

## Completion of a hybrid-theory calculation of the $\Pi_g$ resonance in electron- $N_2$ scattering

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A calculation of  $e$ - $N_2$  scattering in the vicinity of the 2.4-eV ( $\Pi_g$ ) resonance has been completed. The main element of the calculation is a 15-term vibrational close-coupling expansion, reduced to coupled two-dimensional partial differential equations (PDE's), and solved using the noniterative PDE technique. The potential consists of static, exchange, and polarization parts; each part has been (previously) derived in a manner appropriate to its importance in the scattering equation. Results for the absolute total cross section, both in magnitude and shape of the substructure in the resonance region ( $1.5 < k^2 < 3$  eV), are in excellent accord with experiment. Angular distributions are also calculated and found to vary significantly in shape for different energies in the immediate vicinity of the center of the resonance ( $2.05 < k^2 < 2.15$  eV), indicating the need for differential measurements at a finer grid in energy and therefore requiring even better energy resolution. A comparison with other calculations and a discussion of some theoretical aspects are also included.

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### I. INTRODUCTION

The purpose of this paper is to report a calculation of electron scattering from molecular nitrogen ( $e$ - $N_2$ ) using the noniterative partial differential equation (PDE) technique [1]. This calculation is confined to the energy region around the 2.4-eV resonance; it consists of a 15-state vibrational close-coupling expansion for the resonant ( $\Pi_g$ ) partial wave combined with fixed- (plus adiabatic-) nuclei amplitudes for the other (contributing) partial waves. The underlying method is the hybrid theory [2]. We shall concentrate on the angular distributions for the lower vibrational states ( $v=0,1,2$ ), showing that their shapes change very rapidly from one energy to the next as one traverses the energy region in the center of the resonance. Thus, despite the fact that several differential scattering experiments have been reported (to be discussed below), they do not have the energy resolution, nor have they attempted to explore the variation in the angular distributions in this narrow energy region in detail. It is one of our aims to motivate such experimental investigations.

Several important developments in our calculations have been made since the introduction of the hybrid theory [2], which we have reported piecemeal since then. Briefly the most salient of them are as follows: the noniterative PDE technique itself [1], the reduction of the scattering equation to two-dimensional (2D) form, which was first outlined in [3], in addition to which—it turns out—the 2D technique could also be applied to the derivation of the polarization potential [4], as well as to a method for exactly including exchange in the static-exchange approximation [5]. And finally the direct (i.e., nonexchange) static potential could be calculated [6] using a much better multiconfiguration self-consistent-field (MCSCF) approximation of the  $N_2$  ground state than the self-consistent field (SCF) approximation, used originally

[2–5]. Some interim results using a 10-state vibrational expansion were reported in Ref. [7].

### II. THEORETICAL ASPECTS

We start with an antisymmetrized ansatz for the total wave function of the  $e$ - $N_2$  system [2,7]:

$$\Psi^{(m)} = \sum_{i=1}^{15} (-1)^{p_i} F_{N_2}^{(m)}(x_i; R) \Phi_{N_2}(x^{(i)}; R). \quad (2.1)$$

Here  $x_i$  are the coordinates (space and spin) of the  $i$ th electron and  $x^{(i)}$  is the collection of coordinates of the remaining (14) electrons. The factor  $(-1)^{p_i}$  is the parity of a cyclic permutation ( $p_i$ ) of the sequence  $1, 2, \dots, 15$ , thus making  $\Psi^{(m)}$  completely antisymmetric.

We first summarize the analysis, mostly of [5], whereby the basic integro-PDE is derived. (Note, however, that we are here using Rydberg units as opposed to a.u., used in Refs. [5,6].) Insertion of (2.1) into the Schrödinger equation, and premultiplication by the target ground state,  $\Phi_{N_2}$ , yields the (static) exchange approximation. We first consider the ground ( $\Sigma_g^+$ ) to be represented by a single determinant (i.e., SCF approximation):

$$\Phi_{N_2} = \det(1\sigma_g^2 2\sigma_g^2 1\sigma_u^2 2\sigma_u^2 3\sigma_u^2 1\pi_{xu}^2 1\pi_{yu}^2; \Sigma_g^+). \quad (2.2)$$

Labeling the different orbitals  $\psi_\alpha$  [ $\alpha = 1\sigma_g, \dots, 1\pi_{yu}$ ], we recognize that each  $\psi_\alpha$  is an explicit function of the coordinates of a single electron and an implicit function of the internuclear separation  $R$ :

$$\psi_\alpha(x_i) = \phi_\alpha(\mathbf{r}_i; R) \xi_\alpha(\text{spin}). \quad (2.3)$$

