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Study of the Polarized-Orbital Method and Its Application to the Scattering of Electrons by Helium*

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A study has been made of the polarized-orbital method (POM) for electron-atom scattering. Within this framework, an exact calculation has been carried out for the electron–helium-atom case. Our study confirms the importance of the second-order distortion-exchange terms, which provide a nonadiabatic effect. A study is made of the much-criticized step function, and its inclusion within the POM framework is found to be not crucial. An attempt is made to clear up some of the present confusion in the literature by distinguishing between the POM and related methods.

I. INTRODUCTION

In the theoretical study of electron-atom scattering at low energies, one is faced with the essential complexity of a many-body system. Even with present-day high-speed computers, first-principles methods such as the variational approach or the eigenfunction-expansion approach can become impracticable, and one must rely on the art of approximation—the search for a general approximate method that is able to yield, with moderate computational effort, reasonably good results for a large class of atoms.

In a study of low-energy electron–oxygen-atom scattering, Temkin[1] in 1957 introduced the method of polarized orbitals, a method which is similar in concept to the method of perturbed stationary states[2] for atom-atom scattering. The ansatz for the polarized-orbital method (POM) was more clearly defined in the work of Temkin and Lamkin,[3] where it was applied to electron-hydrogen scattering. The resulting s-wave phase shifts and the p-wave phase shifts as corrected by Sloan[4] agree strikingly well with the standard reference, the variational calculations of Schwartz[5] and Armstead,[6] and the d-wave phase shifts are in reasonable agreement with the variational calculation of Gailitis[7] as well. Because of its relative computational simplicity, the POM results are all the more remarkable when compared with the results of much more complicated calculations such as the close-coupling approximation.[8] A large number of calculations for electron-atom scattering have subsequently appeared in the literature under the broad heading of polarized-orbital-method calculation.[9] Recently, certain questions and criticisms have been raised on the validity of the POM, for example, by Mittleman and Peacher.[10] Part of the criticism is formal, that Temkin's ansatz cannot be derived in the framework of the variational principle. Part of the criticism is more on the practical side, that the step function $\epsilon(r_a, r_i)$ used in Temkin's ansatz gives trouble and renders the method "nonpredictive."[10] While it is difficult at present to "derive" the POM prescription in an aesthetically pleasing way, it must be recognized the the POM ansatz is fundamentally based on physical reasonableness rather than a first-principles derivation. As such, the merit of the method must so be judged by the results it produces. Perhaps part of the current confusion with the method could be due to the fact that the large number of existing calculations under the heading of POM actually contain siginficant variations from Temkin's original ansatz and from each other. In fact, in spite of the large number of calculations, the POM in its original prescription has been tested only in two cases: in the electron-hydrogen calculation of Temkin and Lamkin[3] and Sloan,[4] which is exact within the POM framework, and in the electron-oxygen scattering calculation of Henry,[11] where the dominant terms within the POM framework are included. Thus, to truly assess the POM with regard to its usefulness and range of validity, it is necessary to consider "faithful" applications of the POM to cases other than the two just mentioned.

This work is the first part of a systematic study in this direction. Its purpose is twofold. First, we report the results of our application of the POM to the case of electron-helium scattering, rigorously adhering to the original ansatz of Temkin. In particular, we examine two essential points of the method: (i) the importance of the second-order exchange term (the distortion exchange), and (ii) the real effect of the much criticized step function $\epsilon(r_a, r_i)$ introduced by Temkin in his original ansatz.

Second, we attempt to clear up some of the present confusion in the literature by distinguishing between the POM and related methods.

The contents of the following sections are as follows: In Sec. II, the polarized-orbital method with Temkin's original ansatz is reviewed. In addition, the essential features of methods related to, but differing from, the POM are elicited. In Sec. III, the POM is applied to electron-helium scattering at low energies. Results for phase shifts and cross sections are presented. In Sec. IV we discuss the results.

II. THEORY

A. Review of Polarized-Orbital Method (POM)

For an electron scattering from an atom, the Schrödinger equation for the wave function Ψ of the entire system can be written as

$$[H-E]\,\Psi(z_1\ldots z_N;\; z_{N+1})=0\;, \tag{2.1}$$

where z_i denotes the space and spin coordinates $(\vec{r}, \vec{\sigma})$ of the N-electron atom and incident electron. The total Hamiltonian

$$H=H_A+K_{N+1}+V_{N+1,A} \tag{2.2}$$

is composed of H_A, the Hamiltonian of the atom K_{N+1}, the kinetic-energy operator for the incident electron, and $V_{N+1,A}$, the potential energy due to the Coulomb interaction of the incident electron with the atomic electrons and the atomic nucleus. The total energy

$$E=E_A+k_{N+1}^2 \tag{2.3}$$

consists of the initial atomic energy E_A and the incident electron's energy k_{N+1}^2.[12] The prescription that constitutes the POM is given below.[1,3]

1. *Form of Trial Wave Function*

The trial wave function

$$\Psi_t(z_1\ldots z_N;\; z_{N+1})=A\{[\Phi(z_1\ldots z_N)+\Phi^{(\mathrm{pol})}(z_1\ldots z_N;\; z_{N+1})]\,\phi(z_{N+1})\} \tag{2.4}$$

for the solution of Eq. (2.1) is the antisymmetrized product of $\phi(z_{N+1})$, the electron wave function describing the scattering process, and

$$\Phi'(z_1\ldots z_N;\; z_{N+1})=\Phi_0(z_1\ldots z_N)+\Phi(z_1\ldots z_N;\; z_{N+1})\;, \tag{2.5}$$

the distorted (polarized) atomic wave function consisting of the ground-state atomic wave function Φ_0 and a correction function $\Phi^{(\mathrm{pol})}$ due to the polarization of the atomic orbitals caused by the presence of the incident electron.

