Parameter-free model of the correlation-polarization potential for electron-molecule collisions

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A model potential that includes both correlation and polarization effects is proposed for electron-molecule collisions. It is based, as suggested by O'Connell and Lane, on a hybridization of local electron-gas theory for short distances and the asymptotic form of the polarization potential. It is energy independent and very simple to apply, depending only on the molecular charge density and polarizabilities. The potential has been calculated for several molecules (H_2, N_2, CO_2, HF, HCl, and CO); the crossing point between the correlation and polarization potentials is remarkably constant, averaging 0.96 eV. Application in scattering calculations for H_2 and N_2 yields very encouraging results.

I. INTRODUCTION

Polarization effects are known to be important to properly describe low-energy and near-resonant electron collisions with molecules.[1] A variety of schemes, ranging from simple semiempirical analytic formulas to elaborate close-coupling techniques, have been devised to represent the correlation effects that arise from the interaction of the incident electron with the distorted target molecule. Of these approaches, the two most rigorous are the close-coupling method,[1] by which electronically-closed channels are included directly in the many-state expansion of the system wave function, and the optical-potential method,[2,3] by which virtual states introduce an effective potential in the elastic channel. Despite their success in treating electron scattering from H_2 and N_2, the ability of these approaches to handle large molecular systems remains to be demonstrated.

Another set of techniques,[1,4,5] based on the polarized-orbital approach, have also been developed and applied to several molecules. While less rigorous in their treatment of the motion of the incident electron within the charge cloud of the molecule, they are, nonetheless, more easily and efficiently applied than the close-coupling or optical-potential methods.

Finally, the most widely employed and simplest model of the polarization potential is the cutoff asymptotic form.[1] The cutoff parameter is usually determined by adjusting eigenphase sums or cross sections to known results, e.g., the results of more rigorous calculations, or an experimental feature such as a resonance. While easy to apply, this approach suffers from the need for *a priori* knowledge of the system being examined.

Thus a simple model potential which can be efficiently calculated and applied to large systems, yet which is free of adjustable parameters, is highly desirable. We investigate the potential of one such model in this paper.

II. THE MODEL

Recently O'Connell and Lane[6] proposed a simple, parameter-free model based on the free-electron-gas (FEG) correlation energy $\epsilon_{co}(\vec{r})$. $\epsilon_{co}(\vec{r})$ is a function of the molecular charge density $\rho(\vec{r})$ alone, and has very simple forms in the high- and low-density limits. For small r_s [large $\rho(\vec{r})$][7]

$$\epsilon_{co}(\vec{r}) = 0.0311\ln r_s - 0.048 + 0.009 r_s \ln r_s - 0.018 r_s , \quad (1)$$

and for large r_s [small $\rho(\vec{r})$][8]

$$\epsilon_{co}(\vec{r}) = -0.438 r_s^{-1} + 1.325 r_s^{-3/2} - 1.47 r_s^{-2} - 0.4 r_s^{-5/2} , \quad (2)$$

in units of hartree, where

$$r_s = [3/4\pi\rho(\vec{r})]^{1/3} . \quad (3)$$

Since $\epsilon_{co}(\vec{r})$ takes no specific account of the long-range interaction caused by polarization of the target by the incident electron, O'Connell and Lane suggested simply joining the two where they cross near the boundary of the target charge distribution. Defining the correlation potential $v_{co}(\vec{r})$ to be $2\epsilon_{co}(\vec{r})$, they tested this model on elastic electron scattering by noble-gas atoms, with very encouraging results.

In the present work we follow the suggestion of O'Connell and Lane with one minor[9] and one major modification. It has been shown[10] that the relationship between the FEG exchange-correlation potential and exchange energy consistent with a variational principle is
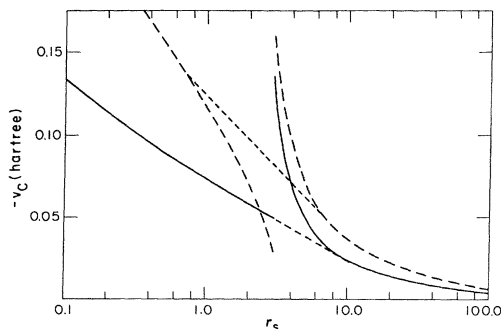

