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Approximations for the exchange potential in electron scattering*

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Four new exchange potentials (the semiclassical exchange approximation, the asymptotically adjusted free-electron–gas exchange approximation, the second-order free-electron–gas exchange approximation, and the high-energy exchange approximation) are derived. Calculations are performed for elastic electron scattering from helium and argon. The results are compared to one another and to calculations using Hara's free-electron–gas approximation and the exact nonlocal exchange potential. Three of the approximations to exchange are in good agreement with the exact exchange —except at very low energy— but are much easier to use. Thus they should be very useful in electron–atom and electron–molecule scattering calculations.

I. INTRODUCTION

The effect of exchange of the scattering electron with the bound electrons is very important in electron scattering from atoms and molecules. This effect can be included in scattering calculations by using antisymetrized trial functions which lead to the continuum Hartree–Fock[1] and close coupling including exchange[2-5] approximations and their modifications. However, the exchange interaction in these equations takes the form of a nonlocal potential, and this adds considerable complication to their solution.[2-5] For this reason, and because of the physical insight which may be afforded, it is desirable to have an approximation to the nonlocal exchange potential. Several previous investigations[6-13] have considered this problem, but the approximations have never been checked against the exact nonlocal exchange potential for scattering. In the present article we wish to examine this problem carefully. We derive a new approximation, called the semiclassical exchange approximation, and we show its relationship to previous work on approximate exchange potentials in both bound state and scattering problems and to previous approximations for calculating exchange amplitudes using plane wave scattering states. We use several approximate exchange potentials in test calculations on electron–helium and electron–argon elastic scattering. The approximate exchange potentials depend only on coordinates and the asymptotic (large radial distance) kinetic energy. Thus they are local in the coordinate representation and are easy to use. We find that three of the approximate exchange potentials provide very good approximations to the nonlocal exchange potential. We also find that the high-energy limit of the exchange potential, which is easiest of all to use, works well over a wide energy range.

II. THEORY

A. Elastic exchange potential

1. Semiclassical and high-energy approximations

The continuum Hartree–Fock equation[1] for the scattering electron's wavefunction $u_0(\mathbf{r})$ may be written in a simplified notation as

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V_s(\mathbf{r}) - E_0 \right] u_0(\mathbf{r})$$

$$= \sum_{i=1}^{n_0} N_i u_i(\mathbf{r}) \int d\mathbf{r}' u_i^*(\mathbf{r}') \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} u_0(\mathbf{r}'), \tag{1}$$

where $V_s(\mathbf{r})$ is the static potential (negative for electron–atom scattering), E_0 is the incident kinetic energy, n_0 is the number of different single-particle spatial states $u_i(\mathbf{r})$ occupied in the target, N_i is a positive or negative constant depending on the state of the target, and m and e are the mass and charge of the electron. For example, for systems with doubly occupied spatial orbitals, N_i is positive and equal to half the occupation number of single-particle state i. The right hand side of Eq. (1) is the exchange term sum. If it is neglected, Eq. (1) yields the static approximation.

We seek an approximation to the exchange term sum such that

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V_s(\mathbf{r}) - E_0 \right] u_0(\mathbf{r}) = - L(\mathbf{r}, E_0) u_0(\mathbf{r}) \tag{2a}$$

or

$$[\nabla^2 + \kappa_0^2(\mathbf{r})] u_0(\mathbf{r}) = 0, \tag{2b}$$

where

$$\kappa_0^2(\mathbf{r}) = 2m [E_0 - V_s(\mathbf{r}) - L(\mathbf{r}, E_0)]/\hbar^2. \tag{3}$$

Consider an integral in the exchange term sum:

$$M(\mathbf{r}) = \int d\mathbf{r}' u_i^*(\mathbf{r}') \, u_0(\mathbf{r}')/|\mathbf{r} - \mathbf{r}'|. \tag{4}$$

If $M(\mathbf{r})$ is written as the product of a slowly varying amplitude $A(\mathbf{r})$ times the rapidly oscillating function $u_0(\mathbf{r})$, there results

$$\nabla^2 M(\mathbf{r}) = - 4\pi u_i^*(\mathbf{r}) u_0(\mathbf{r})$$

$$= [\nabla^2 A(\mathbf{r})] u_0(\mathbf{r}) + 2[\nabla A(\mathbf{r})] \cdot [\nabla u_0(\mathbf{r})] + A(\mathbf{r})\nabla^2 u_0(\mathbf{r}). \tag{5}$$

If $\nabla^2 u_0(\mathbf{r})$ is expressed as $\kappa_0^2(\mathbf{r})$ by the use of Eq. (2b), then Eq. (5) may be solved for $A(\mathbf{r})$ by ordering in inverse powers of κ_0

$$A(\mathbf{r}) = \frac{4\pi u_i^*(\mathbf{r})}{\kappa_0^2(\mathbf{r})} + \frac{2}{\kappa_0^2(\mathbf{r})}\left[\frac{\nabla u_0(\mathbf{r})}{u_0(\mathbf{r})}\right]\cdot\left\{\nabla\left[\frac{4\pi u_i^*(\mathbf{r})}{\kappa_0^2(\mathbf{r})}\right]\right\} + \cdots .\quad (6)$$

If one uses the leading term of Eq. (6) to approximate $A(\mathbf{r})$, then the right-hand side of Eq. (1) becomes

$$\sum_{i=1}^{n_0} N_i\,|u_i(\mathbf{r})|^2\,\frac{4\pi e^2\hbar^2}{\{2m[E_0 - V_s(\mathbf{r}) - L(\mathbf{r},E_0)]\}}\,u_0(\mathbf{r}) .\quad (7)$$

Combining Eqs. (2a) and (7), we have a quadratic equation for $L(\mathbf{r},E_0)$. Its physical solution may be determined using the condition that $L(\mathbf{r},E_0)$ vanish as $E_0 \to \infty$. This yields

$$L(\mathbf{r},E_0) = \tfrac{1}{2}[E_0 - V_s(\mathbf{r})] - \tfrac{1}{2}\{[E_0 - V_s(\mathbf{r})]^2 + \alpha^2\}^{1/2},\quad (8)$$

where

$$\alpha^2 = \frac{8\pi e^2\hbar^2}{m}\sum_{i=1}^{n_0} N_i\,|u_i|^2 .\quad (9a)$$

For targets with doubly occupied spatial orbitals, this becomes

$$\alpha^2 = 4\pi\rho e^2\hbar^2/m ,\quad (9b)$$

where $\rho(\mathbf{r})$ is the total electron density of the target. This attractive potential will be called the *semiclassical exchange approximation* (SCE). In the high-energy limit, we may expand the square root in Eq. (8) to obtain

$$L(\mathbf{r},E_0) \cong -\frac{1}{4}\frac{\alpha^2}{[E_0 - V_s(\mathbf{r})]} + \frac{1}{16}\frac{\alpha^4}{[E_0 - V_s(\mathbf{r})]^3} - \cdots .\quad (10)$$

The first term of Eq. (10) will be called the *high-energy exchange approximation* (HEE). For targets with doubly occupied spatial orbitals, it becomes

$$L(\mathbf{r},E_0) \cong -\frac{\pi e^2\hbar^2}{m}\frac{\rho(\mathbf{r})}{[E_0 - V_s(\mathbf{r})]} ,\quad (11)$$

where $\rho(\mathbf{r})$ is the total electron density of the target.

