# Accurate *Ab Initio* Calculation of Scattering Length and Phase Shifts at Very Low Energies for Electron-Neon Scattering

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The scattering length for electron-neon scattering is calculated very accurately for the first time by an *ab initio* method resulting in a rigorous upper bound of $0.2218a_0$. The calculation uses the multiconfiguration Hartree-Fock method which includes the effects of dynamical target polarization and electron correlation through the configuration interaction procedure. Phase shifts are also calculated for very low energies, an extremely difficult region for accurate theoretical investigation. The results are found to be in excellent agreement with the most accurate experimental results of O'Malley and Crompton.

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The scattering length is a very important quantity in order to determine cross sections of electron-atom collisions at thermal energies. At low energies the cross sections in neon vary very rapidly and as a result extrapolations of the experimental data are difficult and cannot be regarded as having produced accurate results. Because of the small scattering length with neon, accurate *ab initio* calculations are extremely difficult. Moreover, the calculations are made more difficult by the large electron correlations and dynamical polarizations at zero and very low energies. Most accurate methods for electron-atom scattering compute phase shifts in such a way that at zero or very low energies they blow up or give null results. Also at very low energies there is poor convergence and the results are less accurate. Generally the scattering length is determined by computing phase shifts at lower energies with reasonable accuracy and then extrapolating $(\tan\delta_0)/k$ to zero energy. However, this does not guarantee the accuracy of the result.

There have been a number of determinations[1-8] from experimental measurements and few theoretical calculations[9-13] on scattering length with neon. The most accurate determination of scattering length from experimental measurements is due to O'Malley and Crompton.[1] They determined the scattering length and the phase shifts at low energies from an analysis of Robertson's[8] drift-velocity measurements, corresponding to very low swarm energies, through an improved method of analysis employing modified effective-range theory (MERT).[14,15] The MERT is an expansion of the partial-wave phase shifts as a power series in the wave number $k$ with a few coefficients such as the scattering length and one or two others as parameters to be determined by fitting to the best available experimental data. The cross sections are then determined down through the thermal region to zero energy, which is the energy region most difficult to study experimentally. Robertson[8] made drift-velocity measurements in neon at 77 and 300 K and used these data to obtain a momentum-transfer cross section whose accuracy was estimated to be $\pm 3\%$ for low energies between 0.04 and 6.0 eV. Robertson fitted the experimental values of the momentum-transfer cross section by the modified effective-range formula for energies less than 0.2 eV and obtained the scattering length.

As the *ab initio* calculations are very difficult, no reliable data for the scattering length have so far been obtained in this way to verify the experimental results. Thompson[9,10] performed two calculations using a single-state approximation including polarization and exchange but with slightly different polarization potentials. Bottcher[11] adopted a semiempirical approach and constructed model potentials to fit the experimental data. McEachran and Stauffer[12] initially employed the adiabatic-exchange approximation to examine the effects of the polarization potential and the treatment of exchange in the calculation of scattering length. Later they performed calculations[13] using the adiabatic-exchange approximation with the polarization potential scaled to the correct asymptotic form and obtained scattering length and total and momentum-transfer cross sections at low energies, which were in better agreement with experiment.[1] A calculation which includes the exchange polarization terms to assimilate the dynamic polarizability to some extent has been carried out by Dasgupta and Bhatia[16] to obtain total and momentum-transfer cross sections. Their calculations go beyond the adiabatic-exchange calculations of McEachran and Stauffer.[12]

Until now there has been no theoretical verification of the experimental scattering length obtained by O'Malley and Crompton.[1] Moreover, there is no accurate *ab initio* calculation of the scattering length and the phase shifts at very low energies. It is therefore a challenging problem to the theorist to verify the experimental results and thereby to test the accuracy of the theoretical methods.