2. *Perturbation (Polarization) of Atomic Orbitals*

The unperturbed ground atomic state, characterized by a Hartree-Fock-Slater determinant

$$\Phi_0(z_1\ldots z_N)=\frac{1}{\sqrt{N!}}\begin{vmatrix}\phi_1(z_1) & \cdots & \phi_N(z_1)\\ \vdots & & \\ \phi_1(z_1) & \cdots & \phi_N(z_N)\end{vmatrix} \tag{2.6}$$

for an N-electron atom, is assumed to be *adiabatically perturbed*[13] by the incoming electron. The perturbation, being the electrostatic repulsion between the scattering and atomic electrons, is *dipole approximated* and assumed to be *zero when the particle is "inside" the atom*:

$$v(\vec{r}_1\ldots\vec{r}_N;\; \vec{r}_{N+1})\approx\sum_{i=1}^{N}\frac{2r_i}{r_{N+1}^2}\,P_1(\cos\theta_{i,N+1})\,\epsilon(r_i, r_{N+1})\;. \tag{2.7}$$

where the assumption that the atomic distortion is caused mainly by the presence of the perturbing electron in the region outside the atomic electrons is ensured by the introduction of the step function

$$\begin{aligned}\epsilon(r_i, r_{N+1})&=1, \quad r_i<r_{N+1}\\ &=0, \quad r_i>r_{N+1}\;.\end{aligned} \tag{2.8}$$

With these restrictions on the expression for the perturbation, the distorted atomic wave function

$$\Phi'(z_1\ldots z_N;\; z_{N+1})=\begin{vmatrix}\psi_1(z_1;\,\vec{r}_{N+1}) & \cdots & \psi_N(z_1;\,\vec{r}_{N+1})\\ \vdots & & \vdots\\ \psi_1(z_N,\,\vec{r}_{N+1}) & \cdots & \psi_N(z_N,\,\vec{r}_{N+1})\end{vmatrix} \tag{2.9}$$

is determined using Hartree-Fock perturbation theory.[14,15]

The spatial part of the jth atomic orbital ϕ_j, contained in the ground atomic state Φ_0, is perturbed (polarized) into[16]

$$\Psi_j(\vec{r}, \vec{r}_{N+1})=\phi_j(\vec{r})+\chi_j(\vec{r}, \vec{r}_{N+1}) \tag{2.10}$$

to first order, so that

$$\Phi^{(\mathrm{pol})}(z_1\cdots z_N;\; z_{N+1})=\sum_{j=1}^{N}\begin{vmatrix}\phi_1(z_1)\phi_2(z_1) & \cdots & \chi_j(z_1,\, z_{N+1}) & \cdots & \phi_N(z_1)\\ \vdots & & & & \vdots\\ \phi_1(z_N)\phi_2(z_N) & \cdots & \chi_j(z_N,\, z_{N+1}) & \cdots & \phi_N(z_N)\end{vmatrix} \tag{2.11}$$

where the jth term in the sum is a determinant similar to Φ_0 but differing in that the jth column has the ith element replaced by $\chi_j(z_i, z_{N+1})$. The first-order correction to the jth atomic orbital can be written in the form[1]

$$\chi_j(\vec{r}, \vec{r}_{N+1})=\epsilon(r, r_{N+1})\sum_{\substack{l_j'=l_j-1\\ l_j'\neq l_j}}^{l_j+1}\;\sum_{m_j'=-l_j'}^{l_j'}\frac{U_{n_jl_j\to l_j'}(r)}{r}$$

$$\times \frac{C^{(m_j-m_j')}_{n_jl_j-l_j'}}{r^2_{N+1}} Y_{l_j'm_j'}(\Omega_r)Y_{1,m_j-m_j'}(\Omega_{N+1}) \quad , \tag{2.12}$$

where the constants $C^{(m_j-m_j')}_{n_jl_j-l_j'}$ are given by

$$C^{(m_j-m_j')}_{n_jl_j-l_j'} = (-1)^{m_j-m_j'+1}\left[\frac{16\pi}{3}\left(\frac{2l_j+1}{2l_j'+1}\right)\right]^{1/2}$$

$$\times(1\,l_j00|\,l_j'0)(1\,l_j\,m_j'-m_jm_j\,|\,l_j'm_j') \tag{2.13}$$

and the radial functions $U_{n_jl_j-l_j'}(r)$ satisfy Sternheimer's equations

$$\left(-\frac{d^2}{dr^2}+v_{n_jl_j-l_j'}(r)\right)U_{n_jl_j-l_j'}(r)=rU_{n_jl_j}(r) \quad , \tag{2.14}$$

with the potential $V_{n_jl_j-l_j'}(r)$ given by

$$V_{n_jl_j-l_j'}(r)=\frac{U''_{n_jl_j}(r)}{U_{n_jl_j}(r)}+\frac{l_j'(l_j'+1)-l_j(l_j+1)}{r^2} \,. \tag{2.15}$$

Under the influence of the dipole perturbation the ground-state orbital characterized by the radial function $U_{n_jl_j}(r)$ can be thought of as undergoing virtual transitions to the two states characterized by $l_j'=l_j\pm1$.

In the equation that $\chi(\vec{r}, \vec{r}_{N+1})$ satisfies, the presence of the step function $\epsilon(r, r_{N+1})$ gives rise to the δ function containing terms[17] discovered by Sloan:

$$\left(-\nabla_r^2+\frac{\nabla^2\phi_j}{\phi_j}\right)\chi_j(\vec{r}, \vec{r}_{N+1}) = -\epsilon(\vec{r}, \vec{r}_{N+1})\frac{2r}{r^2_{N+1}} P_1(\cos\theta_{r,r_{N+1}})\phi_j(\vec{r})$$

$$\times\sum_{\substack{l_j'=l_j-1\\ l_j'\neq l_j}}^{l_j+1}\left[\frac{U_{n_jl_j-l_j'}(r)}{r}\frac{d}{dr}\,\delta(r-r_{N+1})+2\frac{\delta(r-r_{N+1})}{r}\left(\frac{d}{dr}\,U_{n_jl_j-l_j'}(r)\right)\right]\left[\frac{C^{(m_j-m_j')}_{n_jl_j-l_j'}}{r^2_{N+1}}Y_{l_j'm_j'}(\Omega_r)Y_{1,m_j-m_j'}(\Omega_{N+1})\right] \,. \tag{2.16}$$

3. *Ansatz*: *the Scattering Equation*

The equation of motion of the scattering-electron's wave function $\phi(\vec{r}_{N+1})$ is obtained by projecting on the left-hand side of Eq. (2.1) by the unperturbed atomic wave function Φ_0^* and integrating out the atomic coordinates:

$$\int dz_1\cdots dz_N\,\Phi_0^*(z_1\cdots z_N)\,[H-E]\,\Psi_t(z_1\cdots z_N;\,z_{N+1})=0 \,. \tag{2.17}$$

In the resulting equation for $\phi(\vec{r}_{N+1})$, one has four terms in the effective potential. They are the static, static-exchange, polarization, and polarization-exchange potentials. In a proper polarized-orbital calculation, all terms must be included.