When one includes the  $R$  dependence of  $\phi$  and  $F^{(m)}$ , one derives from the Schrödinger equation, in the usual way [7], a 3D PDE for  $F^{(m)}$ :

$$[-\nabla^2 + H_{\text{vib}} + V(\mathbf{r}, R) - E_{\text{sc}}]F^{(m)}(\mathbf{r}) = \sum_{\alpha=1}^7 W_{\alpha}^{(m)} \phi_{\alpha}, \quad (2.4)$$

where  $V(r, R)$  is (to begin with) the static potential between the scattered electron and the target ( $\text{N}_2$ ):

$$V_{\text{static}}(\mathbf{r}, R) = \langle \Phi_{\text{N}_2} V_{e\text{-mol}} \Phi_{\text{N}_2} \rangle \quad (2.5)$$

and  $W_{\alpha}$  are the (static) exchange kernels

$$W_{\alpha}^{(m)}(\mathbf{r}; R) = \left\langle \phi_{\alpha}(\mathbf{r}'; R) \frac{2}{|\mathbf{r} - \mathbf{r}'|} F^{(m)}(\mathbf{r}'; R) \right\rangle. \quad (2.6)$$

The energy appearing in (2.4) is

$$E_{\text{sc}} = k_v^2 + \epsilon_v \quad (2.7)$$

and  $H_{\text{vib}}(R)$  is the vibrational part of the target Hamiltonian, from whose internuclear potential vibrational wave functions  $[\chi_v]$  and energies  $[\epsilon_v]$  are evaluated. (In this calculation the latter are obtained numerically from the MCSCF potential-energy curve reported in Ref. [6]).

For the static potential (2.5) we use a MCSCF approximation [6] of  $\Phi_{\text{N}_2}$ . A MCSCF wave function is a sum of determinants, whereas the rhs (i.e., the exchange part) of the scattering Eq. (2.4) *assumes* that  $\Phi_{\text{N}_2}$  is a single determinant (i.e., SCF approximation). Thus (2.4) constitutes an admittedly unbalanced approximation, which nevertheless seemed well justified [6,7], because (a) the exchange terms usually have a quantitatively smaller effect than the direct terms, and (b) when written as in (2.4), the exchange terms can be rigorously reduced to a coupled set of ordinary (i.e., nonintegral) PDE's [6]. This comes about by expanding  $W_{\alpha}^{(m)}$  in vibrational states  $\chi_v$  of  $\text{N}_2$ :

$$F^{(m)}(\mathbf{r}; R) = \sum_{v=0}^{N_v} F_v^{(m)}(\mathbf{r}) \chi_v(R), \quad (2.8)$$

$$W_{\alpha}^{(m)}(\mathbf{r}; R) = \sum_{v=0}^{N_v} W_v^{(m, \alpha)}(\mathbf{r}) \chi_v(R),$$

and, using the well-known property of the Coulomb potential as the Green's function of the kinetic energy,

$$\nabla^2 \left[ \frac{1}{|\mathbf{r} - \mathbf{r}'|} \right] = -4\pi \delta(\mathbf{r}' - \mathbf{r}) \quad (2.9)$$

allows the scattering equation (2.4) to be reduced to coupled, but nonintegral, PDE's [7]:

$$[-\nabla^2 + k_v^2]F_v^{(m)}(\mathbf{r}) = \sum_{v'=1}^{N_v} \left[ -V_{vv'}(\mathbf{r})F_{v'}^{(m)}(\mathbf{r}) + \sum_{\alpha} \phi_{vv'}^{(\alpha)}(\mathbf{r}) W_{v'}^{(m, \alpha)}(\mathbf{r}) \right], \quad (2.10)$$

$$-\nabla^2 W_v^{(m, \alpha)}(\mathbf{r}) = 8\pi \sum_{v''} \phi_{vv''}^{(\alpha)}(\mathbf{r}) F_{v''}^{(m)}(\mathbf{r}),$$

where

$$W_{v'}^{(m, \alpha)}(\mathbf{r}) = \sum_{v''} \left\langle \phi_{v'v''}^{(\alpha)}(\mathbf{r}') \frac{2}{|\mathbf{r} - \mathbf{r}'|} F_{v''}^{(m)}(\mathbf{r}') \right\rangle.$$

The double indexed quantities above are vibrational matrix elements of the unsubscripted quantities:

$$V_{vv'}(\mathbf{r}) = \langle \chi_v(R) | V(\mathbf{r}; R) | \chi_{v'}(R) \rangle, \quad (2.11)$$

$$\phi_{vv'}^{(\alpha)}(\mathbf{r}) = \langle \chi_v(R) | \phi_{\alpha}(\mathbf{r}; R) | \chi_{v'}(R) \rangle.$$