Recently, Saha[17,18] applied the multiconfiguration Hartree-Fock[19] (MCHF) method to elastic scattering of electrons from neon and helium atoms at low and intermediate energies. The results were in excellent agreement with the measurements. It is the aim of this paper to apply the same *ab initio* method with proper modification to calculate the scattering length and the phase shifts for electron-neon scattering over the energy range from 0.0 to 7.0 eV, the extremely difficult region for *ab initio* calculation. It will test the accuracy and the

reliability of the present MCHF method. As mentioned earlier, this method considers the dynamical polarization and the electron-correlation effects more accurately and realistically in the *ab initio* method through the configuration interaction procedure. In this approach the dynamical polarization which is energy dependent is considered through the bound configuration representing the multipole polarization and varying the bound and the continuum orbitals simultaneously for each kinetic energy of the scattered electron. The elastic differential, total, and momentum-transfer cross section are calculated from these phase shifts obtained by this novel approach.

In the present calculation, the MCHF method[17] of Saha for scattering states is used to compute the phase shifts $\delta_l$ of various partial waves for very low energies. The method of constructing the phase shifts for various partial waves involves the solution of coupled integro-differential equations of the form[17]

$$\left[\frac{d^2}{dr^2}+\frac{2Z}{r}-\frac{l(l+1)}{r^2}\right]P_i(r) = \frac{2}{r}[Y_i(r)P_i(r)+X_i(r)+I_i(r)]+\sum_{i'}\varepsilon_{ii'}P_{i'}(r) \quad (1)$$

by an iterative method as described in detail earlier.[17] The bound radial functions satisfy the boundary condition

$$P_i(r)\underset{r\to 0}{\longrightarrow} r^{l+1},\quad P_i(r)\underset{r\to\infty}{\longrightarrow} 0. \quad (2)$$

The radial functions for the scattering orbital satisfy the conditions

$$P_i(r)\underset{r\to 0}{\longrightarrow} r^{l+1},$$
$$P_i(r)\underset{r\to\infty}{\longrightarrow} A\sin(kr-l\pi/2+\delta_l). \quad (3a)$$

For $k=0$ and at large $r$, the $s$-wave radial function satisfies the condition

$$P_i(r)\longrightarrow A'(r-a), \quad (3b)$$

where $a$ is the scattering length. Using the explicit zero-energy wave function allows $a$ to be calculated directly, and in addition gives a rigorous upper bound.[20]

The MCHF expansion of the ground-state wave function of the target neon atom consisted of configurations constructed from the single and double replacements of the two outermost orbitals $2s$ and $2p$ of the neon atom by the excited orbitals $3s$, $3p$, $3d$, $4s$, $4p$, $4d$, $4f$, $5s$, $5p$, $5d$, $5f$, $5g$, and $6g$. The $1s$, $2s$, and $2p$ wave functions are obtained from the Hartree-Fock calculation of the $2s^2 2p^6\,{}^1S$ ground state. As the polarization and the correlation of the $2s^2 2p^6$ target atom by the scattering

TABLE I. Comparison of scattering length (in $a_0$) with experiments and other theories.

| | Scattering length ($a_0$) |
|---|---|
| Theory | |
| Present work | 0.2218 |
| McEachran and Stauffer (Ref. 12) | 0.3082 |
| McEachran and Stauffer (Ref. 13) | 0.2012 |
| Thompson (Ref. 9) | 0.172 |
| Thompson (Ref. 10) | 0.347 |
| Bottcher (Ref. 11) | 0.25 |
| Experiment | |
| O'Malley and Crompton (Ref. 1) | 0.2135 |
| Robertson (Ref. 8) | 0.24 |
| Amaldi and Segrè (Ref. 3) | 0.14 |
| O'Malley (Ref. 2) | 0.24 |
| Hoffmann and Skarsgard (Ref. 4) | 0.20 |
| Sol, Devos, and Gauthier (Ref. 5) | 0.24 |
| Salop and Nakano (Ref. 6) | 0.30 |
| McDowell (Ref. 7) | 0.22 |

TABLE II. Comparison of phase shifts with experiment and theory.