To summarize, the essential features of the POM are expression (2.4) for the trial function

$$\Psi_t(z_1\cdots z_N;\,z_{N+1})$$
$$=A\{[\Phi_0(z_1\cdots z_N)+\Phi^{(\text{pol})}(z_1\cdots z_N;\,z_{N+1})]\phi(z_{N+1})\} \,,$$

the dipole approximation (2.7)

$$v(\vec{r}_1\cdots\vec{r}_N;\,\vec{r}_{N+1})$$
$$\approx\sum_{i=1}^{N}\frac{2r_i}{r^2_{N+1}}P_i(\cos\theta_{i,N+1})\epsilon(r_i,\,r_{N+1}) \,,$$

and the scattering ansatz (2.17)

$$\int dz_1\cdots dz_N\,\Phi_0^*(z_1\cdots z_N)[H-E]\Psi_t(z_1\cdots z_N;\,z_{N+1})=0 \,.$$

B. Variations on POM

A large number of calculations that have been referred to as POM calculations in the literature actually contain important deviations from the above prescription. These deviations may be one or more of the following:

a. Omission of distortion exchange terms. The distortion-exchange terms in general add more difficulty in calculation and have, for this reason, been omitted by a large number of authors, a few of whom we cite here.[18–21] This approximation should properly be called the adiabatic-exchange (AE) approximation. With this omission the resulting effective potential, except for the static-exchange term, is local in character and includes a Coulomb interaction term and a polarization potential. As we shall see, the deletion of polarization-exchange terms gives rise to phase-shift and cross-section curves which are significantly shifted with respect to those resulting from application of the exact POM.

b. Inclusion of additional multipole terms in $\chi(\vec{r}, \vec{r}_{N+1})$. Instead of treating only the dipole component of the adiabatic distortion such as was done in the dipole approximation [Eq. (2.7)], one may include the monopole or quadrupole distortion terms as well. This has been done by Garret[22] in the study of the scattering of slow electrons by lithium and sodium. The Dalgarno-Lynn[23] polarization potential is used by Callaway *et al.*,[21] who allow for the effects of higher multipoles in the electron-hydrogen and electron-helium cases. However, it has been pointed out[24] that the inclusion of other multipole terms may not be desirable because of the nonadiabatic condition in the atomic scattering processes.

c. Variationally determined polarization potential. Instead of using an adiabatic distortion function $\chi(\vec{r}, \vec{r}_{N+1})$ to produce a polarization potential, a suitably parametrized function can be introduced to allow variation of a simple form of the atomic wave function so that the energy of the atom is a minimum. For the case where positrons are scattered by hydrogen, Stone[25] allowed the 1*s* function $\Psi_{1s}(\vec{r})$ to distort into $\Psi_{1s}(\vec{r}) + \beta(\vec{r}_{N+1})\,\Psi_{2p}(\vec{r})$, with $\beta(\vec{r}_{N+1})$ varied to minimize the atomic energy. He utilized the same procedure to study not only the scattering of positrons by hydrogen, but the scattering of electrons by lithium as well.

d. Modification of step function. A step function was introduced in Eq. (2.7) by Temkin[1] to express the idea that during the scattering process atomic distortion is appreciable only when the incoming electron does not actually penetrate the atom. In Eq. (2.16), we solve only for the case when $r < r_{N+1}$, since the step function occurring in Eq. (2.12) causes $\chi(\vec{r}, \vec{r}_{N+1})$ to be zero for $r > r_{N+1}$. Some authors[18, 22, 26] prefer to omit the step function and solve Eq. (2.16) for both regions—$r > r_{N+1}$ as well as $r < r_{N+1}$. In this case Sloan terms do not occur. We call this the *modified-polarized-orbital method* (MPOM) and will examine it explicitly in this paper in two special cases.

Still others have replaced the step function by a functional form to be varied for optimum results, as in the work of Oberoi and Callaway[27] or Mittleman and Peacher.[10]

e. Variationally based scattering equation. In the work of Mittleman and Peacher,[10] they set the polarized-orbital method on a variational basis by projecting on the left-hand side of Eq. (2.17) by $\Phi_0(z_1 \cdots z_N) + \Phi^{(\mathrm{pol})}(z_1 \cdots z_N; z_{N+1})$ instead of $\Phi_0(z_1 \cdots z_N)$. That is, they have

$$\int dz_1 \cdots dz_N [\Phi_0(z_1 \cdots z_N) + \Phi^{(\mathrm{pol})}(z_1 \cdots z_N; z_{N+1})] \times [H - E]\,\Psi_t(z_1 \cdots z_N; z_{N+1}) = 0 \; .$$

It may be pointed out that their resulting equation is actually identical to that of the extended-polarization method[20] proposed by us earlier. It can be shown[10] that the essential difference of this variationally based equation is the addition of a new term in the effective potential of the form $\int |\vec{\nabla}_t \chi(\vec{r}, \vec{r}_t)|^2 d^3\vec{r}$.

Mittleman and Peacher introduced a functional form to replace the step function. By varying the functional form, they obtained widely varying results in their phase shifts; and from this they concluded that the POM is nonpredictive. Actually, the trouble comes from this additional term only. This can be seen in a simple way as follows. Because of the gradient operator, this term will yield a large value whenever there exists a "kink" in the distortion wave function χ. In fact, this additional effective potential will become infinite if the χ has a discontinuity in r_t as in the case of the step function. Thus we see the source of Mittleman and Peacher's complaint lies only in this term, which simply does not exist in the proper POM prescription.