Equations (2.10) can be further reduced to 2D PDE's by exploiting the cylindrical symmetry of the various functions. As derived in Ref. [5] they take the form

$$[\Delta(m) + k_v^2]f_v^{(m)}(z) = \sum_{v'=1}^{N_v} \left[ V_{vv'}(z) f_{v'}^{(m)}(z) - \frac{1}{r} \sum_{\alpha=1}^7 \phi_{vv'}^{(\alpha)}(z) w_{v'}^{(m, \alpha)}(z) \right], \quad (2.12)$$

$$\Delta(m - m_{\alpha}) w_{v'}^{(m, \alpha)}(z) = -\frac{4}{r} \sum_{v'} \phi_{vv'}^{(\alpha)}(z) f_{v'}^{(m)}(z),$$

where  $w_{v'}^{(m, \alpha)}$  are reduced exchange orbitals defined in [5], and  $z = (r, \theta)$  and  $\Delta(m)$  is the 2D Laplacian

$$\Delta(m) = \frac{\partial^2}{\partial r^2} + \frac{1}{r^2} \left[ \frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} - \frac{m^2}{\sin^2 \theta} \right]. \quad (2.13)$$

As stated above,  $V_{vv'}$  should be derived from static potential seen by the scattered electron Eq. (2.5). We have shown [6] that the use of a MCSCF  $\Phi$  in (2.14) leads to a slightly less attractive potential than one obtained from a SCF approximation. That result is in qualitative accord with that found by Rumble, Stevens, and Truhlor [8]. Very recently, however, Meyer, Paul, and Riss [9] have carefully examined the  $\Pi_g$  resonance in the static *exchange* approximation and have found that the resonance using a MCSCF ground state, when the consistent exchange terms are included, corresponds to a slightly *more* attractive effect than the corresponding consistent exchange approximation with a SCF ground state. Their conclusion (which we found quite surprising but are forced to agree with; see below) is that the use of SCF orbitals for exchange in Eqs. (2.10) and (2.11) is sufficiently inconsistent with the use of a MCSCF wave function in calculating the direct term, that it gives the opposite effect from what is obtained by using the MCSCF wave function throughout [9].

We now describe how, in this calculation, we deal with this problem. Briefly we make our polarization potential more attractive so as to overcome the under attraction of the exchange potential as we have included it: To our static potential we add a polarization potential, as described in [6]

$$V(\mathbf{r}, R) \rightarrow V_{\text{static}}(\mathbf{r}, R) + V_{\text{pol}}(\mathbf{r}, R), \quad (2.14)$$

where

$$V_{\text{pol}}(\mathbf{r}, R) = \{1 - \exp[-(r/r_0)^2]\} V_{\text{pol}}^{(OT)}(\mathbf{r}, R). \quad (2.15)$$

$V_{\text{pol}}^{(OT)}$  is calculated using the polarized orbital procedure [10], generalized to molecular targets [4], but—as seen in (2.15)—the latter is diminished in magnitude by a tuning factor,  $\{1 - \exp[-(r/r_0)^2]\}$ , in which  $r_0$  was adjusted to give the  $\Pi_g$  resonance at the correct (i.e., experimental) energy.

We found specifically in [6] that a value of  $r_0 = 2.430$  was required, when using  $V_{\text{static}}(\text{MCSCF})$ , whereas  $r_0 = 2.934$  was required for a SCF wave function. (There is an unfortunate typographical error in [6], which reads  $r_0 = 2.394$  for the latter.)

In detail, as one can see from (2.15), a smaller value of  $r_0$  means a smaller effect of the cutoff  $\{1 - \exp[-(r/r_0)^2]\}$ ; and since  $V_{\text{pol}}^{(OT)}$  is attractive, the smaller value of  $r_0$  has the effect of rendering the polarization potential more attractive than it was when it was tuned to a static plus exchange potential based on the SCF target wave function. We will not say more about this alteration here except to repeat that—although it is consistent with Meyer, Pauli, and Riss [9]—it is based on experiment (hence  $r_0$  is phenomenological), and for that reason we have considerable confidence in the angular distributions, particularly in the immediate vicinity of the dominant fine-structure resonance, which will be presented in the next section, and which is the main objective of this paper.

### III. RESULTS AND COMPARISONS

In this calculation we have added (to the resonant  $^1\Pi_g$  partial wave) the nonresonant partial waves ( $^1\Sigma_g, ^1\Sigma_u, ^1\Pi_u, ^1\Delta_g$ ), calculated in the fixed-plus adiabatic-nuclei approximations, as discussed in Ref. [6]. Let us first show and discuss the total cross section  $\sigma_T$  (the sum of all energetically allowed vibrational channels, summed and averaged over rotational states in the usual way). The resonance with its famous substructure [11], is usually compared, as it is here, with the experimental result of Kennerly [12]. The theoretical curves shown are our previous 10-state result [7] (dashed curve), our present 15-state result (solid), compared to experiment and the Schwinger multichannel calculation of Huo *et al.* [13,14] (see Fig. 1).