The semiclassical exchange approximation is similar to that derived by Furness and McCarthy,[13] and indeed, it can be obtained using their method of derivation. However, their derivation contains sign errors indicating a physically unreasonable repulsive potential. Further, in their application to argon they made an error of a factor of 2 (note that N_i should be half the occupation number of single-particle spatial state i), and they treated each exchange term as if it were the only one and then added the potentials instead of obtaining the whole exchange potential as derived here.

2. Free-electron-gas approximations

The exchange potential for an electron in a free-electron gas is

$$V_{FX}(\mathbf{r}) = -\frac{2e^2}{\pi}\,K_F F(\eta) ,\quad (12)$$

where

$$F(\eta) = \frac{1}{2} + \frac{1-\eta^2}{4\eta}\ln\left|\frac{1+\eta}{1-\eta}\right|\quad (13a)$$

and

$$\eta = K/K_F\quad (13b)$$

is the ratio of the magnitude $\hbar K$ of the momentum of the electron considered to the magnitude $\hbar K_F$ of the maximum momentum corresponding to the surface of the Fermi sphere in momentum space. To apply this potential to distributions of electron charge which are not constant, we consider K and K_F to be functions of position. The prescription suggested for bound state problems by Sham and Kohn,[14] Yonei,[15] and Liberman[16] is to give them values corresponding to the values for a uniform electron gas in a constant potential which matches the local density and local potential

$$K_F(\mathbf{r}) = [3\pi^2\rho(\mathbf{r})]^{1/2},\quad (14)$$

$$K(\mathbf{r}) = \{2m[E_0 - V_s(\mathbf{r}) - V_{FX}(\mathbf{r})]/\hbar^2\}^{1/3} .\quad (15)$$

This will be called the semiclassical free-electron exchange approximation. Since $K(\mathbf{r})$ depends on $V_{FX}(\mathbf{r})$, which depends on $K(\mathbf{r})$, various procedures[15-17] have been suggested in atomic bound state calculations to avoid an iterative calculation of $V_{FX}(\mathbf{r})$. For electron scattering problems, we may assume

$$K^2(\mathbf{r}) = (2m/\hbar^2)[E_0 - V_s(\mathbf{r})] .\quad (16)$$

This is most valid when the effect of exchange is small, but it includes higher order effects than the high-energy exchange approximation (see discussion in Sec. III); hence, the use of Eqs. (12)–(14) and (16) will be called the *second-order free-electron-gas exchange approximation* (SOFEGE).

An alternative type of procedure for bound-state problems was suggested earlier by Slater.[18,19] He used the free-electron-gas model to approximate $F(\eta)$. Notice that η and $F(\eta)$ have the values 0 and 1, respectively, at the center and 1 and $\tfrac{1}{2}$, respectively, at the surface of the Fermi sphere. In particular, Slater replaced $F(\eta)$ by its average over the Fermi sphere, which is $\tfrac{3}{4}$. An alternative constant value for $F(\eta)$, $\tfrac{1}{2}$, was obtained by Gaspar,[20] Kohn and Sham,[21] and Cowan et al.[22] by applying the variational method to the energy functional for a free-electron gas. Both these methods then lead to

$$V_{FX}(\mathbf{r}) = -\frac{3e^2}{2\pi}\alpha_X(3\pi^2\rho(\mathbf{r}))^{1/3} ,\quad (17)$$

where α_X is a constant. It is clear from the derivations that this potential is not applicable to electron scattering problems where $\eta > 1$. Although Eq. (17) has been applied to electron–atom scattering several times,[6-10] these applications should be considered to be based on a fundamental misunderstanding. This was pointed out by Hara,[12] who gave a generalization to scattering problems of this type of procedure, viz., using the free-electron-gas model to approximate $K(\mathbf{r})$ and thus η and $F(\eta)$. Hara used the following approximation in Eqs. (12) and (13):

$$K^2(\mathbf{r}) = [2m(E_0 + I)/\hbar^2] + K_F^2(\mathbf{r}) ,\quad (18)$$

where I is the ionization potential of the target. We see that this approximation for K implies that the electron kinetic energy is $E_0 + I$ at large r. Hara suggested that this inconsistency may not be serious since the exchange potential is small at large r. Furthermore, Eq. (18) appears reasonable at small r. The use of the exchange approximation contained in Eqs. (12)–(14) and (18) will be called the *Hara free-electron-gas approximation*

(HFEGE).

An obvious way to correct the Hara formulas for large-r behavior is to remove the ionization energy from Eq. (18). This will give a more attractive exchange approximation everywhere in r. Thus, we set

$$K^2(\mathbf{r}) = 2mE_0/\hbar^2 + K_F^2(\mathbf{r}).\qquad(19)$$

Use of Eqs. (12)–(14) and (19) will be called the *asymptotically adjusted free-electron-gas exchange approximation* (AAFEGE).

A considerable amount of work has been done in finding optimum approximations for $F(\eta)$ for use in bound-state problems.[23] It might be possible to derive improved free-electron-gas approximations for scattering calculations by using similar considerations or by adopting an iterative solution for $F(\eta)$. We have not pursued this, although we do present the $E_0 = 0$ limits in a special discussion section, III. C. The $E_0 = 0$ limit of the exchange potentials is the closest contact that we make with bound-state theories.