III. ELECTRON-HELIUM SCATTERING

A. POM Calculation

The exact POM prescription as outlined in Sec. II is applied to electron-helium scattering in a straightforward manner. The details are given in Appendix A and we give here the resulting equation for the radial wave function $R_l(r)$ for the *l*th partial wave of the scattered electrons:

$$\begin{aligned}
&\left(-\frac{d^2}{dr_3^2} + \frac{l(l+1)}{r_3^2} - \frac{2N}{r_3} + N \cdot V_c(r_3) + N \cdot V_p(r_3) - k^2\right) R_l(r_3) = U_{1s}(r_3)\left(-(-\epsilon_{1s} + k^2)\,\delta_{l0}\int_0^\infty U_{1s}(r) R_l(r)\,dr\right. \\
&\quad \left. + \frac{2}{2l+1}\int_0^\infty \frac{r_<^l}{r_>^{l+1}}\, U_{1s}(r) R_l(r)\,dr\right) - \delta_{l1}\left\{\frac{2}{3}\left[U_{1s\to p}(r_3)\frac{d}{dr_3}\,\frac{U_{1s}(r_3)}{r_3^2} + 2\left(\frac{dU_{1s\to p}(r_3)}{dr_3}\right)\frac{U_{1s}(r_3)}{r_3^2}\right] + \frac{2}{3}\, U_{1s\to p}(r_3)\right. \\
&\quad \left. \times \frac{U_{1s}(r_3)}{r_3^2}\,\frac{d}{dr_3}\right\} R_l(r_3) - \frac{2}{3}\,\delta_{l1} U_{1s}(r_3)\int_{r_3}^\infty \frac{r_3}{r^2}\, U_{1s}(r) R_l(r)\,dr - U_{1s\to p}(r_3)\left[-\frac{2}{3}(-\epsilon_{1s} + k^2)\delta_{l1}\int_{r_3}^\infty \frac{U_{1s}(r) R_l(r)}{r^2}\,dr\right. \\
&\quad \left. + 4\left(\frac{l}{(2l+1)(2l-1)}\, r_3^{l-1}\int_{r_3}^\infty \frac{U_{1s}(r) R_l(r)}{r^{l+2}}\,dr + \frac{l+1}{(2l+1)(2l+3)}\, r_3^{l+1} \times \int_{r_3}^\infty \frac{U_{1s}(r) R_l(r)}{r^{l+4}}\,dr\right)\right] \\
&\quad + U_{1s}(r_3)\left(\delta_{l0}\int_0^\infty U_{1s}(r) V_p(r) R_l(r)\,dr - \frac{4}{9}\,\delta_{l1}\int_0^\infty r_1 \int_{r_1}^\infty \frac{U_{1s}(r_2) R_l(r_2)}{r_2^2}\,dr_2\, U_{1s}(r_1)\frac{r_<}{r_>^2}\,\frac{U_{1s\to p}(r_1)}{r_1}\,dr_1\right) \; . \qquad (3.1)
\end{aligned}$$

TABLE I. Electron-helium partial-wave phase shifts (in rad).

k	Energy (eV)	Static exchange η_0	Static exchange η_1	Static exchange η_2	Adiabatic exchange η_0	Adiabatic exchange η_1	Adiabatic exchange η_2	Polarized orbitals η_0	Polarized orbitals η_1	Polarized orbitals η_2
0[a]	0	1.482			1.121			1.110		
0.10	0.14	2.9937	0.00042	0.00000	3.0192	0.00335	0.00044	3.0203	0.00332	0.00044
0.197	0.50	2.8595	0.00289	0.00001	2.8978	0.0131	0.00164	2.8997	0.0128	0.00164
0.25	0.85	2.7757	0.00627	0.00004	2.8193	0.0229	0.00281	2.8216	0.0224	0.00280
0.30	1.22	2.7049	0.0106	0.00009	2.7520	0.0338	0.00407	2.7546	0.0327	0.00405
0.40	2.18	2.5673	0.0236	0.00034	2.6196	0.0617	0.00732	2.6223	0.0594	0.00727
0.50	3.40	2.4358	0.0425	0.00092	2.4918	0.0971	0.0116	2.4942	0.0926	0.0115
0.60	4.90	2.3113	0.0667	0.00201	2.3701	0.1375	0.0170	2.3719	0.1302	0.0167
0.70	6.66	2.1943	0.0947	0.00376	2.2556	0.1803	0.0234	2.2564	0.1696	0.0228
0.75	7.65	2.1388	0.1095	0.00492	2.2011	0.2015	0.0270	2.2012	0.1891	0.0262
0.80	8.70	2.0852	0.1246	0.00627	2.1485	0.2223	0.0307	2.1479	0.2081	0.0298
1.00	13.60	1.8901	0.1831	0.0136	1.9571	0.2959	0.0477	1.9530	0.2749	0.0458
1.10	16.46	1.8037	0.2093	0.0184	1.8722	0.3254	0.0570	1.8662	0.3016	0.0544
1.25	21.25	1.6868	0.2430	0.0266	1.7572	0.3600	0.0712	1.7483	0.3332	0.0676
1.50	30.60	1.5220	0.2843	0.0419	1.5943	0.3967	0.0943	1.5811	0.3671	0.0890
1.75	41.65	1.3883	0.3105	0.0579	1.4610	0.4152	0.1152	1.4445	0.3852	0.1086
2.00	54.40	1.2789	0.3267	0.0735	1.3507	0.4232	0.1333	1.3321	0.3941	0.1256

[a] $k=0$ entries are scattering lengths.

The terms on the left-hand side of the equation are, respectively, the kinetic-energy operator term, the centrifugal-barrier term, the nuclear coulomb term, the static-potential term, the direct polarization potential and the incident-electron energy term. On the right-hand side of the equation, terms associated with the first large parentheses are the first-order static exchange terms while those associated with the first curly brackets are the Sloan terms. The other terms are the second-order distortion-exchange contributions which constitute the unique feature of the POM. The 1s radial wave function U_{1s} used in this calculation is the Hartree-Fock helium wave function of Roothaan, Sachs, and Weiss.[28] The dipole distortion $U_{1s\to p}$ satisfies the Sternheimer equation

$$\left(-\frac{d^2}{dr^2}+\frac{U_{1s}''(r)}{U_{1s}(r)}+\frac{2}{r^2}\right)U_{1s\to p}(r)=rU_{1s}(r)\ . \qquad (3.2)$$

The calculation is exact and no deletions are made in Eqs. (3.1) and (3.2).