FIG. 1. Two models of the FEG correlation potential plotted as a function of the density parameter r_s: variational form of Eqs. (6), (———); and $2\epsilon_{co}(\vec{r})$, the model of O'Connell and Lane (Ref. 6), (———). The curve (— — —) is the result of interpolation from $0.7 \leq r_s \leq 10.0$.

$$v_{ec}(\vec{r}) = \frac{\partial}{\partial \rho}[\rho \epsilon_{ec}(\vec{r})] \ . \qquad (4)$$

$$v_{co}(\vec{r}) = \frac{\partial}{\partial \rho}[\rho \epsilon_{co}(\vec{r})] \ . \qquad (5)$$

By analogy, Kohn and Sham[10] take the FEG correlation potential to be

Using (1) and (2), and bridging the high- and low-density limits of $v_{co}(\vec{r})$ by a two-parameter interpolation formula, we obtain

$$v_{co}(\vec{r}) = \begin{cases} 0.0311\ln r_s - 0.0584 + 0.006 r_s \ln r_s - 0.015 r_s, & r_s \leq 0.7 \\ -0.07356 + 0.02224\ln r_s, & 0.7 \leq r_s \leq 10.0 \\ -0.584 r_s^{-1} + 1.988 r_s^{-3/2} - 2.450 r_s^{-2} - 0.733 r_s^{-5/2}, & r_s \geq 10.0 \ . \end{cases} \qquad (6)$$

The form (6) and $2\epsilon_{co}(\vec{r})$ are compared in Fig. 1. The former is approximately $\frac{3}{5}$ the latter, reminiscent of the $\frac{2}{3}$ factor introduced by the variational treatment of exchange.[10]

For molecules the correlation potential is not, as for the noble gases, spherically symmetric, but may be expanded in Legendre polynomials as

$$v_{co}(\vec{r}) = \sum_{\lambda} v_{co}^{\lambda}(r)P_{\lambda}(\cos\theta) \ . \qquad (7)$$

For large r, the dipole polarization potential is

$$v_p(\vec{r}) = v_p^0(r) + v_p^2(r)P_2(\cos\theta)$$
$$= -\frac{1}{2}\left[\frac{\alpha_0}{r^4} + \frac{\alpha_2}{r^4}P_2(\cos\theta)\right] \ . \qquad (8)$$

For homonuclear molecules, only even moments $(\lambda = 0, 2, \dots)$ appear in the expansion (7). We therefore join the curves $v_{co}^{\lambda}(r)$ and $v_p^{\lambda}(r)$ for $\lambda = 0$ and 2 at the point r_c^{λ} where they first cross, thereby defining the correlation-polarization potential $v_{cop}(\vec{r})$.

The model potential $v_{cop}(\vec{r})$ has been calculated for several molecules at their equilibrium internuclear separation. The sources of wave functions, and values of polari-

zabilities, r_c^{λ}, and v_{cop}^{λ} at the crossing points for six molecules studied to date are given in Table I. The consistency in the values of $v_{cop}^0(r_c^0)$ is remarkable, and was also noted by O'Connell and Lane for the noble gases. We can offer no explanation for this effect, but it immediately suggests a useful, if ad hoc, method for estimating values of α_0 for molecules. To illustrate this point, also given in Table I are the values of α_0 obtained by equating $v_{co}^0(r)$ and α_0/r^4 at that value of r where the former is 0.96 eV (the average of the values in Table I).

Moments with $\lambda > 2$ in the expansion (7) proved, for H_2, N_2, and CO_2, to be negligible in comparison to the static-exchange potential (SE) at all r, and could be ignored. For the heteronuclear molecules (HCl, HF, CO), moments with $\lambda = 1$ and $\lambda > 2$ were also negligible compared with the static-exchange potential. It will be interesting to see if this applies to more complex molecular systems.

III. TESTS OF THE MODEL FOR ELECTRON SCATTERING

The obvious molecular systems for a first test of this correlation-polarization model for electron scattering are H_2 and N_2. One can hardly imagine a more stringent test

TABLE I. Sources of wave functions, and values of polarizabilities (a.u.), $r_c^{\lambda}(a_0)$, and v_{cop}^{λ} (eV) at the crossing points r_c^{λ}.