B. Inelastic exchange potential

The close coupling equation[2-5] for the scattering electron wavefunction in channel q contains not only the diagonal nonlocal exchange potential considered in subsections II. A. 1 and II. A. 2 but nondiagonal nonlocal exchange terms of the form

$$\hat{L}_{ij}^q u_q(\mathbf{r}) = -u_j(\mathbf{r}) \int d\mathbf{r}' u_i^*(\mathbf{r}') \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} u_q(\mathbf{r}'),$$

where $u_i(\mathbf{r})$ and $u_j(\mathbf{r})$ are bound-state orbitals. In a fashion similar to the derivation of Eq. (11), we may derive the following high-energy approximation to these terms,

$$L_{ij}^q(\mathbf{r}, E_q) \cong -\frac{2\pi e^2 \hbar^2}{m} \frac{\rho_{ij}(\mathbf{r})}{[E_q - V_{s,q}(\mathbf{r})]},\qquad(20)$$

where E_q and $V_{s,q}(\mathbf{r})$ are the incident kinetic energy and static potential in channel q and $\rho_{ij}(\mathbf{r})$ is the transition density

$$\rho_{ij}(\mathbf{r}) = u_i^*(\mathbf{r}) u_j(\mathbf{r}).$$

Such approximations to these nondiagonal exchange terms do not appear to have been considered in the context of close coupling calculations and they deserve future study.

C. Plane wave approximations for the scattering electron

If the plane wave approximation is used for $u_0(\mathbf{r})$ in (5), i.e.,

$$(\nabla^2 + k^2) u_0 = 0,$$

where $k^2 = 2mE_0/\hbar^2$, then Eqs. (6), (11), and (20) become

$$A(\mathbf{r}) = \frac{4\pi u_i^*(\mathbf{r})}{k^2} + \frac{2i}{k^3} 4\pi \mathbf{k} \cdot \nabla u_i^*(\mathbf{r}) + \cdots,\qquad(21)$$

$$L(\mathbf{r}, E_0) = -\frac{2\pi e^2 \rho(\mathbf{r})}{k^2},\qquad(22)$$

and

$$L_{ij}^q(\mathbf{r}, E_q) \cong -\frac{4\pi e^2 \rho_{ij}(\mathbf{r})}{k_q^2}\qquad(23)$$

where $k_q^2 = 2mE_q/\hbar^2$, respectively. Equations (21) through (23) are related to the Bonham approximation[24] for exchange scattering, which was derived by Bonham entirely within the framework of the Born approximation. The approximation has also been derived by Bonham and Fink[25] using plane wave states for all electrons. Thus, the free-electron-gas exchange theories give equivalent results for high energy scattering. This approximation was rederived by Ochkur.[26] Use of Eqs. (22) and (23) and the first Born approximation with plane wave scattering states leads immediately to their approximation. The difference between K^2 [see Eqs. (16) and (18)] appearing in the denominators of the local potentials of subsections II. A. 1, II. A. 2, and II. B and k^2 appearing in the denominators of Eqs. (22) and (23) are reminiscent of the extra terms that appear in the denominators of the Bonham–Ochkur-like theories of Rudge,[27,28] Crothers,[29] and Bely,[30] although these terms entered their expressions based on different considerations.

III. DISCUSSION OF THE ELASTIC EXCHANGE POTENTIALS

A. Region of validity of the Thomas–Fermi equation

We recall the notation that $k^2 = 2mE_0/\hbar^2$, that $\hbar K(\mathbf{r})$ is the approximation to the electron momentum entering the free-electron-gas formulas, that $\hbar K_F(\mathbf{r})$ is the Fermi momentum, and that $\eta(\mathbf{r}) = K/K_F$. In Table I we present $V_s(\mathbf{r})$ and $\rho(\mathbf{r})$ for the argon atom; these quantities are obtained directly from the Hartree–Fock wavefunction of Mann.[31] In addition, Table I contains $K_F(\mathbf{r})$ and $\eta(\mathbf{r})$, where η is $(-2m V_s)^{1/2}/(\hbar K_F)$, which is the $E_0 = 0$ value calculated from Eqs. (13b), (14), and (16) in the SOFEGE approximation. The deviation of this η from unity is a measure of how much the Hartree–Fock wavefunction for argon deviates from the Thomas–Fermi (TF) equation,[32] $K_F^2 = -2m V_s/\hbar^2$. Thus, from an r less

TABLE I. The static potential, electron density, Fermi momentum, η (in the SOFEGE approximation at $E_0 = 0$), and the $L^{HEE}(r, 0)$ limit for the argon atom, all in hartree atomic units. V_S and ρ are obtained from the data of Ref. 31.

r (a_0)	$-V_S$ (hartree)	ρ (a_0^{-3})	K_F (a_0^{-1})	η (dimensionless)	$-\pi\rho/V_S$ (a_0^{-3} hartree^{-1})
0.02	8.326 + 2	1.873 + 3	3.813 + 1	1.070	7.067
0.05	2.992 + 2	6.503 + 2	2.680 + 1	0.913	6.828
0.10	1.287 + 2	1.343 + 2	1.584 + 1	1.013	3.278
0.20	4.937 + 1	3.445 + 1	1.007 + 1	0.987	2.192
0.40	1.588 + 1	8.565 + 0	6.330 + 0	0.890	1.694
0.50	1.075 + 1	3.563 + 0	4.725 + 0	0.981	1.041
0.60	7.722 + 0	1.517 + 0	3.555 + 0	1.106	0.617
0.80	4.320 + 0	5.400 − 1	2.519 + 0	1.167	0.393
1.00	2.512 + 0	4.094 − 1	2.297 + 0	0.976	0.512
1.20	1.477 + 0	3.176 − 1	2.111 + 0	0.814	0.676
1.40	8.740 − 1	2.242 − 1	1.879 + 0	0.703	0.806
1.60	5.198 − 1	1.485 − 1	1.638 + 0	0.622	0.898
1.80	3.110 − 1	9.489 − 2	1.411 + 0	0.559	0.959
2.00	1.872 − 1	5.949 − 2	1.208 + 0	0.507	0.998
2.50	5.392 − 2	1.798 − 2	8.105 − 1	0.405	1.048
3.00	1.603 − 2	5.429 − 3	5.437 − 1	0.329	1.064
3.50	4.885 − 3	1.664 − 3	3.666 − 1	0.270	1.070
4.00	1.518 − 3	5.180 − 4	2.485 − 1	0.222	1.072
6.00	1.638 − 5	5.448 − 6	5.444 − 2	0.105	1.045

than $0.02\ a_0$ (a_0 is the Bohr radius) to r greater than 1 a_0, the TF equation holds well for argon. We refer to this as the TF region and note that it contains a large fraction of the electron density. It should be reiterated that all of our results are computed with the Hartree–Fock electron density rather than the Thomas–Fermi density which might be preferred in the free-electron-gas approximation.