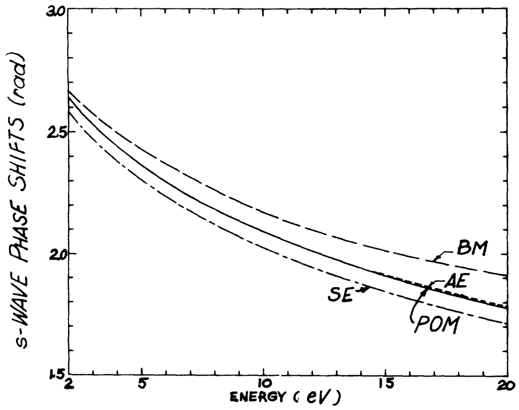

FIG. 1. s-wave phase shifts for the elastic scattering of electrons by helium.

B. Comparison of POM with MPOM

In a study of the effect of the step function ϵ, we have compared, in both the e^--H and e^--He cases, the POM results with those of the MPOM in which

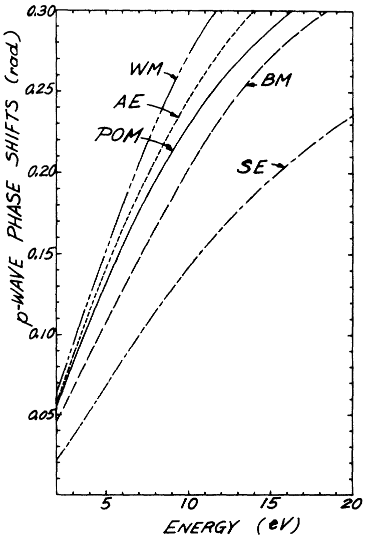

FIG. 2. p-wave phase shifts for the elastic scattering of electrons by helium.

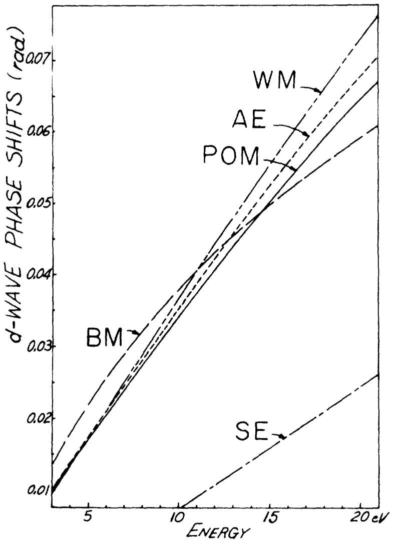

FIG. 3. d-wave phase shifts for the elastic scattering of electrons by helium.

the step function is not employed.

For the e^--H case, the atomic distortion function $U_{1s\rightarrow p}$ can be obtained analytically[29] and the calculations are exact. For the e^--He case, we have employed a slight approximation such that the function $U_{1s\rightarrow p}$ becomes analytic. This small approximation is further justified by the fact that the POM result with this approximation is nearly identical to the exact POM calculation and that we are interested in the difference between the POM and the MPOM results. Details of the approximation, known as the SCF-hydrogenic approximation, are given in Appendix B. In Appendix C we give comments pertinent to the numerical methods employed.

IV. RESULTS AND DISCUSSION

We first present our results for the case of e^--He scattering. The polarized-orbital-method prescription, as discussed in Sec. III, has been rigorously followed. The phase shifts for s, p, and d waves are tabulated in Table I and displayed in Figs. 1–3. For comparison we give the static-exchange (SE) results and the adiabatic-exchange (AE) results. Also included is a theoretical fit of experimental data by Bransden and McDowell[30] (BM). The total-cross-section curves are given in Fig. 4, where the experimental curve of Golden and Bandel is also presented.

The dominant characteristics of the POM calculations are readily apparent. The POM curves in general lie between the SE curves and the AE curves. A variational lower bound is provided in the SE case, but polarization effects are not taken into account, while the adiabatic long-range potential of the AE case tends to provide too much attraction. Since the main difference between the POM and AE calculations comes from the second-order distortion-exchange term, we conclude, as in the case of e^--H scattering, that the second-order exchange term is important and provides a nonadiabatic effect, shifting from the AE results toward the SE results.

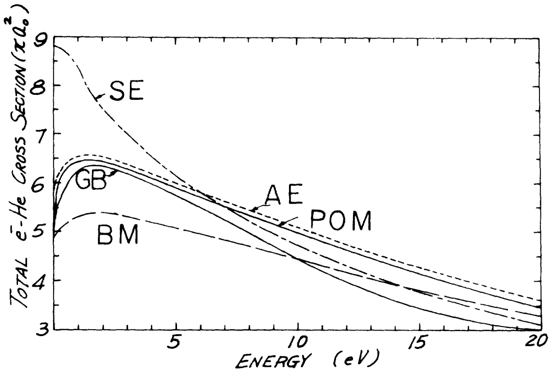

FIG. 4. Total elastic scattering cross section for the scattering of electrons by helium.

On the whole, the POM result for the e^--He case agrees quite well with presently available experimental data. It also compares well with other theoretical methods. Thus our study supports the usefulness of the POM as a general approximate method for obtaining relatively accurate phase shifts with a minimum effort. Since in the e^--He case the s-wave phase shift is rather insensitive to the various theoretical methods, the higher partial waves are more important in distinguishing between the different methods. More accurate experiments of the differential-cross-section type are needed in this regard.

We now turn to the question of the "predictiveness" of the POM calculation. As explained in Sec. II B,

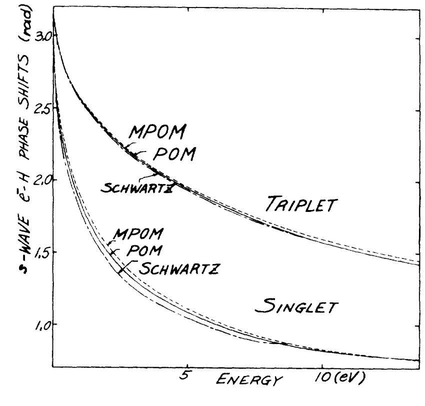

FIG. 5. Comparison of POM and MPOM s-wave phase shifts for the elastic scattering of electrons by hydrogen.

the widely varying results obtained by Mittleman and Peacher come from an additional term in the effective potential which simply does not arise in the proper POM ansatz. However, it is still of interest to examine the effect of the step function *within* the POM prescription. In this direction we have made two MPOM calculations, which differ from the POM only in that the step function is not used in the distortion function χ. For the e^--He case the MPOM phase-shift values differ so little from those of the POM that they are not discernible in the figures. The MPOM calculation for the e^--H case is illustrated in Fig. 5. Here the POM and MPOM are slightly different and the POM results seem to be preferred. These results suggest that the effect of the step function in the POM is not really severe.

