\gamma}_{\lambda}^1, \quad (28)$$

where

$$\gamma_{\lambda}^1 = \sum_{\alpha=1}^{\beta-1} \omega_{\alpha} \phi_{l''m_i}^{i,m_i}(r_{\alpha}) r_{\alpha}^{\lambda} \hat{j}_l(k_j r_{\alpha}), \quad (29)$$

and

$$\bar{\gamma}_{\lambda}^1 = \sum_{\alpha=\beta}^{N_p} \omega_{\alpha} \phi_{l''m_i}^{i,m_i}(r_{\alpha}) r_{\alpha}^{-\lambda-1} \hat{j}_l(k_j r_{\alpha}). \quad (30)$$

A computer program based on the LA method is utilized to find the FONDA K matrix. The original version of this program, which was developed by Collins and Schneider, finds the exact exchange BF-FN radial wave functions. As a result, this code had to be modified for the FONDA theory.

III. RESULTS AND DISCUSSIONS

Before discussing the results, it is important to comment on Eqs. (16) and (24), which give the exchange kernel in rigorous and separable forms, respectively. From these equations, it is clear that the number of sums that must be performed in (16) is smaller than in (24). This reduction, however, is not as dramatic as it might seem, because the summations in (24) extend only over the occupied molecular orbitals. The expansions of the bound orbitals usually require only a few terms since the exchange interaction depends on the diffuse electronic charge density and not on the nuclear potential, which is strongly singular (in the rigid-rotor approximation). This, however, does not apply to the expansion in Eq. (16). This equation forms an approximate representation of the exchange kernel, the accuracy of which improves as more basis functions are added. Consequently, using the separable form of the exchange kernel will be compositionally more efficient only if the number of basis functions needed to get accurate results is smaller than the total number of terms that appear in Eq. (24).

In this paper, we present exact exchange FONDA results for the electron- H_2 system. The static part of the interaction potential has been included in the scattering calculations by averaging the Coulomb potential energy over the $X^1\Sigma_g^+$ electronic target wave function. This potential has been expanded in terms of Legendre polynomials in which four terms ($\lambda=0,2,4,6$) have been retained. For induced polarization, we have used Morrison

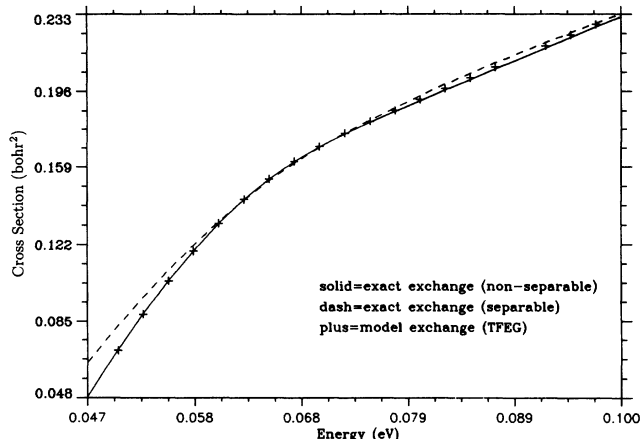


FIG. 1. Integrated LF-FONDA cross sections for rotational excitation $j_0=0$ to $j=2$ of H_2 , using exact (nonseparable) exchange (solid curve), separable exchange (dashed curve), and Σ_u tuned TFEG model exchange (pluses).

and Gibson's BTAD (better than adiabatic) potential [33], which incorporates the effects due to the distortion of probability density of the target electrons caused by the scattering electron in the calculations. The equilibrium internuclear distance is $R = 1.4a_0$ with spherical and nonspherical polarizabilities equal to $5.1937a_0^3$ and $1.3053a_0^3$, respectively. The quadrupole moment of H_2 has been set to $0.45174a_0^2$ with rotational constant equal to $0.27727 \times 10^{-3} E_h$.

The radial equation has been integrated to $r_{\max} = 600a_0$ to ensure convergence of the cross sections and eigenphase sums for Σ, Π symmetries to within 1% [43]. The LA method has been used throughout the whole region ($r=0.0-600.0a_0$) [44]. It consists of 95 points for all 9 channels used in these calculations. The points are divided between these regions as follows: 9 points from 0.0 to 0.7, 26 points from 0.7 to 1.5, 10 points from 1.5 to 2.5, 10 points from 2.5 to 10.0, 20 points from 10.0 to 130.0, and 20 points from 130.0 to 600.0. This arrangement of

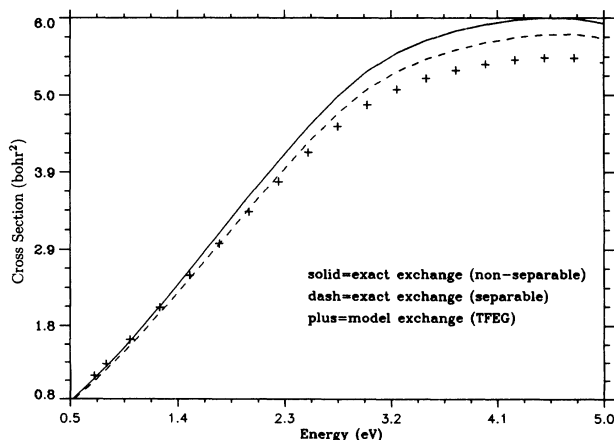


FIG. 2. Integrated LF-FONDA cross sections for rotational excitation $j_0=0$ to $j=2$ of H_2 , using exact (nonseparable) exchange (solid curve), separable exchange (dashed curve), and Σ_n tuned TFEG model exchange (pluses).