| | $\delta_0$ | | $\delta_1$ | | $\delta_2$ | |
|---|---|---|---|---|---|---|
| Energy (eV) | Present work | Experiment (Ref. 1) | Present work | Experiment (Ref. 1) | Present work | Experiment (Ref. 1) |
| 0.003 | −0.0039 | −0.0038 | 0.000 10 | 0.0001 | 0.000 008 | 0.0 |
| 0.01 | −0.0080 | −0.0077 | 0.000 34 | 0.004 | 0.000 03 | 0.0001 |
| 0.02 | −0.0122 | −0.0119 | 0.000 67 | 0.007 | 0.000 07 | 0.0001 |
| 0.03 | −0.0159 | −0.0156 | 0.000 97 | 0.0010 | 0.000 132 | 0.0002 |
| 0.04 | −0.0193 | −0.0189 | 0.001 24 | 0.0013 | 0.000 19 | 0.0002 |
| 0.05 | −0.0222 | −0.0219 | 0.001 52 | 0.0016 | 0.000 25 | 0.0003 |
| 0.07 | −0.0281 | −0.0276 | 0.000 20 | 0.0022 | 0.000 37 | 0.0004 |
| 0.10 | −0.0359 | −0.0354 | 0.002 72 | 0.0029 | 0.000 54 | 0.0006 |
| 0.136 | −0.0445 | −0.0440 | 0.003 44 | 0.0036 | 0.000 78 | 0.0008 |
| 0.20 | −0.0583 | −0.0578 | 0.004 47 | 0.0047 | 0.001 10 | 0.0012 |
| 0.30 | −0.0776 | −0.0773 | 0.005 54 | 0.0059 | 0.001 76 | 0.0018 |
| 0.40 | −0.0952 | −0.0949 | 0.006 15 | 0.0065 | 0.002 33 | 0.0024 |
| 0.544 | −0.1175 | −0.118 | 0.006 52 | 0.0070 | 0.003 03 | 0.003 |
| 0.70 | −0.1412 | −0.141 | 0.005 80 | 0.0060 | 0.003 91 | 0.004 |
| 1.00 | −0.1812 | −0.181 | 0.003 43 | 0.0040 | 0.005 74 | 0.006 |
| 1.224 | −0.2086 | −0.208 | 0.000 40 | 0.0 | 0.007 03 | 0.007 |
| 1.5 | −0.2396 | −0.240 | −0.003 98 | −0.004 | 0.008 69 | 0.009 |
| 2.0 | −0.2913 | −0.292 | −0.014 86 | −0.015 | 0.011 76 | 0.012 |
| 2.176 | −0.3082 | −0.310 | −0.017 74 | −0.019 | 0.013 04 | 0.013 |

electron are extremely important at these very low energies, all the configurations which account for polarization and correlation are considered in the expansion of the scattering wave function. The dipole polarizability obtained in this calculation is $2.613a_0^3$ which is in excellent agreement with the experimental value[21] of $2.66a_0^3$.

In Table I, the present scattering length is compared with results derived from experiments[1-8] and with other theoretical data.[9-12] The present result agrees to within 4% with the most accurate results derived from experiment by O'Malley and Crompton.[1] These authors applied MERT to analyze the drift-velocity data of Robertson[8] for very-low-energy electron swarms, using data for the $p$-wave phase shift $\delta_1$ derived by an application of MERT to Williams' data[22] for $\delta_1$ obtained from low-energy differential cross-section measurements. However, in the range 0–2.25 eV $\delta_1$ is less than 8% of $\delta_0$, so O'Malley and Crompton's results rest heavily on the swarm data which extend to much lower energies. This outstanding agreement suggests the accuracy of the MCHF method. The present result also agrees very well with the result of McDowell[7] derived from an analysis of experimental data from a number of sources. The earlier theoretical result obtained by McEachran and Stauffer[12] is higher than the present and the O'Malley and Crompton's results whereas their later result[13] is lower. The present scattering length lies in between Thompson's theoretical results[9,10] obtained from two calculations using a single-state approximation including polarization and exchange but with slightly different polarization potentials.