In Sec. II B we discussed the distinguishing features of the wide range of approximate methods which contain significant deviations from the POM but are nevertheless often referred to under the same heading in the literature. For illustration we show the "POM"[9] calculation of Williamson and McDowell[19] in Figs. 2 and 3. Thus, careful differentiation must be exercised in surveying the literature, especially when assessing the validity of the POM itself.

Regarding the theoretical justification of Temkin's method, it must be made clear that no one has yet provided for the POM a derivation resting upon first principles. Rather, the method remains a "prescription" as we have referred to it throughout this paper. Further investigation is needed along two fronts. Attempts, such as the one by Mittleman and Peacher,[10] to justify it on a formal basis should be continued. However, to provide the impetus for such attempts, one must explore the range of validity of the POM in a number of applications.

Our work, along with the e^--H result,[3] indicates that the second-order distortion-exchange term contributes significantly. Thus a more stringent test on the POM would be the application to highly polarizable atoms. A POM calculation on e^--Li is presently being carried out which should further help in assessing the usefulness of the POM as a general tool for electron-atom scattering calculations.

APPENDIX A: ELECTRON-HELIUM SCATTERING (EXACT POM PRESCRIPTION)

For helium the unperturbed ground state is taken to be the self-consistent restricted Hartree-Fock-Slater determinant

$$\Phi_0(z_1, z_2) = \frac{1}{\sqrt{2!}} \begin{vmatrix} \phi_{1s}(\vec{r}_1)\alpha(\vec{\sigma}_1) & \phi_{1s}(\vec{r}_2)\alpha(\vec{\sigma}_2) \\ \phi_{1s}(\vec{r}_1)\beta(\vec{\sigma}_1) & \phi_{1s}(\vec{r}_2)\beta(\vec{\sigma}_2) \end{vmatrix}, \tag{A1}$$

where ϕ_{1s} is the $1s$ helium ground-state orbital and α and β are spin functions. Under the influence of the incoming (polarizing) electron, the atomic orbitals are polarized so that the new atomic state to first order is

$$\Phi_0'(z_1, z_2, z_3) = \Phi_0(z_1, z_2) + \frac{1}{\sqrt{2!}} \begin{vmatrix} \chi(\vec{r}_1, \vec{r}_3)\alpha(\vec{\sigma}_1) & \phi_{1s}(\vec{r}_2)\alpha(\vec{\sigma}_2) \\ \chi(\vec{r}_1, \vec{r}_3)\beta(\vec{\sigma}_2) & \phi_{1s}(\vec{r}_2)\beta(\vec{\sigma}_2) \end{vmatrix} + \frac{1}{\sqrt{2!}} \begin{vmatrix} \phi_{1s}(\vec{r}_1)\alpha(\vec{\sigma}_2) & \chi(\vec{r}_2, \vec{r}_3)\alpha(\vec{\sigma}_2) \\ \phi_{1s}(\vec{r}_1)\beta(\vec{\sigma}_1) & \chi(\vec{r}_2, \vec{r}_3)\beta(\vec{\sigma}_2) \end{vmatrix}. \tag{A2}$$

The orbital distortion $\chi(\vec{r}_3, \vec{r}_2)$ satisfies

$$\begin{aligned} [-\nabla_3^2 - 4/r_3 + V_c(r_3) - \epsilon_{1s}]\, \chi(\vec{r}_3, \vec{r}_2) = {} & -\epsilon(r_3, r_2)\,(2r_3/r_2^2)\, P_1(\cos\theta_{32})\, \phi_{1s}(\vec{r}_3) \\ & - \left[\frac{U_{1s\to p}(r_3)}{r_3} \frac{d}{dr_3} \delta(r_3 - r_2) + 2\,\frac{\delta(r_3 - r_2)}{r_3} \left(\frac{d}{dr_3}\, U_{1s\to p}(r_3)\right)\right] \left(\frac{P_1(\cos\theta_{32})}{\pi^{1/2} r_2^2}\right), \end{aligned} \tag{A3}$$

and has a form identical with that for the case of electron-hydrogen scattering[29]

$$\chi(\vec{r}_3, \vec{r}_2) = -\frac{\epsilon(r_3, r_2)}{r_2^2} \frac{U_{1s\to p}(r_3)}{r_3} \frac{P_1(\cos\theta_{32})}{\pi^{1/2}}, \tag{A4}$$

where $U_{1s\to p}(r)$ satisfies Sternheimer's equation

$$\left(-\frac{d^2}{dr^2} + \frac{U_{1s}''(r)}{U_{1s}(r)} + \frac{2}{r^2}\right) U_{1s\to p}(r) = r U_{1s}(r). \tag{A5}$$

with $U_{1s}(r)$ taken to be the $1s$ radial wave function for helium provided by Roothaan, Sachs, and Weiss.[28] Their $1s$ energy is denoted by ϵ_{1s}. $V_c(r_3)$ is defined in Eq. (A10). It should be noted that Eqs. (A3) and (2.16) are equivalent[31] since, for the case of helium, Sternheimer's approximation is exact. In fact, Eq. (A3) is the complete Hartree-Fock 1st-order perturbation equation within the constraint of our dipole approximation except for the deletion of a single intrashell $1s$-$1s$ correlation term.