With reference to our calculations the comparison of the 10- and 15-term results gives a good idea of the convergence of the close-coupling expansions: we would say that our calculations are well converged to just beyond the first resonance ( $k^2 < 1.95$  eV), reasonably well converged to just beyond the second ( $\sim 2.2$  eV), and approximately converged to  $\sim 2.5$  eV. Of particular note, therefore, is the fact that ours is the only calculation which describes the magnitude of the first peak ( $\sigma_T \approx 27 \text{ \AA}^2$  at  $k^2 \approx 1.95$  eV) and gives the ratio of the first two peaks accurately. The calculation of Huo *et al.* [14] is almost as satisfactory, while their adjoining paper [13] gives the whole sequence of vibrational excitation cross sections whose shapes are in remarkable accord with experiment [15].

The ability of such theories [13,14] to achieve a detailed description of the entire substructure goes back to the physical ideas underlying the boomerang model (so

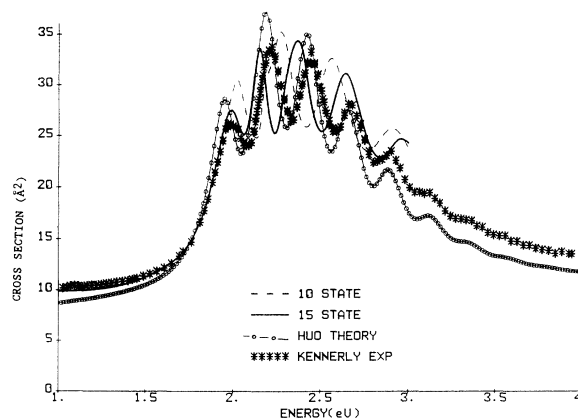


FIG. 1. Total integrated cross section in square Angstroms ( $\text{\AA}^2$ ): Experiment: (\*\*\*) Ref. [12]. Theory: (—) present [15-state results]; (- - -) our 10-state results (Ref. [7]); (-○-○-) Ref. [14].

called because the nuclei execute only a single vibrational cycle during the limited lifetime of the  $\text{N}_2^-$  ion; cf. [16]), which have been given their most rigorous justification in the *R*-matrix calculations of Schneider, LeDourneuf, and Vo Ky Lan [17]. More discussions of those theories and calculations (Ref. [18], for example) will be included in the latter parts of this paper.

In this (hybrid-theory) calculation we shall concentrate on angular distributions. Figure 2 shows the elastic differential cross section at 1.50 eV, just below the onset of the  $\Pi_g$  resonance. Also shown are various other theoretical [2,14,19] and experimental [20,21,22] results. Both similarities and differences are evident. The results continue into the heart of the resonance region ( $k^2 \approx 2.1$  eV): Figs. 3 and 4. We have divided those results into two parts: in Fig. 3 we show our present results at three energies surrounding 2.10 eV; one sees how *significantly*

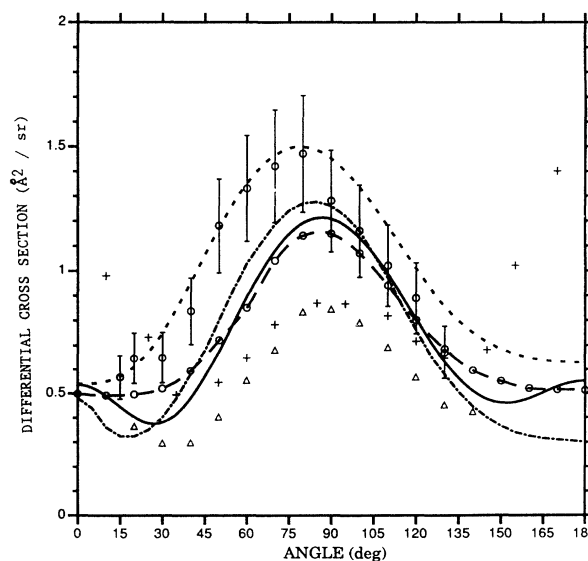


FIG. 2.  $d\sigma_{00}/d\Omega$  for  $e^- + \text{N}_2: v(0 \rightarrow 0)$  at 1.50 eV: Theory: (—) present; (-○-○-) Ref. [14]; (- - -) Ref. [2]; (—○—) Ref. [19]. Experiment: (ΦΦΦ) Ref. [22]; (+ + +) Ref. [20]; (Δ Δ Δ) Ref. [21].

the shape varies over 0.1 eV. That is particularly relevant to the fact that the latest experiment [22] only claims an energy uncertainty of just that amount. Nevertheless the discrepancy between all these results and the original hybrid calculation [2] is clear. (In this and future comparisons with experiment in this narrow energy region around 2.1 eV it is to be emphasized that it is not the absolute energies but rather the energy differences that are essential. Thus "2.10 eV" means the experimental energy at the second (major) peak in  $\sigma_T$ , and the other two energies correspond to energies 0.05 eV below or above it.)