The properties of the TF region facilitate the comparison of the SCE and HEE approximations. From Eqs. (9b) and (10), we see that, if

$$\theta = m(E_0 - V_s)^2/(\pi\rho e^2 \hbar^2) \qquad (24)$$

and θ is a number greater than unity, the SCE potential may be replaced with the HEE potential with a relative error of size θ^{-1}. In the TF region, Eq. (24) becomes

$$\theta = m[E_0 + (3\pi^2\rho)^{2/3}\hbar^2/(2m)]^2/(\pi\rho e^2\hbar^2\ ). \qquad (25)$$

It is evident that the SCE potential may be replaced by the HEE potential under fairly mild conditions on the on the size of E_0: at large r, E_0^2 is larger than $\pi e^2\rho\hbar^2/m$ since the electron density is small; in the TF region, $(3\pi^2\rho)^{4/3}(\hbar^2/2m)^2$ is larger than $\pi\rho e^2\hbar^2/m$ since the density is large there. For argon with $\theta \approx 2$, these r regions overlap for E_0 on the order of 1 hartree and the HEE potential is a valid approximation to the SCE potential for any energy greater than about 1 hartree. We assume this occurs for any atom. In addition, a pleasing and important result is obtained: for $E_0 \gtrsim 1$ hartree, one need not retain L in the $\kappa_0^2(r)$ expression [Eq. (3)] used in the derivation of the SCE potential. This avoids the quadratic expression discussed after Eq. (7) and gives $L^{\mathrm{HEE}}\ (\mathbf{r}, E_0)$ directly by the asymptotic expansion for the exchange integrals developed in Eqs. (4)–(7). This is important in connection with the development of local exchange approximations in close coupling (Sec. II. B) since it is awkward to formulate the full SCE approximation for coupled equations.

B. Comparison of exchange potentials at nonzero E_0

The various free-electron-gas exchange potentials bear little obvious resemblance to the semiclassical exchange potential and its high-energy limit. For $E_0 > 0$, the parameter η used in the free-electron-gas formulas increases from unity near $r = 0$ to infinity at large r. The SOFEGE is anomalous at small E_0, and this will be discussed later in detail. At sufficiently large r, we may use the power series expansion in $1/\eta$ of $F(\eta)$

$$F(\eta) \underset{\eta > 1}{=} \tfrac{1}{3}\eta^{-2} + \tfrac{1}{15}\eta^{-4} + \cdots \qquad (26)$$

to simplify the free-electron-gas potentials. Correct up to a relative error η^{-2}, we have

$$F(\eta) \underset{\eta \gg 1}{\cong} (3\pi^2\rho)^{2/3}/(3K^2) \qquad (27)$$

and

$$V_{FX} \underset{\eta \gg 1}{\cong} -2\pi\rho e^2/K^2. \qquad (28)$$

Using Eqs. (16), (18), and (19), we obtain for the individual approximations,

$$L^{\mathrm{SOFEGE}} \underset{\eta \gg 1}{\cong} -2\pi\rho e^2/(k^2 - 2mV_s/\hbar^2),$$

$$L^{\mathrm{HFEGE}} \underset{\eta \gg 1}{\cong} -2\pi\rho e^2/(k^2 + (3\pi^2\rho)^{2/3} + 2mI/\hbar^2),$$

$$L^{\mathrm{AAFEGE}} \underset{\eta \gg 1}{\cong} -2\pi\rho e^2/(k^2 + (3\pi^2\rho)^{2/3}). \qquad (29)$$

The restriction $\eta \gg 1$ is satisfied at any nonzero E_0 as $r \to \infty$ or any nonzero r as $E_0 \to \infty$. From the preceding subsection, we see that, if $E_0 \gtrsim 1$ hartree,

$$L^{\mathrm{SCE}} \underset{E_0 > 1\,\mathrm{hartree}}{\cong} L^{\mathrm{HEE}} = -2\pi\rho e^2/(k^2 - 2mV_s/\hbar^2). \qquad (30)$$

Thus, as $E_0 \to \infty$ ($k^2 \to \infty$), all the exchange potentials become equal, ultimately to the Bonham result given by Eq. (22). They are also all equal as $r \to \infty$ at nonzero E_0, except for the HFEGE potential, which is smaller by a factor of $E_0/(E_0 + I)$, as may be seen from Eq. (29).

As $r \to 0$, the exchange approximations differ from one another. We do not consider the region very close to $r = 0$ where the TF model breaks down, but rather the small-r part of the TF region (for argon, the TF region covers at least $0.02\ a_0$ to $1\ a_0$). In the TF region, $-E_0/V_s \cong k^2/(3\pi^2\rho)^{2/3}$, so by keeping only the leading terms in E_0/V_s or $k^2/(3\pi^2\rho)^{2/3}$, we have

$$\eta \underset{\substack{r \to 0 \\ \mathrm{TF\ region}}}{\sim} 1, \quad F(\eta) \underset{\substack{r \to 0 \\ \mathrm{TF\ region}}}{\sim} 1/2$$

and $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (31)$

$$L \underset{\substack{r \to 0 \\ \mathrm{TF\ region}}}{\sim} -e^2(3\pi^2\rho)^{1/3}/\pi$$

for all the free-electron-gas exchange potentials. This limit agrees with the $F(\eta) = 1/2$ exchange potential of Refs. 20–22. The SCE and HEE approximations become, as $r \to 0$ at any finite E_0,

$$L^{\mathrm{SCE}} \underset{r \to 0}{\sim} L^{\mathrm{HEE}} \underset{r \to 0}{\sim} \pi\rho e^2\hbar^2/(mV_s). \qquad (32)$$

Using the fact that we are in the TF region, Eq. (32) may be expressed

$$L^{\mathrm{SCE}} \underset{\substack{r \to 0 \\ \mathrm{TF\ region}}}{\sim} L^{\mathrm{HEE}} \underset{\substack{r \to 0 \\ \mathrm{TF\ region}}}{\sim} -\tfrac{2}{3}e^2(3\pi^2\rho)^{1/3}/\pi. \qquad (33)$$

Thus the SCE and HEE potentials are smaller than the free-electron-gas exchange potentials by a factor of $\tfrac{2}{3}$ in the innermost part of the TF region.