To obtain the desired scattering equation, one substitutes the expressions for the total Hamiltonian

$$H = -\nabla_1^2 - \nabla_2^2 - \nabla_3^2 - \frac{4}{r_1} - \frac{4}{r_2} - \frac{4}{r_3} + \frac{2}{r_{12}} + \frac{2}{r_{13}} + \frac{2}{r_{23}}, \tag{A6}$$

the total energy

$$\begin{aligned}E &= E_A + k^2\\ &= 2\epsilon_{1s} - \langle \phi_{1s}(\vec{r}_1)\phi_{1s}(\vec{r}_2)(2/r_{12})\phi_{1s}(\vec{r}_1)\phi_{1s}(\vec{r}_2)\rangle_{1,2} + k^2\\ &= 2\epsilon_{1s} - \langle \phi_{1s}(\vec{r}_1)V_c(\vec{r}_1)\phi_{1s}(\vec{r}_1)\rangle_1 + k^2,\end{aligned} \tag{A7}$$

and the trial wave function

$$\Psi_t(z_1, z_2; z_3) = [\Phi'(z_1, z_1; z_3)\phi(z_3)] \tag{A8}$$

into the ansatz (2.17). One finds that the scattering equation satisfied by $\phi(\vec{r}_3)$ is

$$\begin{aligned}&[-\nabla_3^2 - 4/r_3 + 2\langle \phi_{1s}(\vec{r}_1)(2/r_{13})\phi_{1s}(\vec{r}_1)\rangle_1 + 2\langle \phi_{1s}(\vec{r}_1)(2/r_{13})\chi(\vec{r}_1, \vec{r}_3)\rangle_1 - k^2]\,\phi(\vec{r}_3) = (\epsilon_{1s} - k^2)\langle \phi_{1s}(\vec{r}_2)\,\phi(\vec{r}_2)\rangle_2\,\phi_{1s}(\vec{r}_3)\\ &\quad + \langle \phi_{1s}(\vec{r}_2)(2/r_{23})\phi(\vec{r}_2)\rangle_2\,\phi_{1s}(\vec{r}_3) + (\epsilon_{1s} - k^2)\langle \phi_{1s}(\vec{r}_2)\,|\,\chi(\vec{r}_3, \vec{r}_2)\phi(\vec{r}_2)\rangle_2 + \langle \phi_{1s}(\vec{r}_2)\,|\, -\epsilon(r_3, r_2)(2r_3/r_2^2)\\ &\quad \times P_1(\cos\theta_{32})\,\phi(\vec{r}_2)\rangle_2\,\phi_{1s}(\vec{r}_3) + \langle \phi_{1s}(\vec{r}_1)\,\phi_{1s}(\vec{r}_2)(2/r_{13})\chi(\vec{r}_1, \vec{r}_2)\phi(\vec{r}_2)\rangle_{1,2}\,\phi_{1s}(\vec{r}_3)\\ &\quad + \langle \phi_{1s}(\vec{r}_2)\phi_{1s}(\vec{r}_1)(2/r_{12})\chi(\vec{r}_1, \vec{r}_2)\,\phi(\vec{r}_2)\rangle_{1,2}\,\phi_{1s}(\vec{r}_3) - \langle \phi_{1s}(\mathrm{r}_2)\,|\\ &\quad \times \left[\frac{U_{1s\text{-}p}(r_3)}{r_3}\,\frac{d}{dr_3}\,\delta(r_3 - r_2) + 2\,\frac{\delta(r_3 - r_2)}{r_3}\left(\frac{d}{dr_3}\;U_{1s\text{-}p}(r_3)\right)\right]\left(\frac{P_1(\cos\theta_{32})}{\pi^{1/2}r_2^2}\right)\,|\,\phi(\vec{r}_2)\rangle_2\,.\end{aligned} \tag{A9}$$

By retaining in the effective potential only the direct-Coulomb static term[32]

$$2V_c(r_2) = \langle \phi_{1s}(\vec{r}_1)(2/r_{12})\phi_{1s}(\vec{r}_1)\rangle, \tag{A10}$$

and the static-exchange terms

$$(\epsilon_{1s} - k^2)\langle \phi_{1s}(\vec{r}_2)\,|\,\phi(\vec{r}_2)\rangle\;\phi_{1s}(\vec{r}_3)$$
$$+\langle \phi_{1s}(\vec{r}_2)(2/r_{23})\phi(\vec{r}_2)\rangle\;\phi_{1s}(\vec{r}_3),$$

one has the static-exchange approximation. Static-exchange phase shifts were calculated in 1953 by Morse and Allis.[33] Inclusion of the polarization-potential term[32]

$$2V_p(r_2) = 2\langle \phi_{1s}(1)(2/r_{12})\chi(\vec{r}_1, \vec{r}_2)\rangle \tag{A11}$$

results in the *adiabatic-exchange* approximation. Further inclusion of the Sloan terms and the remaining distortion-exchange terms leaves one with what is properly called the polarized-orbital method (POM).

By expressing $\phi(\vec{r})$ as

$$\phi(\vec{r}) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{R_l(r)}{r}\,Y_{lm}(\Omega), \tag{A12}$$

a partial-wave analysis of Eq. (A9) results in the radial equation (3.1).

Note that the Temkin-Sloan[3,4] electron-hydrogen equation for the triplet case can be recovered by setting $N = 1$ and deleting the last two terms in large parentheses on the right. For the singlet case the entire right-hand side must change sign also and for the electron-helium case $N = 2$.

APPENDIX B: SCF HYDROGENIC APPROXIMATION

This approximation[34,35] constitutes a slight modification which yields very similar results with greater simplicity by providing an analytic solution for $U_{1s\text{-}p}(r)$, and thus making numerical solution of Sternheimer's equation unnecessary. It is in the framework of this approximation that we will compare the POM and MPOM in the electron-helium scattering case.

1. POM *Prescription*

With the aim of obtaining an atomic distortion function $\chi(\vec{r}, \vec{R})$ in the SCF hydrogenic approximation, we transform Eq. (A5) by introducing a function f such that

$$U_{1s\text{-}p}(r) = f(r)\,U_{1s}(r)\;, \tag{B1}$$

whereby Sternheimer's equation becomes

$$\left(-\frac{d^2}{dr^2} - 2\,\frac{U_{1s}'(r)}{U_{1s}(r)}\,\frac{d}{dr} + \frac{2}{r^2}\right)f(r) = r\;. \tag{B2}$$

The approximation of this section is to let $U_{1s}'(r)/U_{1s}(r) = -z + 1/r$, our justification of the introduction of the screening parameter z having been demonstrated previously by one of us (LaBahn).[35] Since this approximation is exact for the electron-hydrogen scattering problem (with $z = 1$) and since in Eq. (A14) as well as elsewhere the proper SCF orbital is still retained, it is called the SCF hydrogenic approximation.