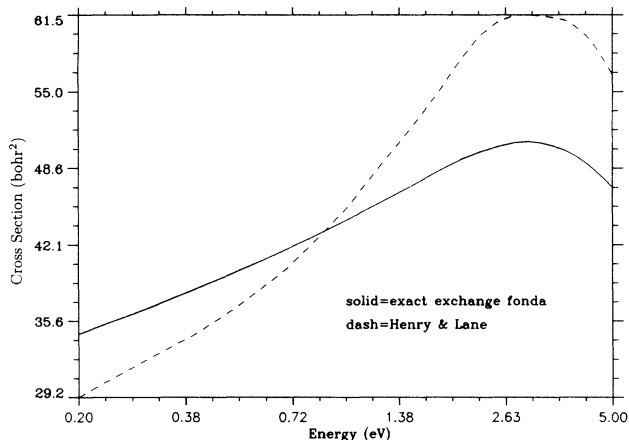


FIG. 3. Total integrated elastic, $j_0=0$ to $j=0$, cross sections of H_2 using LF-FONDA method (solid curve) and Henry and Lane results (dashed curve).

regions and points has been obtained after extensive convergence tests on the cross sections. Finally, five terms have been retained in the expansion of the occupied orbitals in terms of spherical harmonics [34].

The integrated LF-FONDA cross sections for $j_0=0$ to $j=2$ rotational excitation are shown in Figs. 1 and 2. Figure 1 shows these cross sections in the low energy range. From this figure, it is clear that the cross sections obtained using exact (rigorous) and model (TFEG) exchange are in excellent agreement. This is because of strong influence of p ($l=1$) waves on these cross sections; the tuning of the TFEG exchange potential used in these calculations is performed in the Σ_u symmetry [45]. At higher energies, however, there could be noticeable differences between the exact and model exchange FONDA results, as is obvious from Fig. 2 which shows the $j_0=0$ to $j=2$ cross sections at these energies. This is due to the fact that the tuning of the TFEG exchange potential is performed at one energy, which makes this potential inaccurate for energies far from the tuning energy. The difference between the results obtained from separable exchange and exact (rigorous) exchange near threshold and high energies indicates that the basis used to expand the exchange kernel needs improvement. Finally, in Figs. 3 and 4, the exact exchange LF-FONDA results are compared to the elastic and rotational excitation cross sections calculated by Henry and Lane [11]. These figures indicate that there is a significant difference be-

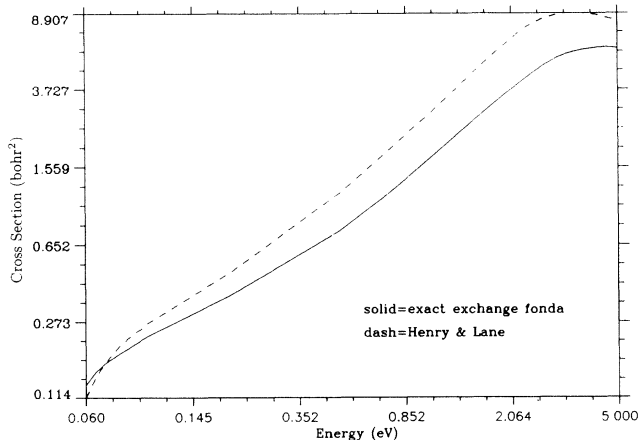


FIG. 4. Total integrated cross sections of H_2 for rotational excitation $j_0=0$ to $j=2$ using LF-FONDA method (solid curve) and Henry and Lane results (dashed curve).

tween the results of these two studies especially for elastic scattering cross sections. For $j_0=0$ to $j=2$ rotational excitation cross sections, the results obtained from LF-FONDA theory is lower than the results from Henry and Lane, except very near threshold.

IV. CONCLUSION

The results discussed above reveal that the method used to implement the exchange effect in the FONDA theory could noticeably affect the cross sections. Some of these implementations simplify the procedure for calculating the cross sections, but the results may not be as accurate as desired. Treating exchange rigorously gives the most accurate cross sections at the cost of requiring solution of integrodifferential equations involving double integrals. However, because of recent advances in numerical techniques and computer technology, this is not a significant problem especially for small systems.

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- [39] The tuning process is not required for larger molecules. For small systems we can also avoid tuning if we impose orthogonality constraints, as required by the continuum Hartree-Fock theory for scattering from closed-shell targets. However, this is not always accurate enough.
- [40] This means that as far as exchange is concerned, we neglect the distortion of the molecular orbitals by the scattering electron. This would allow us to write the total wave function as the product of the molecular wave function and the scattering wave function. For more information see Ref. [41].
- [41] K. Jung *et al.*, J. Phys. B **80**, L327 (1987).
- [42] M. A. Morrison and L. A. Collins, Phys. Rev. A **17**, 918 (1978).
- [43] Lower value for r_{\max} (130 bohr) and number of channels (5) should be sufficient if 1% accuracy is desired for the total cross sections and eigenphase sums (summed over the Σ and Π symmetries). It should be noted that setting r_{\max} to such a high value does not increase the demands for computer resources drastically. This is because the potential in the outer region is very slowly varying and only a few Gaussian quadrature points are needed in this region for convergence.
- [44] To find the BF-FN K matrix, one can use the more efficient R -matrix propagation technique in the outer region where the potential is slowly varying. To find the FONDA K matrix, however, one needs the wave function in the entire region ($0-r_{\max}$) as is evident from Eq. (5). After extensive studies, we found the LA method to be the most appropriate in this region (see Ref. [43]) because the propagative techniques (e.g., Numerov) are extremely sensitive to the initial value of the wave function in the outer region.
- [45] The tuning of the TFEG model exchange should be done in Σ_g symmetry if the elastic cross sections are desired.