Molecule	Wave functions	α_0[a]	α_2[a]	r_c^0	r_c^2	v_{cop}^0	v_{cop}^2	α_0 (est.)[b]
H_2	c	5.18[d]	1.20[d]	2.9	4.7	-0.94	-0.03	5.1
N_2	e	11.74[f]	3.1[g]	3.5	3.4	-1.03	-0.30	13.2
HCl	h	17.22[i]	1.15[i]	4.0	4.7	-0.90	-0.03	15.7
HF	j	5.48[i]	0.82[i]	2.9	3.9	-1.06	-0.05	6.5
CO	k	13.13[l]	2.61[l]	3.7	3.2	-0.95	-0.35	13.0
CO_2	k	17.75[g]	9.45[g]	4.05	3.65	-0.90	-0.72	16.6

[a]References given as superscripts.
[b]The values of α_0 (est.) are estimated using Eqs. (6) and (8), as discussed in the text.
[c]Reference 11.
[d]Reference 12.
[e]Reference 13.
[f]Reference 14.
[g]Reference 15.
[h]Reference 16.
[i]Reference 17.
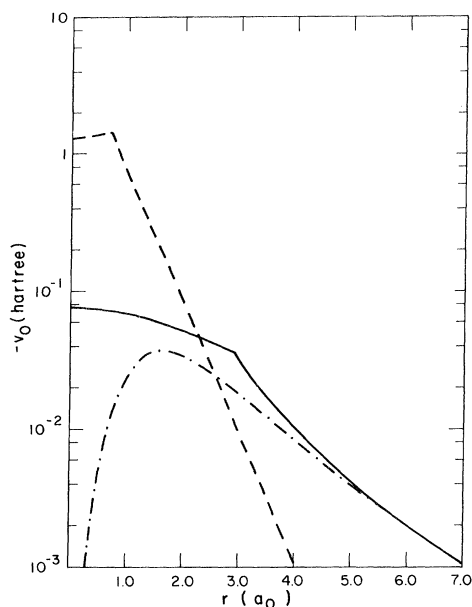[j]Reference 18.
[k]Reference 19.
[l]Reference 20.

FIG. 2. Spherically symmetric terms in the interaction potential for electron-H_2 scattering: the SE potential (using the FEG exchange approximation), (— — —); the polarization model of Gibson and Morrison (Ref. 4), (—·—); the present correlation-polarization model, (———).

of a FEG approximation than H_2, and N_2 has a prominent and oft-studied shape resonance that severely tests any model. There are also extensive, essentially exact, results in the fixed-nuclei approximation for these two molecules available for comparison.

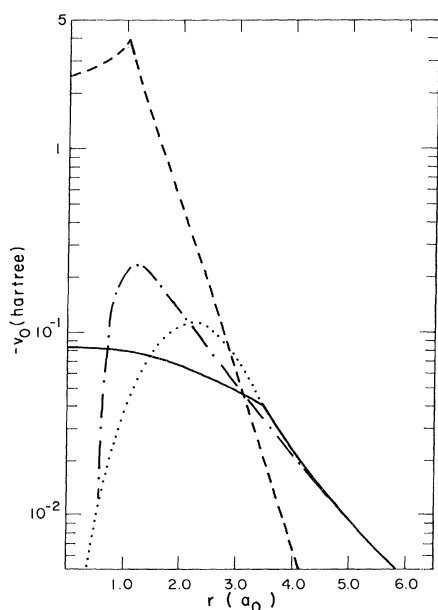In order to complete the form of the electron-molecule

FIG. 3. As Fig. 2, for electron-N_2 scattering. The curve (···) is the tuned cutoff asymptotic polarization potential of Morrison and Collins (Ref. 23), and the curve (—·—) is the result of the polarized-orbital calculation of Onda and Temkin (Ref. 5). The latter results change sign for $r \lesssim 0.5a_0$, but remain less than 0.1 hartree in magnitude.

TABLE II. Parameters used in scattering calculations.

		l_m	λ_m^{el}	λ_m^n	λ_m^{ex}	r_m
SECOP						
H_2,	gerade	12	12	24	12	20.0
	ungerade	11	12	22	12	20.0
N_2,	gerade	28	20	56	20	113.6
	ungerade	27	20	54	20	113.6
ESECOP						
H_2,	gerade	10	12	20	6	50.0
	ungerade	11	12	22	7	50.0
N_2,	gerade	24	20	48	8	75.0
	ungerade	23	20	46	10	75.0

interaction, we must add a representation of the static and exchange terms to the polarization potential. We calculate the static potential exactly by averaging the electrostatic electron-molecule interaction over the ground state of the target molecule.[21] Calculations have been made with two treatments of exchange: a local, FEG model potential[22] (denoted SE); and an exact treatment [denoted ESE (exact static exchange)]. The results of calculations in which the static-exchange interaction was augmented by $v_{cop}(\vec{r})$ are denoted SECOP (static-exchange correlation polarization) and ESECOP (exact static-exchange correlation polarization).