Figure 4 contains the same experimental information but here compared to the present calculation and that of Huo *et al.* [14] at 2.10 eV. The similarity of the calculated results, both of which provide absolute values of the cross section, is the most striking feature. (It should be noted, however, that a SCF target representation was used by Huo *et al.* [4]). The agreement between calculations suggests that the recent experiment [22] is dominated by the particular energy in the composite beam which gives the dominant cross section at the particular angle.

Comparison of experiment and theory at 3.0 eV is shown in Fig. 5. The similarity of the recently calculated results continues, but—referring back to Fig. 1—we emphasize that at 3 eV one is definitely pressing the outer edge of reliability of the present calculation. The other interesting, but enigmatic, feature of the latest experi-

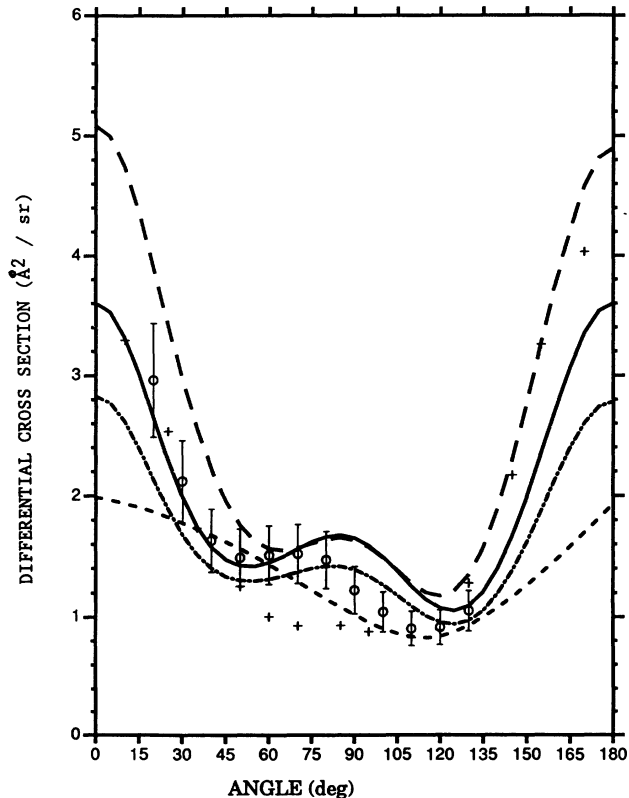


FIG. 3.  $d\sigma_{00}/d\Omega$  for  $e^- + N_2$ ;  $v(0 \rightarrow 0)$ . Theory: (—) present at 2.05 eV; (—) present at 2.10 eV; (- - -) present at 2.15 eV; (· · ·) Ref. 2. Experiment: ( $\Phi\Phi\Phi$ ) Ref. [22]; (+ + +) Ref. [20].

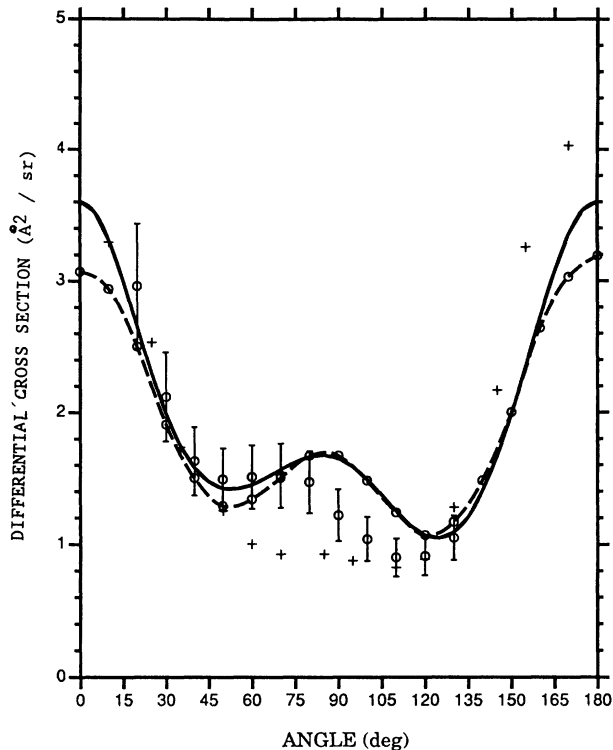


FIG. 4.  $d\sigma_{00}/d\Omega$  for  $e^- + N_2$ ;  $v(0 \rightarrow 0)$  at 2.10 eV. Theory: (—) present; (- - -) Ref. [14]. Experiment: ( $\Phi\Phi\Phi$ ) Ref. [22]; (+ + +) Ref. [20].

ment [22], noted there as well, is that the absolute magnitude in the directions  $\theta < 110^\circ$  favors the original hybrid result [2].