We then have as an analytic solution[29] for f in the POM prescription

$$f(r) = (1/2z^2)\left(\tfrac{1}{2}zr^2 + r\right), \quad r < R \tag{B3}$$

whereupon

$$U_{1s\text{-}p}(r) = [U_{1s}(r)/2z^2]\left(\tfrac{1}{2}zr^2 + r\right)\;. \tag{B4}$$

Z is chosen to give the polarizability of 1.395 in accordance with the experimental value provided by Johnston, Oudemans, and Cole.[36] That this value differs from the Sternheimer value[37] of 1.487 is of no consequence in the particular comparative study we are concerned with. It is interesting to note that in Figs. 1–3 the POM curves with and without the SCF hydrogenic approximation coincide to the accuracy of the graphs (consequently only the POM results are shown).

The equation now satisfied by χ is the same as Eq. (A3) with the addition to the right-hand side of a so-called logarithmic-derivative-correction (LDC) term

$$\epsilon(r_2, r_3)\, 2\frac{r_3}{r_2^2}\, \frac{1}{U_{1s\to p}(r_3)} \left[\left(1 - \frac{1}{z^2 r_3^2}\right) U_{1s}(r_3) + \frac{(zr_3+1)}{z^2 r_3}\, U'_{1s}(r_3)\right] \frac{U_{1s\to p}(r_3)}{r_3}\, \frac{P_1(\cos\theta_{32})}{(4\pi)^{1/2}} \;. \qquad \text{(B5)}$$

This causes the addition to the right-hand side of the radial equation (3. 1) of the expression

$$\delta_{l1}\, \frac{2}{3} \left[\left(1 - \frac{1}{z^2 r_3^2}\right) U_{1s}(r_3) + \frac{zr_3+1}{z^2 r_3}\, U'_{1s}(r_3)\right] \times \int_{r_3}^{\infty} \frac{U_{1s}(r) r_3 R_1(r)}{r^2}\, dr \qquad \text{(B6)}$$

to account for the fact that the SCF hydrogenic approximation is used. Note that both of the above expressions reduce to zero if $U_{1s}(r)$ is the radial function for the hydrogen atom.

2. *Modified Polarized-Orbital Method* (MPOM)

In this case we consider both of the regions $r < R$ and $r > R$ instead of setting $\chi(\vec{r}, \vec{R}) = 0$ for $r > R$ by use of the step function $\epsilon(r, R)$. The POM is now modified in the following manner.

In Eq. (A3), the Sloan term is omitted since that is due solely to the operation of ∇^2 on the step function. The form of χ is the same as in Eq. (A4) except that ϵ is replaced by unity. Equation (B3) is now replaced with expressions found by Reeh[38] and also by Bethe.[39] Reeh found solutions for $r < R$ and $r > R$ and then matched them by mixing in appropriate multiples of the two independent homogeneous solutions. We have

$$f(r) = \frac{1}{z(zR)^2}\left[\frac{3(zR+1)^2}{4}\, e^{-2zR}\left(\frac{e^{2zr}-1}{(zr)^2} - \frac{2}{zr} - 2\right) - \frac{(zr)^2}{2} - zr\right], \qquad r < R$$

$$f(r) = \frac{1}{z}\left[\frac{3'\,3}{4(zR)^2}\left[1 - (zR)^2 - e^{-2zR}\,(zR+1)^2\right]\left(\frac{1}{(zr)^2} + \frac{2}{zr} + 2\right) + \frac{zR}{2}\left(\frac{1}{(zr)^2} + \frac{2}{zr}\right)\right], \qquad r > R \;. \qquad \text{(B7)}$$

$U_{s\to p}(r)$ for each region, inside and out, is specified by Eq. (B1). For the electron-hydrogen case, where $z = 1$, Eq. (B7) is exact and yields for $V_p(r)$ the so-called Bethe potential.[25] Callaway[25] compares this form of $V_p(r)$ with that obtained by use of Eq. (B3).

In Eq. (A9), $\epsilon(r_3, r_2)$ is replaced by unity and the Sloan term is dropped. A radial equation is obtained after carrying out the integration in Eq. (A9) just as Eq. (3. 1) follows from Eq. (A9). It contains an LDC term different from that of (B6).

APPENDIX C: NUMERICAL PROCEDURE

Sternheimer's equation [(A5)] for the electron-helium case was solved numerically by the use of the procedure outlined by Sternheimer.[40] An outward integration routine was fed starting values which were varied appropriately until a well-behaved solution was obtained. Equation (3. 1) was solved by use of the noniterative method described by Temkin[3] and modified by Sloan.[4] Mesh sizes used were 0.01 for $r \le 0.2$, 0.02 for $0.2 < r \le 2$, and 0.03 for $r > 2$. Integrations were carried out to $r = 20$. All calculations were performed on an IBM 360 computer. Two exceptions to Temkin's procedure are listed below. The orthogonality term $\int_0^\infty U_{1s}(r) R_0(r)\, dr$ is set equal to zero in the static-exchange and polarized-orbital cases. That this is a rigorous result and not an approximation can be seen by multiplying the radial equation on the left by $U_{1s}(r_3)$ and integrating over r_3. Retention of the orthogonality term allows R_0 to contain multiples of spurious solutions which increase numerical errors in the asymptotic form of R_0 and hence in resulting phase shifts.[41] For example, in the static-exchange case, if $\phi(r)$ is a solution, then $\phi(r) + c\phi_{1s}(r)$ is also a solution for any constant c. "Forcing" orthogonality by deleting the orthogonality term gives the best results by ensuring that $c = 0$ instead of some arbitrary value generated by random errors occurring in the numerical analysis used to solve the scattering equation.

To account for the fact that the long-range polarization potential is still appreciable at the limits of integration, the Levy-Keller[33] method is used as explained previously by LaBahn and Callaway[34] to correct phase shifts and scattering lengths for a truncation necessitated by computational considerations.

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$$\hbar^2 k_i^2 / 2m_e = k_i^2 .$$

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[17] Use is made of the following identity: For $f(r) = [R(r)/r]\, Y_{lm}(r)$, we have

$$\nabla_r^2 \epsilon(r, R) f(r) = \epsilon(r, R) \nabla_r^2 f(r) + \left[\frac{1}{r} \left(\frac{d}{dr}\, \delta(r-R) \right) R(r) + \frac{2\delta(r-R)}{r} \left(\frac{d}{dr}\, R(r) \right) \right] .$$

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