TABLE III. Comparison of total elastic cross sections (in Å$^2$) with other theory and experiment.

| $E$ (eV) | Present work | Theory McEachran and Stauffer (Ref. 13) | Experiment (Ref. 1) |
|---|---|---|---|
| 0.0 | 0.173 | | 0.161 |
| 0.003 | 0.243 | | 0.227 |
| 0.01 | 0.307 | | 0.287 |
| 0.02 | 0.359 | | 0.346 |
| 0.03 | 0.407 | | 0.392 |
| 0.04 | 0.451 | | 0.432 |
| 0.05 | 0.478 | 0.438 | 0.468 |
| 0.07 | 0.548 | | 0.532 |
| 0.10 | 0.627 | 0.578 | 0.613 |
| 0.136 | 0.710 | 0.660 | 0.695 |
| 0.20 | 0.828 | 0.781 | 0.820 |
| 0.30 | 0.976 | 0.934 | 0.970 |
| 0.40 | 1.098 | 1.059 | 1.090 |
| 0.544 | 1.225 | 1.208 | 1.240 |
| 0.70 | 1.369 | 1.341 | 1.370 |
| 1.00 | 1.565 | 1.547 | 1.570 |
| 1.224 | 1.688 | 1.671 | 1.680 |
| 1.50 | 1.813 | 1.804 | 1.820 |
| 2.00 | 2.009 | 2.003 | 2.020 |
| 2.176 | 2.069 | | 2.090 |

Table II presents the $s$-, $p$-, and $d$-wave phase shifts which are compared with the experimental results of O'Malley and Crompton.[1] The present results are in excellent agreement with the phase shifts obtained by O'Malley and Crompton.[1] The present total cross section $\sigma_T$ is presented in Table III for energies from 0.0 to 2.176 eV and compared with that of McEachran and Stauffer[13] and that derived by O'Malley and Crompton.[1] The present results are in remarkably excellent agreement with the results of O'Malley and Crompton.[1] The results of McEachran and Stauffer[13] are a little less than the present values but the differences decrease with increasing energy.

TABLE IV. Comparison of momentum-transfer cross sections (in Å$^2$) with other theory and experiments.

| Energy (eV) | Present work | Theory McEachran and Stauffer (Ref. 13) | Experiment O'Malley and Crompton (Ref. 1) | Experiment Robertson (Ref. 8) |
|---|---|---|---|---|
| 0.0 | 0.173 | | 0.161 | |
| 0.003 | 0.255 | | 0.241 | |
| 0.01 | 0.333 | | 0.314 | |
| 0.02 | 0.398 | | 0.386 | |
| 0.03 | 0.456 | | 0.442 | 0.469 |
| 0.04 | 0.507 | | 0.491 | 0.504 |
| 0.05 | 0.541 | 0.501 | 0.535 | 0.536 |
| 0.06 | 0.575 | | | 0.566 |
| 0.07 | 0.623 | | 0.611 | 0.601 |
| 0.08 | 0.656 | | | 0.636 |
| 0.09 | 0.676 | | | 0.669 |
| 0.10 | 0.718 | 0.670 | 0.707 | 0.701 |
| 0.12 | 0.776 | | | 0.754 |
| 0.136 | 0.813 | 0.765 | 0.803 | |
| 0.15 | 0.857 | 0.798 | | 0.828 |
| 0.18 | 0.905 | | | 0.893 |
| 0.20 | 0.947 | 0.903 | 0.940 | 0.930 |
| 0.25 | 1.035 | 0.994 | | 1.018 |
| 0.30 | 1.105 | 1.072 | 1.11 | 1.091 |
| 0.40 | 1.229 | 1.202 | 1.23 | 1.225 |
| 0.50 | 1.334 | 1.306 | | 1.321 |
| 0.544 | 1.349 | 1.346 | 1.37 | |
| 0.60 | 1.404 | 1.392 | | 1.402 |
| 0.70 | 1.470 | 1.464 | 1.48 | 1.472 |
| 0.80 | 1.521 | 1.525 | | 1.528 |
| 0.90 | 1.571 | 1.577 | | 1.580 |
| 1.00 | 1.615 | 1.622 | 1.62 | 1.619 |
| 1.20 | 1.677 | 1.694 | | 1.685 |
| 1.224 | 1.689 | 1.701 | 1.69 | |
| 1.50 | 1.752 | 1.773 | 1.75 | 1.753 |
| 1.80 | 1.794 | 1.829 | | 1.793 |
| 2.0 | 1.822 | 1.857 | 1.83 | 1.815 |
| 2.176 | 1.842 | | 1.86 | |
| 2.5 | 1.865 | | | 1.860 |
| 3.0 | 1.898 | | | 1.906 |
| 4.0 | 1.952 | | | 1.984 |
| 5.0 | 2.007 | 2.071 | | 2.070 |
| 6.0 | 2.059 | | | 2.144 |
| 7.0 | 2.117 | | | 2.213 |