C. Comparison at $E_0 = 0$

The HEE approximation breaks down severely at $E_0 = 0$ as seen, for example, in the last column of Table I, where the large r values of $L^{\mathrm{HEE}}(r, 0) = \pi\rho e^2\hbar^2/(mV_s)$ approach -1 hartree. The SCE approximation gives

$$L^{\mathrm{SCE}}(\mathbf{r}, 0) = -\tfrac{1}{2}V_s - \tfrac{1}{2}(V_s^2 + 4\pi\rho e^2\hbar^2/m)^{1/2}, \qquad (34a)$$

$$r \approx \infty \quad -(\pi\rho e^2\hbar^2/m)^{1/2}, \qquad (34b)$$

$$r \approx 0 + \pi\rho e^2\hbar^2/(mV_s). \qquad (34c)$$

If r is assumed to be in the TF region for a given atom and $\rho^{1/3} \gg 1 a_0^{-1}$, Eq. (34a) becomes

$$L^{SCE}(\mathbf{r}, 0) \underset{\text{T F region}}{=} -\tfrac{2}{3} e^2 (3\pi^2 \rho)^{1/3}/\pi, \tag{35}$$

which also can be obtained from Eq. (34c) using the TF equation since $\rho^{1/3} \gg 1 a_0^{-1}$ and $r \to 0$ give the same limit.

As $E_0 \to 0$, the AAFEGE potential assumes the particularly simple form

$$L^{AAFEGE}(\mathbf{r}, 0) = -e^2 (3\pi^2 \rho)^{1/3}/\pi, \tag{36}$$

since η is unity and $F(\eta)$ is exactly $\tfrac{1}{2}$ for all r. Again, this limit agrees with the exchange potential of Refs. 20–22 using $F(\eta) = \tfrac{1}{2}$. The HFEGE potential closely follows the AAFEGE potential at small r, but at large r it reduces to

$$L^{HFEGE}(\mathbf{r}, 0) \underset{r \to \infty}{\sim} -\pi \rho e^2 \hbar^2/(mI). \tag{37}$$

The SOFEGE approximation at $E_0 = 0$ possesses an anomaly that is illustrated in Table I: owing to the fact that the actual electron density does not satisfy the TF equation, η oscillates slightly above and below unity, even in the TF region. $F(\eta)$ is a strong function of η near $\eta = 1$, and $L^{SOFEGE}(\mathbf{r}, 0)$ oscillates about $L^{AAFEGE}(\mathbf{r}, 0)$ as a function of r. At very large r it becomes

$$L^{SOFEGE}(\mathbf{r}, 0) \underset{r \to \infty}{\sim} -2e^2 (3\pi^2 \rho)^{1/3}/\pi \tag{38}$$

since $\eta \to 0$ and $F(\eta) \sim 1$. This is a factor of 2 larger than the AAFEGE potential. We also note that, near $r = 0$, the aforementioned oscillation can persist to fairly high energy.

Comparison of Eqs. (34b), (36), (37), and (38) shows that, at vanishing energy and large distances, the approximate exchange potentials are in the following order of increasing attractiveness: HFEGE, SCE, AAFEGE, SOFEGE.

IV. APPLICATIONS

A. Helium

For helium we use the wavefunction of Green et al.,[23] which closely approximates the Hartree–Fock wavefunction of helium. In this case $N_{1s} = 1$,

$$\rho(\mathbf{r}) = 2 |u_{1s}(\mathbf{r})|^2,$$

and the static potential has been given by Khare and Moiseiwitsch.[34] We carried out phase shift calculations using the static approximation and, also, using five different approximations to the exchange potential, viz., the semiclassical exchange approximation (SCE), the high-energy exchange approximation (HEE), the second-order free-electron-gas exchange approximation (SOFEGE), the Hara free-electron-gas exchange approximation (HFEGE), and the asymptotically adjusted free-electron-gas exchange approximation (AAFEGE).

The numerical calculations were carried out using both the Gordon method[35] and variable-step Runge–Kutta integration[36] of the phase equation.[37] The results are given in Tables II, III, and IV, where they are compared to accurate phase shifts computed in the continuum Hartree–Fock approximation (which is designated as the exchange approximation[1]) by Duxler et al.[38]

B. Argon

The static interaction and charge density for the argon atom were obtained from the Hartree–Fock calculations

TABLE II. Electron–helium partial wave phase shifts (in rad) for $l = 0$.

Energy (eV)	k (a_0^{-1})	Static	Exchange[a]	HEE[b]	SCE[c]	AAFEGE[d]	HFEGE[e]	SOFEGE[f]
0.14	0.100	2.648	2.994	5.775	3.006	3.032	2.957	3.337
0.53	0.197	2.297	2.859	3.212	2.863	2.887	2.782	3.142
0.85	0.250	2.157	2.776	3.015	2.783	2.806	2.691	3.043
1.22	0.300	2.050	2.705	2.901	2.708	2.731	2.607	2.956
2.18	0.400	1.884	2.567	2.723	2.562	2.583	2.449	2.794
3.40	0.500	1.761	2.436	2.570	2.422	2.442	2.304	2.648
4.90	0.600	1.664	2.311	2.429	2.291	2.309	2.174	2.514
6.67	0.700	1.584	2.194	2.295	2.168	2.184	2.056	2.390
7.65	0.750	1.549	2.139	2.231	2.111	2.126	2.001	2.332
8.70	0.800	1.517	2.085	2.170	2.055	2.069	1.950	2.276
13.60	1.000	1.405	1.890	1.945	1.856	1.867	1.769	2.071
16.46	1.100	1.358	1.804	1.845	1.769	1.779	1.691	1.978
21.26	1.250	1.296	1.687	1.713	1.653	1.662	1.589	1.848
30.61	1.500	1.209	1.522	1.530	1.491	1.500	1.446	1.654
41.67	1.750	1.137	1.388	1.387	1.362	1.371	1.331	1.481
54.42	2.000	1.076	1.279	1.273	1.257	1.262	1.236	1.328
108.84	2.828	0.923		1.023	1.019	1.026	1.015	1.038
163.26	3.464	0.839		0.904	0.902	0.908	0.902	0.911
217.68	4.00	0.782		0.829	0.828	0.832	0.829	0.833

[a]Static-exchange approximation from Ref. 38.
[b]High-energy exchange approximation.
[c]Semiclassical exchange approximation.
[d]Asymptotically adjusted free-electron-gas exchange approximation.
[e]Hara free-electron-gas exchange approximation.
[f]Second-order free-electron-gas exchange approximation.