Typical results for $v_{cop}^0(r)$ are shown in Figs. 2 and 3. Here the exchange interaction was approximated by the FEG model potential. The present model is seen to differ most significantly from the parameter-free models of Gibson and Morrison[4] for H_2 and Onda and Temkin[5] for N_2 when both are negligible compared to the model SE potential. For both molecules $v_{cop}^0(r)$ is a bit stronger in the crossing region [$\sim (3-4)a_0$]. For N_2, the present model is also compared with the cutoff asymptotic form used by Morrison and Collins.[23] They used the FEG exchange potential and chose the adjustable parameter in their polarization model so as to reproduce the position of the $^2\Pi_g$ resonance.

We performed scattering calculations in the molecular body-fixed frame, with the fixed-nuclei approximation, and restricted our detailed comparisons to other calculations of this type that also employed target wave functions of comparable accuracy. The scattering equations with the FEG model were solved using an integral equation formulation of the close-coupling equations.[23] The ESE and ESECOP calculations were done with the linear-algebraic program of Collins and Schneider.[24]

The most important parameters in the potential expansions and scattering calculations are given in Table II. These are l_m, the maximum order of partial wave in the continuum channels; λ_m^{el} (λ_m^n, λ_m^{ex}), the order of the expansion of the static electron-electron (electron-nuclear, exchange) interaction; and r_m, the asymptotic matching radius. These provided a level of numerical precision at least as good as in any work to the results of which ours will be compared. Orthogonality of the scattering wave function to all bound orbitals of like symmetry was imposed throughout.

Our results for e-H_2 partial scattering cross sections are presented in Figs. 4 and 5 and compared with other re-

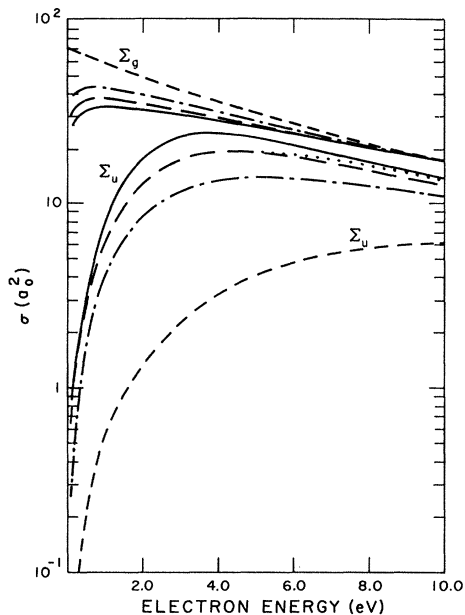FIG. 4. Partial cross sections for Σ_g and Σ_u elastic scattering of electrons by H_2: SE results, (— — —); results of Gibson and Morrison (Ref. 4), (———); results of Schneider and Collins (Ref. 3), (···); present SECOP, (—·—), and ESECOP, (———) results.

sults. In the calculations of Gibson and Morrison,[4] exchange was treated exactly and polarization accounted for by their parameter-free model. The results of Schneider and Collins[3] are from benchmark calculations in which exchange was treated exactly and polarization was treated rigorously using the optical-potential approach.

For the Σ_g symmetry, the SECOP results are about 10% higher than those of the optical-potential calculation,[25] while the ESECOP results are about the same
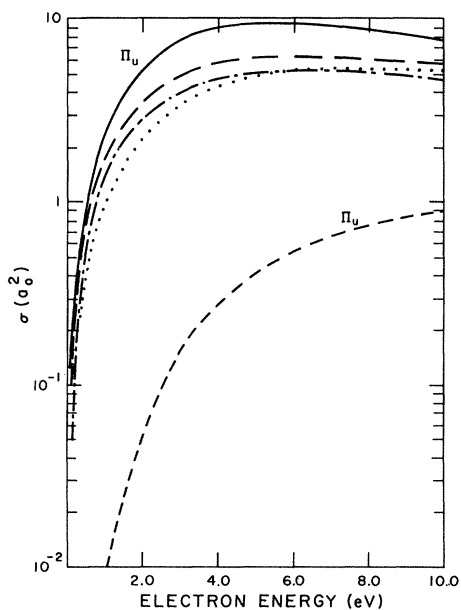