In the next three figures (Figs. 6–8) we show differential cross sections in the excitation transition to the first vibrational state. At the lowest energy (1.50 eV)

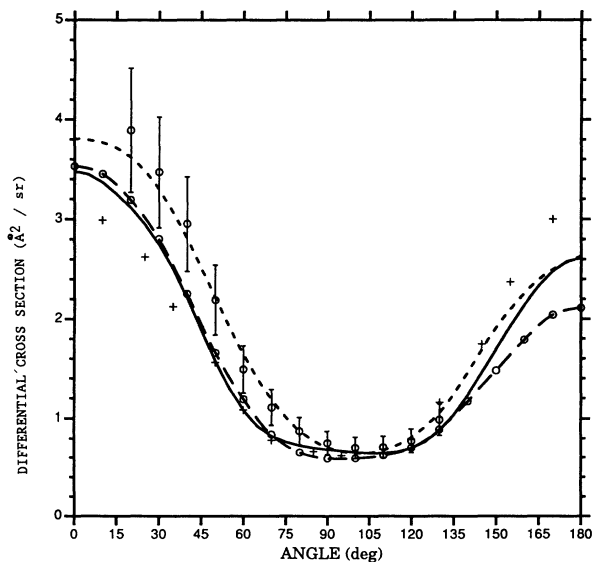


FIG. 5.  $d\sigma_{00}/d\Omega$  for  $e^- + N_2$ ;  $v(0 \rightarrow 0)$  at 3.00 eV. Theory: (—) present; (- - -) Ref. [2]. Experiment: ( $\Phi\Phi\Phi$ ) Ref. [22]; (+ + +) Ref. [20].

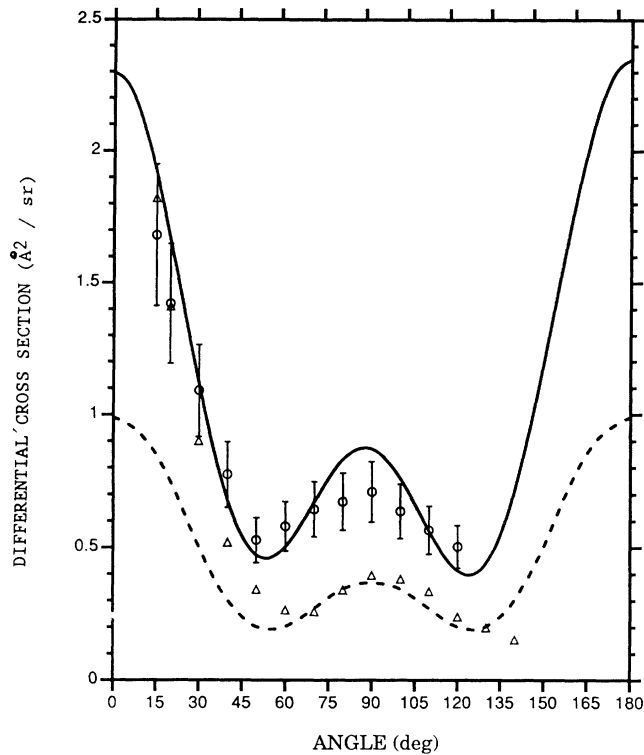


FIG. 6.  $d\sigma_{01}/d\Omega$  for  $e^- + N_2$ :  $v(0 \rightarrow 1)$  at 1.50 eV. Theory: (—) present; (- - -) Ref. [2]. Experiment: ( $\Phi\Phi\Phi$ ) Ref. [22]; ( $\Delta\Delta\Delta$ ) Ref. [21].