TABLE III. Electron–helium partial wave phase shifts (in rad) for $l=1$.

Energy (eV)	k (a_0^{-1})	Static	Exchange[a]	HEE[b]	SCE[c]	AAFEGE[d]	HFEGE[e]	SOFEGE[f]
0.14	0.100	0.00009	0.00042	3.135	0.00169	0.00244	0.000222	0.0101
0.53	0.197	0.00070	0.00289	2.952	0.00989	0.0113	0.00166	0.0455
0.85	0.250	0.00142	0.00687	0.338	0.0176	0.0186	0.00333	0.0729
1.22	0.300	0.00242	0.0106	0.191	0.0267	0.0268	0.00565	0.102
2.18	0.400	0.00556	0.0236	0.167	0.0495	0.0461	0.0127	0.162
3.40	0.500	0.0104	0.0425	0.178	0.0762	0.0680	0.0233	0.218
4.90	0.600	0.0171	0.0667	0.195	0.104	0.0911	0.0374	0.265
6.67	0.700	0.0256	0.0947	0.212	0.132	0.114	0.0544	0.302
7.65	0.750	0.0305	0.1095	0.221	0.146	0.126	0.0638	0.316
8.70	0.800	0.0359	0.125	0.229	0.159	0.137	0.0736	0.329
13.60	1.000	0.0605	0.183	0.256	0.205	0.178	0.116	0.359
16.46	1.100	0.0743	0.209	0.268	0.223	0.196	0.137	0.366
21.26	1.250	0.0959	0.243	0.283	0.248	0.221	0.167	0.370
30.61	1.500	0.132	0.284	0.302	0.279	0.254	0.212	0.367
41.67	1.750	0.166	0.3105	0.315	0.300	0.279	0.247	0.359
54.42	2.000	0.196	0.327	0.325	0.315	0.279	0.274	0.352
108.84	2.828	0.263		0.340	0.337	0.329	0.320	0.349
163.26	3.464	0.289		0.342	0.340	0.337	0.332	0.347
217.68	4.000	0.300		0.340	0.339	0.337	0.334	0.343

[a-f]See footnotes of Table II.

of Mann.[31] The phase shifts were obtained by numerical integration of the radial Schrödinger equation using automatic error control integration[39] and by matching to spherical Bessel functions at sufficiently large distance. The phase shifts were obtained modulo π directly, but were converted to an absolute scale by adding the multiple of π that gave the best agreement to the Langer–JWKB phase shift.[40] This procedure fails in the event that three turning points occur in the radial motion; these few cases are noted by an asterisk in the argon tables and the absolute phase shift is estimated by continuity from higher energy. The numerical accuracy of the phases should be all reported digits, except for a possible additive multiple of π in the noted cases (Tables V–VII).

The calculations of Pindzola and Kelly[41] furnish the continuum-Hartree–Fock standard for testing the various exchange approximations. These, of course, do not include the correlation correction developed in that study. The static and exchange calculations of Thompson[42] at $k=1.7$ a_0^{-1} on argon agree very well with our static calculations and Pindzola and Kelly's exchange calculations. The Furness and McCarthy paper[13] contains errors (see Sec. II. A. 1), so we do not compare to their results.

V. RESULTS AND DISCUSSION

At high energy, all of the local exchange potentials give the same accurate exchange correction to the phase

TABLE IV. Electron–helium partial wave phase shifts (in rad) for $l=2$.

Energy (eV)	(a_0^{-1})	Static	Exchange[a]	HEE[b]	SCE[c]	AAFEGE[d]	HFEGE[e]	SOFEGE[f]
0.85	0.250	0.00001	0.00004	0.000501	0.000214	0.000223	0.0000250	0.000485
1.22	0.300	0.00002	0.00009	0.000851	0.000430	0.000431	0.0000603	0.000897
2.18	0.400	0.00009	0.00034	0.00195	0.00123	0.00117	0.000234	0.00225
3.40	0.500	0.00026	0.00092	0.00367	0.00263	0.00243	0.000648	0.00436
4.90	0.600	0.00061	0.00201	0.00604	0.00472	0.00431	0.00144	0.00723
6.67	0.700	0.00119	0.00376	0.00907	0.00752	0.00681	0.00273	0.0108
7.65	0.750	0.00160	0.00492	0.0108	0.00918	0.00830	0.00360	0.0128
8.70	0.800	0.00210	0.00627	0.0127	0.0110	0.00994	0.00462	0.0150
13.60	1.000	0.00511	0.0136	0.0216	0.0197	0.0179	0.0104	0.0247
16.46	1.100	0.00729	0.0184	0.0266	0.0244	0.0225	0.0146	0.0301
21.26	1.250	0.0114	0.0266	0.0347	0.0326	0.0301	0.0211	0.0384
30.61	1.500	0.0204	0.0419	0.0489	0.0471	0.0438	0.0346	0.0527
41.67	1.750	0.0314	0.0579	0.0633	0.0617	0.0581	0.0494	0.0667
54.52	2.000	0.0437	0.0735	0.0772	0.0759	0.0721	0.0644	0.0802
108.84	2.828	0.0854		0.116	0.115	0.113	0.108	0.118
163.26	3.464	0.1123		0.138	0.138	0.136	0.133	0.140
217.68	4.000	0.1303		0.152	0.152	0.150	0.148	0.153

[a-f]See Footnotes of Table II.

TABLE V. Electron—argon partial wave phase shifts (in rad) for $l = 0$.