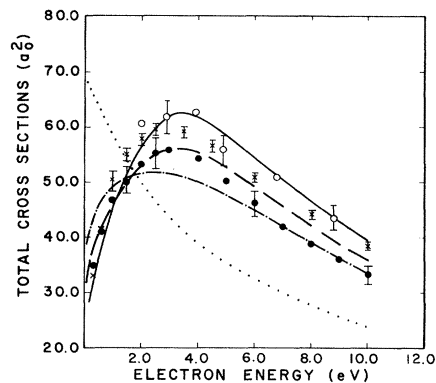FIG. 5. As Fig. 4, for the Π_u scattering symmetry.

FIG. 6. Total cross sections for scattering of electrons by H_2: SE results, (···); results of Gibson and Morrison, (———); present SECOP, (—·—), and ESECOP, (———) results; experimental data of Golden et al. (Ref. 26), (●); of Hoffman et al. (Ref. 27), (○); and of Dalba et al. (Ref. 28), (×).

amount lower. This finding is reversed for Σ_u scattering, with the ESECOP results being a little high and the SECOP results somewhat low. Still the agreement for Σ_g and Σ_u symmetries is good given the nature of the COP model. For the Π_u symmetry the SECOP cross section is in reasonable agreement with the optical-potential results while the ESECOP values are almost a factor of 2 too high. We should note that in the Π_u symmetry the two more elaborate techniques also show their largest disagreement. We found that the cross sections depend strongly on the correlation potential in the range $2.0a_0$ to $5.0a_0$ (see Fig. 2). If we reduce v_{co}^0 by 30% [consequently $r_c^0 = 3.4a_0$, $v_{cop}^0(r_c) = -0.52$ eV], we get a reduction of up to 30% in
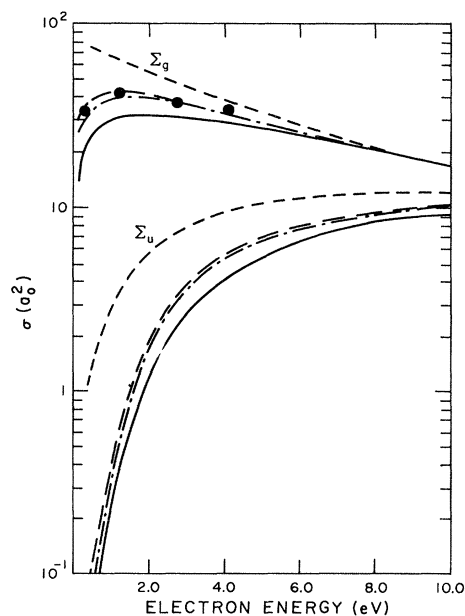

FIG. 7. Partial cross sections for Σ_g and Σ_u elastic scattering by N_2: ESE results of Collins et al. (Ref. 29), (— — —); results of Morrison and Collins (Ref. 23), (———); results of Schneider and Collins (Ref. 3), (●); present SECOP, (—·—), and ESECOP, (———) results.
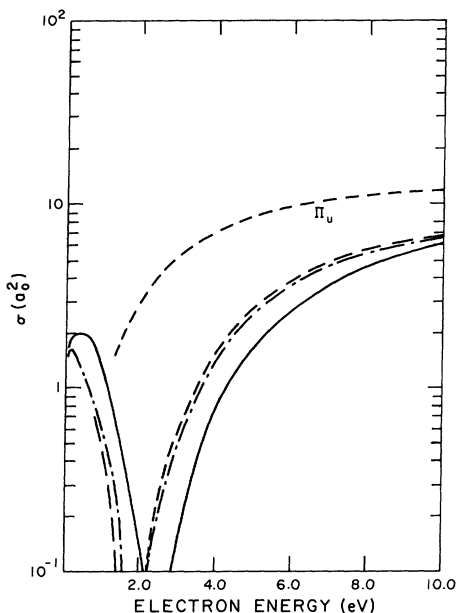
FIG. 8. As Fig. 7, for the Π_u scattering symmetry.

the Π_u cross sections and up to 10% in the Σ_u.

