# Scattering of positronium by H, He, Ne, and Ar

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## Abstract

The low-energy scattering of ortho positronium (Ps) by H, He, Ne, and Ar atoms has been investigated in the coupled-channel framework by using a recently proposed time-reversal-symmetric nonlocal electron-exchange model potential with a single parameter $C$. For H and He we use a three-Ps-state coupled-channel model and for Ar and Ne we use a static-exchange model. The sensitivity of the results is studied with respect to the parameter $C$. Present low-energy cross sections for He, Ne and Ar are in good agreement with experiment.

Low-energy collision of ortho positronium (Ps) atom with neutral gas atoms and molecules is of interest in both physics and chemistry. Recently, there have been precise measurements of low-energy ortho-Ps scattering by $H_2$, $N_2$, He, Ne, Ar, $C_4H_{10}$, and $C_5H_{12}$ [1, 2, 3]. Due to internal charge and mass symmetry, Ps atom yields zero elastic and even-parity transition potentials in the direct channel. Ps scattering is dominated mainly by exchange correlation at low energies. If $N$ basis states are included for both Ps and target in a coupled-channel formalism, the number of channels grow as $N^2$. This complicates the tractability of the Ps scattering process in a coupled channel scheme compared to the electron scattering. The dominance of the short-range interaction in Ps scattering causes serious trouble towards the convergence of any coupled-channel formalism with a truncated basis [4, 5]. The use of 22 coupled Ps pseudostates for Ps-H system in the R-matrix approach has indicated convergence difficulties [5, 6] in Ps-H binding and resonance energies.

To find a solution to the nonconvergence problem, we have suggested a nonlocal electron-exchange model potential [4, 5] with a single parameter $C$ and demonstrated its effectiveness by performing quantum coupled-channel calculations using the ab initio framework of close coupling approximation. Two versions of this potential were suggested: one is time-reversal-symmetric and the other nonsymmetric. The nonsymmetric potential has been applied for the study of Ps scattering by H [7], He [4] and $H_2$ [8] using a three-Ps-state coupled-channel model. For He and $H_2$ these studies yielded total cross sections in good agreement with experiments [1, 2, 3] in addition to producing the correct pick-off quenching rate for Ps-He at low energies [9]. Higher Ps-excitation and ionization cross sections were also calculated in these cases to reproduce the total cross sections at medium and high energies. Previous theoretical studies [10, 11] on Ps-He produced results in strong disagreement [4] with experiment [1, 2, 3].

In a subsequent application of this model potential to Ps scattering by H [5], it was found that the symmetric form leads to by far superior result than the nonsymmetric form. The symmetric form was able to reproduce accurate variational results very precisely for singlet Ps-H binding and resonance energies; the nonsymmetric form failed to yield such results.

In view of this we reinvestigate the problem of low-energy Ps scattering by He [4] using the symmetric exchange potential employing the three-Ps-state model used before. We study how the low-energy cross sections for Ps-H and Ps-He change with the variation of the parameter $C$ of the potential. Then we also apply this exchange potential to the study of low-energy Ps scattering by Ne and Ar using a static-exchange model. The present calculation accounts for the measured low-energy cross sections [1, 2, 3] satisfactorily for He, Ne, and Ar.

The total wave function of the Ps-target system is expanded in terms of the Ps eigenstates

as

$$\Psi^{\pm}(\mathbf{r_1}, ..., \mathbf{r_N}; \mathbf{r_{N+1}}, \mathbf{x}) = \sum_{\nu} \Big[ F_{\nu}(\rho_{\mathbf{N+1}}) \chi_{\nu}(\mathbf{t_{N+1}}) \phi_0(\mathbf{r_1}, ..., \mathbf{r_j}, ..., \mathbf{r_N})$$
$$+ \sum_{j=1}^{N} (-1)^{S_{N+1,j}} F_{\nu}(\rho_{\mathbf{j}}) \chi_{\nu}(\mathbf{t_j}) \phi_0(\mathbf{r_1}, ..., \mathbf{r_{N+1}}, ..., \mathbf{r_N}) \Big], \qquad (1)$$