Energy (eV)	k (a_0^{-1})	Static	Exchange[a]	HEE[b]	SCE[c]	AAFEGE[d]	HFEGE[e]	SOFEGE[f]
0.053	0.0625	9.253*[g]	9.331	12.317	9.407*	9.807	9.315*	12.133
0.14	0.10	9.149*		12.121	9.374	9.679	9.249	11.858
0.31	0.15	9.016		11.777	9.310	9.538	9.162	11.463
0.54	0.20	8.886		11.202	9.230	9.411	9.074	11.042
0.85	0.25	8.759	9.045	10.371	9.141	9.291	8.987	10.628
3.40	0.50	8.200	8.647	8.847	8.658	8.756	8.561	9.250
7.65	0.75	7.758	8.249	8.290	8.206	8.293	8.162	8.536
13.60	1.00	7.401	7.875	7.858	7.808	7.888	7.798	8.030
21.26	1.25	7.104	7.455	7.495	7.463	7.535	7.472	7.624
30.61	1.5	6.847	7.252	7.185	7.163	7.227	7.182	7.288
54.4	2.0	6.417	6.722	6.676	6.664	6.716	6.692	6.758
85.1	2.5	6.061		6.270	6.262	6.304	6.291	6.340
122.5	3.0	5.756		5.931	5.926	5.960	5.952	5.992
217.7	4.0	5.252		5.385	5.381	5.406	5.403	5.427
340.1	5.0	4.847		4.953	4.951	4.971	4.969	4.984

[a]Static-exchange approximation from Ref. 41.
[b]High-energy exchange approximation.
[c]Semiclassical exchange approximation.
[d]Asymptotically adjusted free-electron-gas exchange approximation.
[e]Hara free-electron-gas exchange approximation.
[f]Second-order free-electron-gas exchange approximation.
[g]* denotes possible error of additive multiple of π.

shifts. This is evident in the tables, especially Tables VI–IX for argon, where the continuum Hartree–Fock calculations were performed up to 340 eV $(k = 5 a_0^{-1})$. This also confirms the analysis of Sec. III. B, which indicated that the local exchange potentials tend to the same limit at high energy.

In all cases that we have studied, the SOFEGE approximation overestimates the exchange effects. As mentioned in Sec. II. C, the ratio η for the SOFEGE potential can oscillate about unity in the TF region for zero (and larger) E_0. An examination of $L^{SOFEGE}(r, E_0)$ for argon reveals that it is too strong for $k \leq 1 a_0^{-1}$ in the region of r between 1.0 and 2.0 a_0. This is, in fact, the region of r containing the last maximum of $F(\eta)$ (at nonzero E_0)

as a function of r in the SOFEGE approximation. As $E_0 \rightarrow 0$, this maximum in $F(\eta)$ broadens to infinite r at a plateau value of 1 as compared to a value of $\frac{1}{2}$ for the AAFEGE approximation. This accounts for the factor-of-2 error discussed with regard to Eq. (38) and for the excess attraction. Much the same problem must occur in helium as well as argon. Although the SOFEGE approximation possessed all the qualities that we expected of it, it is unsatisfactory and not given further detailed discussion.

Examination of the tables shows that the HEE, SCE, AAFEGE, and HFEGE approximations produce phase shifts in error by less than 0.1 rad down to k on the order of $1.5 a_0^{-1}$ (30.6 eV) in all tested cases. The HEE

TABLE VI. Electron—argon partial wave phase shifts (in rad) for $l = 1$.

Energy (eV)	k (a_0^{-1})	Static	Exchange[a]	HEE[b]	SCE[c]	AAFEGE[d]	HFEGE[e]	SOFEGE[f]
0.053	0.0625	3.143*[g]	6.283	9.413*	6.282*	6.285*	6.281*	6.297*
0.14	0.10	3.146*		8.977*	6.279*	6.286*	6.275*	6.318*
0.31	0.15	3.156*		6.353*	6.267*	6.284*	6.258*	6.349*
0.54	0.20	3.177*		6.327*	6.246*	6.275*	6.230*	6.373*
0.85	0.25	3.214*	6.227	6.301*	6.213*	6.257*	6.192*	6.381*
3.40	0.50	3.882*	6.001	6.057	5.938	6.042	5.909	6.214
7.65	0.75	4.576	5.702	5.713	5.613	5.734	5.604	5.901
13.60	1.00	4.650	5.411	5.387	5.320	5.434	5.333	5.575
21.26	1.25	4.571	5.151	5.111	5.069	5.171	5.098	5.266
30.61	1.5	4.457	4.923	4.881	4.854	4.943	4.892	4.996
54.4	2.0	4.215	4.548	4.513	4.500	4.570	4.544	4.597
85.1	2.5	3.990	4.248	4.223	4.215	4.271	4.256	4.291
122.5	3.0	3.787	3.999	3.980	3.974	4.021	4.012	4.038
217.7	4.0	3.445	3.601	3.588	3.585	3.619	3.615	3.627
340.1	5.0	3.170	3.291	3.283	3.281	3.306	3.304	3.310

[a]–[g]See footnotes of Table V.

TABLE VII. Electron–argon partial wave phase shifts (in rad) for $l=2$.

Energy (eV)	k (a_0^{-1})	Static	Exchange[a]	HEE[b]	SCE[c]	AAFEGE[d]	HFEGE[e]	SOFEGE[f]
0.053	0.0625	~0		div	~0	~0	~0	0.0001*[g]
0.14	0.10	~0		div	0.0001	0.0001*	~0	0.0006*
0.31	0.15	~0		div	0.0004	0.0006*	0.0001*	0.0036*
0.54	0.20	0.0001		div	0.0015	0.0018*	0.0003*	0.0122*
0.85	0.25	0.0004	0.002	0.101*	0.0038	0.0043*	0.0009*	0.0312*
3.40	0.50	0.0098	0.045	0.164*	0.0608	0.0609*	0.0241*	0.8147*
7.65	0.75	0.0604	0.277	0.520*	0.284*	0.285*	0.150*	1.963
13.60	1.00	0.208	0.860	1.070	0.782	0.830	0.536*	2.008
21.26	1.25	0.514	1.393	1.473	1.315	1.424	1.171	1.921
30.61	1.5	0.936	1.644	1.684	1.614	1.724	1.594	1.877
54.4	2.0	1.498	1.837	1.859	1.840	1.916	1.873	1.943
85.1	2.5	1.687	1.912	1.921	1.911	1.961	1.940	1.981
122.5	3.0	1.754	1.943	1.938	1.931	1.965	1.953	1.988
217.7	4.0	1.780	1.935	1.919	1.914	1.931	1.926	1.952
340.1	5.0	1.760	1.885	1.870	1.867	1.877	1.874	1.892

[a]–[g]See footnotes of Table V; div indicates that the HEE shifts were too large to convert to absolute scale by method described in Sec. IV.B of text.

results begin to diverge for lower energies as predicted in Sec. III.C and shown in the last column of Table I. We regard the fact that the HEE approximation is as good as the SCE approximation down to $k \cong 1.5a_0^{-1}$ as an important result of this study for two reasons. First, a simple exchange correction is now available for elastic electron scattering above a few 10's of eV. Second, the asymptotic expansion of the exchange integrals in terms of an ordering in powers of inverse local wave number easily generalizes to inelastic scattering. We do not discuss the HEE form further, as it reproduces the SCE approximation and the exact results at moderately high energy.