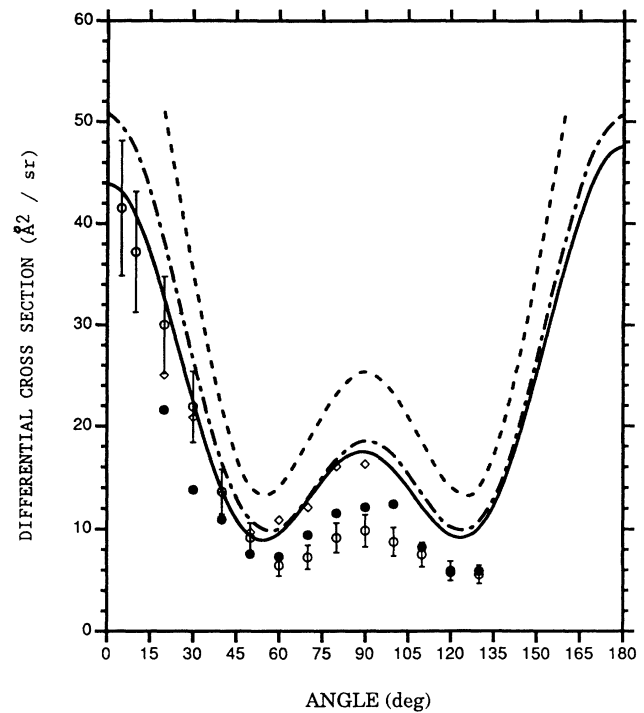


FIG. 8.  $d\sigma_{01}/d\Omega$  for  $e^- + N_2$ :  $v(0 \rightarrow 1)$  at 3.00 eV. Theory: (—) present; (- - -) Ref. [2]; (- · - ·) Ref. [24]. Experiment: ( $\Phi\Phi\Phi$ ) Ref. [22]; ( $\diamond\diamond\diamond$ ) Ref. [23]; ( $\bullet\bullet\bullet$ ) Ref. [25].

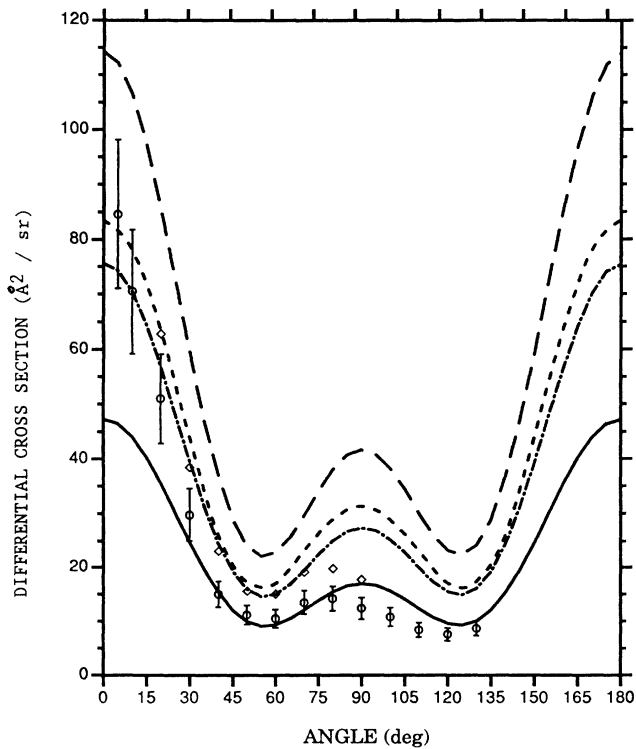


FIG. 7.  $d\sigma_{01}/d\Omega$  for  $e^- + N_2$ :  $v(0 \rightarrow 1)$ . Theory: (—) present at 2.05 eV; (—) present at 2.10 eV; (—) present at 2.15 eV; (- - -) Ref. [2]. Experiment: ( $\Phi\Phi\Phi$ ) Ref. [22]; ( $\diamond\diamond\diamond$ ) Ref. [23].

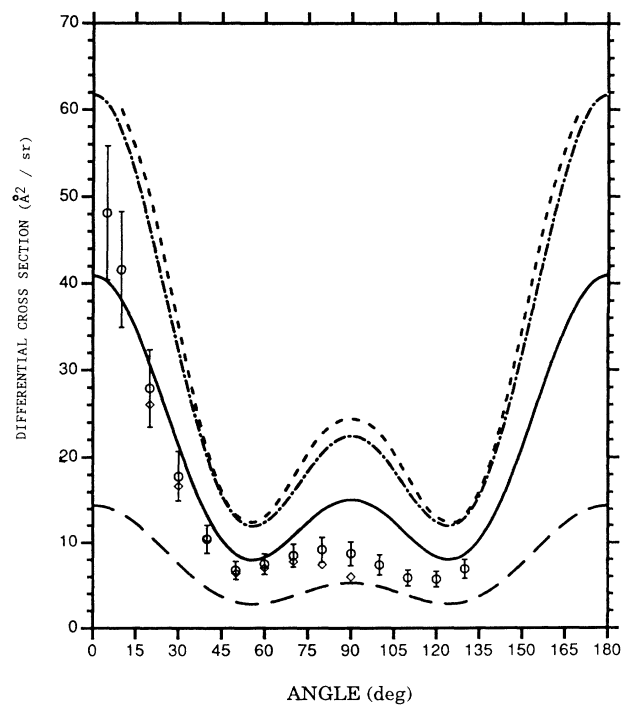


FIG. 9.  $d\sigma_{02}/d\Omega$  for  $e^- + N_2$ :  $v(0 \rightarrow 2)$ . Theory: (—) present at 2.05 eV; (—) present at 2.10 eV; (—) present at 2.15 eV; (- - -) Ref. [2]. Experiment: ( $\Phi\Phi\Phi$ ) Ref. [22]; ( $\diamond\diamond\diamond$ ) Ref. [23].