In Fig. 6, we compare the total cross section with that of Gibson and Morrison,[4] and with experimental results.[26–28] The general features of the cross-section curve are reproduced well by both the SECOP and ESECOP models. The peak is slightly shifted to lower energies in the SECOP model. The difference between the total cross section of Gibson and Morrison and the SECOP model is never more than 20%, while for the ESECOP model it is less than 12%.

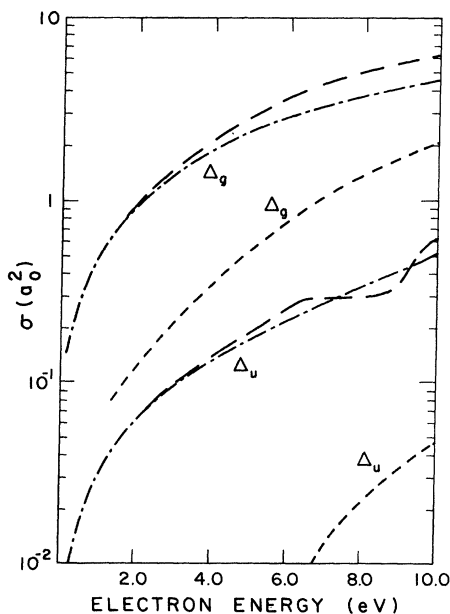Our results for e-N_2 partial scattering cross sections are

FIG. 9. As Fig. 7, for the Δ_g and Δ_u scattering symmetries.

presented in Figs. 7—9. The results of Collins et al.[29] are from a calculation in which exchange was treated exactly, but polarization neglected. In the work of Morrison and Collins,[23] the Hara FEG model of the exchange potential was employed, but they did not impose orthogonality of bound and continuum orbitals. Recall also that in their work the polarization potential was tuned based on the $^2\Pi_g$ resonance. The results of the exact static-exchange plus optical-potential calculations of Schneider and Collins[3] are also shown in Fig. 7. The results of calculations[2] employing a similar approach to an essentially exact result are, given differences in target wave functions, in reasonable agreement with those of Schneider and Collins above 3.0 eV. (Closer to zero energy very large differences are noted, which may[30] be due to the neglect of Δ virtual orbitals in the work of Burke et al.[2])

For all the nonresonant symmetries, agreement of the SECOP results with those of Morrison and Collins[23] is remarkably good. Since both calculations employed the same exchange model and similar polarization potentials (see Fig. 3), this is not unexpected. The ESECOP cross sections are a little lower in the Σ_g and Σ_u symmetries, and shifted to slightly higher energies in the Π_u symmetry.

The agreement between the results of Collins and Schneider[3] and the SECOP calculation for Σ_g scattering is quite good while the ESECOP results are somewhat lower. We should point out that at $k^2=0.1,0.2,0.3$ our ESE (no polarization) cross section values are 58.04,45.71,36.69 as compared to 60.57,48.72,41.95 for Collins and Schneider,[3] if we use the same convergence parameters. Making this systematic correction would bring our ESECOP results into better agreement with those of the optical-potential calculations. In addition, the optical-potential calculation was performed to demonstrate the efficiency of a new technique, and a detailed study on the sensitivity to such parameters as AO and MO basis size remains to be thoroughly tested.

The most stringent test of the model is the resonant $^2\Pi_g$ scattering channel. Our results for the width and position of the resonance are compared with those of other calculations at the fixed-nuclei level in Table III. More elaborate models,[32] in which polarized N_2 targets were used, yield results for the resonance position and width closer to 2.2 and 0.4 eV, respectively. When we use the ESECOP model, our results for the resonant parameters move into excellent agreement with these more elaborate calculations.

Total cross sections for N_2 are given in Fig. 10. The results labeled ESECOP in this figure were formed from ESECOP calculations for the Σ_g, Σ_u, Π_g, and Π_u sym-

TABLE III. Characteristics of the Π_g resonance in e-N_2 scattering.

	SE	ESE[a]	SETP[b]	SECOP	ESECOP
E_r (eV)	5.11	3.90	2.39	3.03	2.17
Γ (eV)	1.75	1.33	0.48	0.76	0.47

[a]References 29 and 31—ESE.