where antisymmetrization with respect to Ps- and target-electron coordinates has been made. Here $\rho_{\mathbf{i}} = (\mathbf{x} + \mathbf{r_i})/2$, $\mathbf{t_i} = (\mathbf{x} - \mathbf{r_i})$, where $\mathbf{r_i}, i = 1, ..., N$ denote the target electron coordinates, and $\mathbf{r_{N+1}}$ and $\mathbf{x}$ are the electron and positron coordinates of Ps; $\phi_0$ and $\chi_{\nu}$ denote the target and Ps wave functions, and $F_{\nu}$ is the continuum orbital of Ps with respect to the target. $S_{N+1,j}$ is the total spin of the Ps electron $(N+1)$ and target electron $(j)$ undergoing exchange and can have values of 1 or 0. The spin of the positron is conserved in this process and the exchange profile of the Ps-target system is analogous to the corresponding electron-target system. Projecting the resultant Schrödinger equation on the Ps eigenstates and averaging over spin states, the resulting momentum-space Lippmann-Schwinger scattering equation for a particular total electronic spin state $S$ can, in general, be written as [11, 12]

$$f_{\nu'\nu}^{S}(\mathbf{k'}, \mathbf{k}) = \mathcal{B}_{\nu'\nu}^{S}(\mathbf{k'}, \mathbf{k})$$
$$- \frac{1}{2\pi^2} \sum_{\nu''} \int d\mathbf{k''} \frac{\mathcal{B}_{\nu'\nu''}^{S}(\mathbf{k'}, \mathbf{k''}) f_{\nu''\nu}^{S}(\mathbf{k''}, \mathbf{k})}{k_{\nu''}^2/4 - k''^2/4 + i0}, \qquad (2)$$

where $f_{\nu'\nu}^{S}$ is the scattering amplitude, and $\mathcal{B}_{\nu'\nu}$ is the corresponding Born potential, $\nu$ and $\nu'$ denote initial and final Ps states, $k_{\nu''} = \sqrt{2m(\mathcal{E} - \epsilon'')/\hbar^2}$ is the on-shell relative momentum of Ps in the channel $\nu''$ with $\epsilon''$ the total binding energy of the intermediate Ps and target states, and $\mathcal{E}$ the total energy of the Ps-target system and $m$ the reduced mass. Here

$$\mathcal{B}_{\nu'\nu}^{S}(\mathbf{k'}, \mathbf{k}) = B_{\nu'\nu}^{D}(\mathbf{k'}, \mathbf{k}) + \sum_{j=1}^{N} (-1)^{S_{N+1,j}} B_{\nu'\nu}^{E_j}(\mathbf{k'}, \mathbf{k}); \qquad (3)$$

where $B^D$ is the direct Born potential and $B^{E_j}$ is the model potential for exchange between the Ps electron (denoted by $N+1$) with the $j$th target electron. For Ps-H scattering both $S \equiv S_{2,1}$ $= 0, 1$ will contribute [12]; the corresponding potentials and amplitudes are usually denoted by $\mathcal{B}_{\nu'\nu}^{\pm}$ and $f_{\nu'\nu}^{\pm}$, respectively [5]. For Ps scattering from He, Ne, and Ar etc. there will be only one scattering equation (2) corresponding to total electronic spin $S = 1/2$. For these targets with doubly occupied spatial orbitals, in the sum over $j$ in Eq. (3) only half of the occupied target electrons in each sub-shell will contribute when the target is frozen to its ground state [13]. Consequently, only $S_{N+1,j} = 1$ ($f^-$ and $\mathcal{B}^-$) will contribute to target-elastic scattering [11] for targets with doubly occupied spatial orbitals.

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For Ps-H scattering, the differential cross section is given by $d\sigma/d\Omega = [|f^+|^2 + 3|f^-|^2]/4$. For target-elastic Ps scattering by He, Ne, and Ar, the differential cross section is given by $d\sigma/d\Omega = |f^-|^2$. In all Ps-scattering the direct potential, $B^D$, is zero for elastic and all even-parity-state transitions of Ps. Thus the nonorthogonal exchange kernel alone dominates the solution of Eq. (2) and this dominance is possibly responsible for convergence difficulties to conventional approaches based on Eq. (2).

The present exchange model was derived using Slater-type orbital for the H-atom, so that a generalization from a H-target to a complex target represented by a Hatree-Fock wave function becomes straight-forward. For Ps scattering from a H orbital, the model exchange potential between the Ps-electron ($\mathbf{r_2}$) and the orbital electron ($\mathbf{r_1}$) was derived from the $1/r_{12}$ term and is given by [4, 5]:

$$
\begin{aligned}
B^E_{\mu'\nu'\mu\nu} &= \frac{4(-1)^{l+l'}}{<D>} \int \phi^*_{\mu'}(\mathbf{r_2}) \exp(i\mathbf{Q}.\mathbf{r_2})\phi_\mu(\mathbf{r_2})\mathrm{d}\mathbf{r_2} \\
&\times \int \chi^*_{\nu'}(\mathbf{t_2}) \exp(i\mathbf{Q}.\mathbf{t_2}/2)\chi_\nu(\mathbf{t_2})\mathrm{d}\mathbf{t_2},
\end{aligned}
\tag{4}
$$