our present calculation (Fig. 6) is definitely favored by the experiment of Brennan *et al.* [22], whereas in the vicinity of the dominant peak ( $k^2=2.1$  eV, Fig. 7), that is only true in the middle of the angular range. Note that a different set of experimental results from Brunger *et al.* has also been included [23]. It is clear that differences between the experiments can easily be explained by a slight difference ( $\sim 0.05$  eV) in their energy calibrations. At the highest energy, 3 eV the graph also includes results of an *R*-matrix calculation [24] and yet another experiment [25]. Here the similarity of the present results with those of the *R*-matrix calculation is the most notable feature, particularly at middle angles, where they agree best with the experimental results of Ref. [23].

Finally we show in Fig. 9 the angular distribution associated with the excitation of the second vibrational state in the vicinity of the dominant peak. Here the two experimental results [22,23] are in agreement with each other within their experimental errors, and they agree best with our present result at the experimental energy (2.10 eV), rather than at its fringes (2.05 and 2.15 eV).

#### IV. DISCUSSION

This completes the presentation of results of this calculation. (More results are available on request.) Although the method (the hybrid theory) is *ab initio* in principle, it contains here one phenomenological parameter, the polarization cutoff  $r_0$  [cf. Eq. (2.15)]. The main practical purpose for doing this is to provide reliable cross sections for (several space) applications. It will be recalled that our (hybrid) theory was developed in the context of stable auroral red (SAR) arcs [2]. The numerical results of that calculation were collected as a NASA document [26]. The present (more accurate) cross sections are additionally intended for the understanding of secondary electron flux in the *F* region of the ionosphere. The specific question concerns whether or not there is a dip in the electron distribution function [27]. Relevant ionospheric calculations are now ongoing at the Goddard Space Flight Center [28], using our cross sections and those of others, principally Huo *et al.* [13,14].

From a more fundamental point of view the present results are intended to provide a better comparison, particularly with experimental angular distributions in the resonance region. As we have seen from the comparisons in the preceding section, there is still insufficient agreement among experiments themselves to provide a definitive check at this time. In addition future experiments will require even finer energy resolution, at a finer energy grid, to be compelling in this regard. This having been said, it is important to acknowledge that great progress in experimental angular distributions has already been made, culminating in the recent work of Brennan and Brunger and co-workers [22,23].

With regard to calculational methodologies, specifically hybrid vs *R*-matrix type theories, we remark—in addition to what was said above and elsewhere [29]—that it is clear the latter are capable of giv-

ing the greater overall accuracy, as is exemplified by the results of Refs. [13,14,17]. (In further detail, for example, other *ab initio* calculations [30] show that the  $\Pi_g$  resonance is dominated by shorter-range correlations rather than the long-range polarizability.) However if *insufficient* correlation is included, the *R*-matrix method can yield noticeable inaccuracy (cf. [18], for example).

The essential point, however, is that the basic tenet of the hybrid theory is common to both approaches [2,29]: it is the fact that if the interaction time of the resonance is comparable to the vibrational time scale of the target molecule, but short compared to rotation, then in one way or another a dynamical treatment of vibration, but not rotation, is required. That treatment can be either a dynamical coupling of the incident particle with the vibrational motion of the target, *or* a recalculation of the Born-Oppenheimer problem of the ( $N+1$ )-electron system followed by a calculation of the vibrational spectrum in the (necessarily complex) potential energy well of the compound system. In both cases the rotational motion can be ignored in the dynamics and only be included adiabatically at the end. (In addition, the adiabatic part, because it is rotation, can and has been done analytically; cf. the second references of [34].)

The drawback of the present methodology is due to the slow convergence of the vibrational close-coupling expansion. In principle that can be overcome by going to a (3D PDE) approach in which the internuclear separation (*R*) becomes the third dynamical variable. Such a (3D PDE) theory has already been outlined [31], and the noniterative PDE method [1] has been generalized to 3D and higher dimensional equations and applied to a soluble model [32].

The implementation of the 3D PDE approach for the real *e*-N<sub>2</sub> problem is in progress, however its completion will not be easy; in particular, the detailed substructure that such a calculation will reveal will depend critically on the range and mesh size with which the *R* variable can be covered.

Perhaps the most exciting potential application of the 3D PDE technique, also discussed in [31], is the fact that it can be applied to scattering from (in principle) arbitrary *polyatomics* in the fixed-nuclei approximation [33]. Augmented by the adiabatic-nuclei approximation [34], such a method would be an invaluable tool in studying scattering processes in galactic environments, such as the Orion nebula, where it is known that exotic molecules can form (cf. [35], for example) which may not be amenable to laboratory experimentation, so that theoretical calculation provides the only reasonable alternative.

#### ACKNOWLEDGMENTS

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