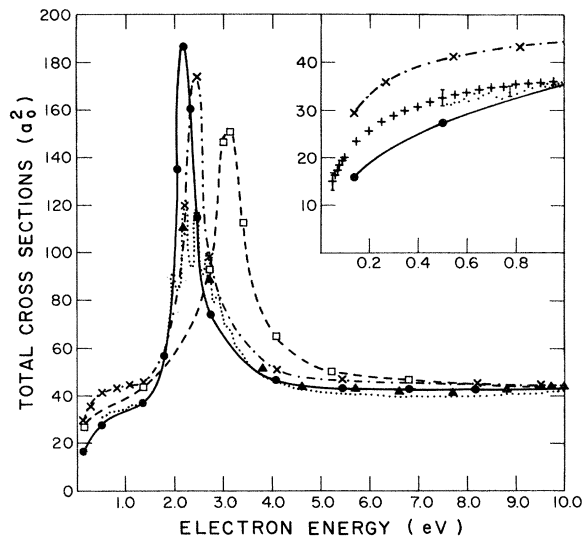[b]Reference 23—FEG exchange, tuned polarization.

FIG. 10. Total cross sections for scattering of electrons by N_2: results of Morrison and Collins (Ref. 23), (—·—); present SECOP, (———), and ESECOP, (———) results; experimental data of Hoffman *et al.* (Ref. 27), (▲); Kennerly (Ref. 33), (· · · ·); and of Jost *et al.* (Ref. 34), (+). The results of Refs. 33 and 34 are in excellent agreement above 1.0 eV; only the former are shown.

metries, and SECOP calculations for Δ symmetries. The location of the resonance peak in the ESECOP results is a little lower, and its maximum much higher, than the experimental results;[27,33,34] the observed structure is also missing in the calculated results. Since nuclear dynamics was neglected in the calculations, much better agreement cannot be expected. Away from the resonance, agreement

with measurements is remarkably good.

IV. CONCLUSIONS

We have tested a new, parameter-free model of the correlation-polarization contribution to the electron-molecule interaction potential. One of its main attractions is the ease with which it can be applied to polyatomic molecules, and in calculations requiring treatment of nuclear dynamics, e.g., vibrational excitation. It shows promise as a crude method for estimating molecular polarizabilities; further tests, particularly at other than equilibrium molecular geometries, should be undertaken.

Applied in electron scattering calculations for H_2 and N_2, the correlation-polarization model employed [Eqs. (6)] occasionally gives better agreement with the results of more elaborate calculations when used in combination with the FEG exchange potential (SECOP) than in combination with an exact treatment of exchange (ESECOP). Since the FEG model of exchange is known[35] to be too weak for H_2 and N_2, this is fortuitous and suggests that the correlation-polarization model compensates by being too strong. Other evidence points in the same direction: it is stronger than the polarized orbital models (Figs. 2 and 3) in the important crossing region, and the corrections to the ESE results for partial cross sections in the ESECOP calculations are consistently too large. This leads to the suspicion that an *ad hoc* reduction of $v_{\mathrm{cop}}(\vec{r})$ could yield improved results, at least for H_2 and N_2, but tests on other systems with more electrons should first be undertaken.

Note added. Subsequent to completion of the work described above, we discovered the paper by Perdew and Zunger,[36] in which a new form for $v_{\mathrm{co}}(\vec{r})$ is given. This form, the results of a parametric fit to more accurate calculations of the correlation energy, is

$$v_{\mathrm{co}}(\vec{r})=\begin{cases} 0.0311\ln r_s-0.0584+0.00133r_s\ln r_s-0.0084r_s, & r_s<1 \\[2mm] \dfrac{\gamma(1+\frac{7}{6}\beta_1 r_s^{1/2}+\frac{4}{3}\beta_2 r_s)}{(1+\beta_1 r_s^{1/2}+\beta_2 r_s)^2}, & r_s\geq 1 \end{cases} \tag{9}$$

where $\gamma=-0.1423$, $\beta_1=1.0529$, and $\beta_2=0.3334$. The result is slightly smaller ($\sim 15\%$) for $r_s \lesssim 10$ than given by (6), and leads to a slightly weaker potential (e.g., $\sim 10\%$ for H_2). Given the conclusions reached above, we recommend the use of (9) rather than (6) in future work.

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