What remains is to characterize the SCE, AAFEGE, and HFEGE approximations at lower energy where they differ the most, but nevertheless work well compared to the exact results. In most cases the HFEGE form gives too weak an approximation to the exchange interaction and gives phase shifts that are too small. One may easily show that $|L^{AAFEGE}(r, E_0)| > |L^{HFEGE}(r, E_0)|$ and infer that the phase shifts for the AAFEGE approxi-

mation are always greater than those of the HFEGE approximation. This is because $F(\eta)$ is a monotonic function dropping from 1 at $\eta = 0$ to 1/2 at $\eta = 1$ to zero at large η. In terms of a fractional correction to $V_s(r)$, the HFEGE and AAFEGE potentials differ the most at large r, where, from Eq. (29),

$$L^{AAFEGE}(r, E_0) = -\pi \rho e^2 \hbar^2/(mE_0)$$

$$L^{HFEGE}(r, E_0) = L^{AAFEGE}(r, E_0)\frac{E_0}{E_0 + I} \tag{39}$$

providing $(3\pi^2\rho)^{1/3} \ll k$. For high l, the scattering electron only samples the interaction into a separation of about $(l + \frac{1}{2})/k$; thus, we may choose between the HFEGE and AAFEGE approximations where they differ the most by examining the larger-l, lower-k phases to see if the $E_0/(E_0 + I)$ ratio is evident. For example, using the argon data from Tables I, VII, VIII, and IX, the fact that the HFEGE potential is weaker than the AAFEGE potential by a factor of roughly $E_0/(E_0 + I)$ is quite obvious. Most important, the AAFEGE approximation is a better result. This confirms Hara's statement about the in-

TABLE VIII. Electron–argon partial wave phase shifts (in rad) for $l=3$.

Energy (eV)	k (a_0^{-1})	Static	Exchange[a]	HEE[b]	SCE[c]	AAFEGE[d]	HFEGE[e]	SOFEGE[f]
0.54	0.20			~0	~0	~0		~0
0.85	0.25	~0		0.0001	0.0001	0.0001	~0	0.0001
3.40	0.50	0.0003	0.001	0.0032	0.0024	0.0023	0.0008	0.0039
7.65	0.75	0.0038	0.011	0.018	0.016	0.014	0.008	0.022
13.60	1.00	0.017	0.042	0.055	0.050	0.046	0.032	0.065
21.26	1.25	0.049	0.105	0.118	0.111	0.104	0.083	0.134
30.61	1.5	0.104	0.197	0.206	0.198	0.187	0.164	0.224
54.4	2.0	0.284	0.428	0.426	0.419	0.408	0.386	0.445
85.1	2.5	0.506	0.645	0.639	0.635	0.631	0.616	0.653
122.5	3.0	0.701	0.806	0.804	0.801	0.804	0.795	0.812
217.7	4.0	0.937	0.994	0.997	0.996	1.001	0.998	1.001
340.1	5.0	1.040	1.083	1.085	1.084	1.089	1.087	1.089

[a]–[f]See footnotes of Table V.

TABLE IX. Electron–argon partial wave phase shifts (in rad) for $l=4$.

Energy (eV)	k (a_0^{-1})	Static	Exchange[a]	HEE[b]	SCE[c]	AAFEGE[d]	HFEGE[e]	SOFEGE[f]
0.85	0.25			~0	~0	~0		~0
3.40	0.50	~0		0.0001	0.0001	0.0001	~0	0.0002
7.65	0.75	0.0003		0.0016	0.0015	0.0014	0.0007	0.0017
13.60	1.00	0.0023		0.0073	0.0070	0.0067	0.0045	0.0078
21.26	1.25	0.009		0.021	0.020	0.019	0.015	0.022
30.61	1.5	0.022	0.040	0.044	0.043	0.041	0.035	0.046
54.4	2.0	0.079	0.119	0.121	0.120	0.116	0.109	0.124
85.1	2.5	0.173	0.228	0.227	0.226	0.222	0.215	0.231
122.5	3.0	0.286	0.344	0.342	0.341	0.338	0.333	0.346
217.7	4.0	0.496	0.540	0.538	0.538	0.538	0.536	0.540
340.1	5.0	0.639	0.666	0.667	0.667	0.668	0.667	0.668

[a–f]See footnotes of Table V.

correct large-r behavior of L^{HFEGE}.[12] However, there is a tendency of the HFEGE approximation to be as good or better than the others, in terms of a fractional correction to the static phase shifts, at very low energy and smaller l. The phase shift tables also confirm the order of attractiveness of the local approximations at large r and low energy as given at the end of Sec. III: HFEGE, SCE, AAFEGE, SOFEGE.

The Yates and Strand[7] calculation on argon at $k = 1.214$ a_0^{-1} (20 eV) uses an energy-independent "$\rho^{1/3}$" exchange potential of the form Eq. (17) and gives an exchange correction to the $l = 0$, 1, and 2 phase shifts which is at least a factor of 2 too large. This illustrates our point about the inappropriateness of bound-state-type exchange corrections for electron scattering calculations.

The final comparison involves the SCE and AAFEGE forms; these two generally appear to be the best of the tested approximations. The only major defect in the AAFEGE potential occurs for $k < 0.5 a_0^{-1}$ for $l = 0$ in argon, where the L^{AAFEGE} interaction is too strong. Since this problem disappears at higher l, the excessive attraction must be at small r, which is classically excluded from the electron motion at nonzero l. The problem is also obviously energy dependent. We recall Eqs. (31) and (33) which show that the SCE potential is only $\frac{2}{3}$ the size of the free-electron-gas potentials at small r; moreover, the extent of this region in r is inversely related to k. If we accept the premise that the AAFEGE potential is too strong at small r, then the HFEGE potential is also, and the HFEGE approximation phase shifts appear good in this region of k and l due to a cancellation of errors between excess attraction at small r and insufficient attraction at large r (second preceding paragraph).

It recently came to our attention that an additional method exists for the determination of a local effective potential for electron scattering based on the integral Hartree–Fock equation in momentum space.[43] Unfortunately, we did not include a study of this method in our work.

To conclude, we point out that one other test of exchange approximations exists for scattering conditions.[44] This compared the HEE and SOFEGE approximations for

relativistic elastic electron scattering from mercury to the continuum–relativistic-exchange calculations of Walker at 300 eV.[45] The local exchange potentials were added into the Dirac equation and the results were quite analogous to those found here for light atoms.

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