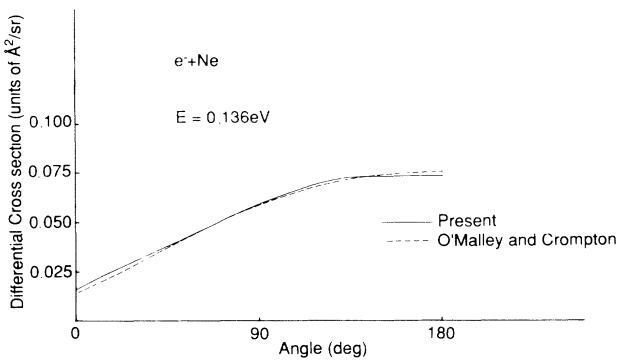


FIG. 1. Differential cross sections at 0.136 eV.

The present momentum-transfer cross sections are shown in Table IV and compared with the experimental results of O'Malley and Crompton[1] and of Robertson[8] and the theoretical results of McEachran and Stauffer.[13] The present results are seen to be in excellent agreement with the results obtained by O'Malley and Crompton[1] and of Robertson.[8] From 3.5 to 5.0 eV, Robertson's results are slightly higher. The results obtained by McEachran and Stauffer are slightly lower except for energies greater than 0.70 eV, where the results are a little higher.

Figures 1 and 2 show present differential cross sections for energies 0.136 and 2.176 eV. They are compared with the results of O'Malley and Crompton[1] and the experimental results of Williams[22] where available. At energy 0.136 eV, the present results show excellent agreement with the experimental results of O'Malley and Crompton. At 2.176 eV, the present results are again in excellent agreement with the results obtained by O'Malley and Crompton except for $\theta$ from 40° to 110° where the present results are a little lower. Williams' results are higher than the present results for $\theta$ less than 70° and slightly lower for $70° < \theta < 120°$ and higher afterwards.

In conclusion, we would like to mention that the scattering length of $0.2218a_0$ is calculated and bounded for the first time very accurately in the *ab initio* manner using the MCHF method. This method, which optimizes both bound and continuum wave functions simultaneously at each kinetic energy of the continuum electron, produces very accurate values of the scattering length and the phase shifts at very low energies, an extremely difficult region for theoretical investigation. The beauty of the present method is that it takes into account the electron correlation and the dynamical polarization in an *ab initio* way very efficiently through the configuration interaction procedure. The present values of the scattering length and the phase shifts are in excellent agreement with the most accurate experimental result of O'Malley and Crompton which verifies the accuracy of the present theoretical method.[19]

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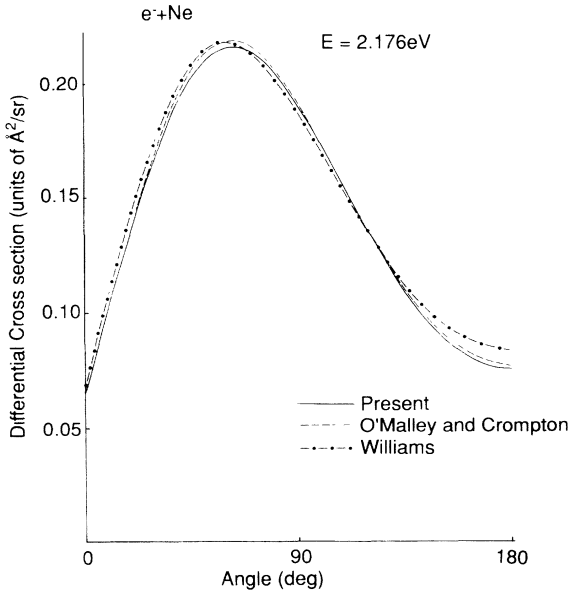


FIG. 2. Differential cross sections at 2.176 eV.

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