where $l$ and $l'$ are angular momenta of the initial ($\chi_\nu$) and final ($\chi_{\nu'}$) Ps states, $\phi_\mu$ and $\phi_{\mu'}$ are initial and final H states, and $\mathbf{Q} = \mathbf{k_i} - \mathbf{k_f}$. Here $\mathbf{k_i}$ and $\mathbf{k_f}$ are initial and final Ps momenta, respectively. In Eq. (4) the symmetric form of the averaged quantity $<D>$ is [4, 5]

$$
<D> = \frac{k_i^2 + k_f^2}{8} + C^2 \left[ \frac{\alpha_\mu^2 + \alpha_{\mu'}^2}{2} + \frac{\beta_\nu^2 + \beta_{\nu'}^2}{2} \right],
\tag{5}
$$

where $\alpha_{\mu'}^2/2$ and $\beta_\nu^2$ are the binding energies of the final target and initial Ps states, respectively, and $C$ is the only parameter of the potential. Normally, the parameter $C$ is taken to be unity [4, 5] which leads to reasonably good numerical results. However, it can be varied slightly from unity to obtain a precise fit of a low-energy scattering observable (experimental or variational), as have been done in some applications of model potentials [14, 15]. A variation of $C$ from unity leads to a variation of the binding energy parameters ($\alpha^2, \beta^2$ etc.) used as average values for square of momentum [4] in the expression for $\langle D \rangle$ of Eq. (5). This, in turn, tunes the strength of the exchange potential (4) at low energies. At high energies this model potential is insensitive to this parametrization and leads to the well-known Born-Oppenheimer form of exchange [16]. We have turned this flexibility to good advantage by obtaining precise agreement with low-energy results of Ps scattering by H, He, Ne, and Ar, as we shall see in the following.

For a complex target the space part of the HF wave function [17] is given by $\Psi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_j,- ..., \mathbf{r}_N) = \mathcal{A}[\phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_2)...\phi_j(\mathbf{r}_j)...\phi_N(\mathbf{r}_N)]$, where $\mathcal{A}$ is the antisymmetrization operator. The position vectors of the electrons are $\mathbf{r}_i, i = 1, 2, ..., N$ and $\phi_j$'s have the form: $\phi_j(\mathbf{r_j}) =$

$\sum_\kappa a_{\kappa j}\phi_{\kappa j}(\mathbf{r_j})$. The orbital $\phi_{\kappa j}(\mathbf{r_j})$ is a Slater-type orbital. Considering proper antisymmetrization with respect to Ps and target electrons, the final model exchange potential obtained from (4) is given by [4]

$$
\begin{aligned}
B^{E_j}_{\nu'\nu} & = \sum_{\kappa\kappa'} \frac{4a_{\kappa j}a_{\kappa'j}(-1)^{l+l'}}{<D_{\kappa\kappa'}>} \\
& \times \int \phi^*_{\kappa'j}(\mathbf{r}_j)\exp(i\mathbf{Q}.\mathbf{r}_j)\phi_{\kappa j}(\mathbf{r}_j)\mathrm{d}\mathbf{r}_j \\
& \times \int \chi^*_{\nu'}(\mathbf{t}_j)\exp(i\mathbf{Q}.\mathbf{t}_j/2)\chi_\nu(\mathbf{t}_j)\mathrm{d}\mathbf{t}_j.
\end{aligned}
\tag{6}
$$

with

$$
<D_{\kappa\kappa'}> = (k_i^2 + k_f^2)/8 + C^2[(\alpha^2_{\kappa j} + \alpha^2_{\kappa'j})/2 + (\beta^2_\nu + \beta^2_{\nu'})/2],
$$

where $\alpha_{\kappa j}$ is the energy parameter corresponding to the orbital $\phi_{\kappa j}(\mathbf{r_j})$ [17].

We use exact wave functions for H and Ps, HF wave functions for He, Ne, and Ar [17]. After a partial-wave projection, the one-dimensional scattering equations are solved by the method of matrix inversion.

First we study the effect of the variation of the parameter $C$ of the exchange potential in the Ps-H system using a three-Ps-state model with Ps(1s,2s,2p) states [7]. We start our discussion with the singlet S-wave resonance. In Fig. 1 we plot the S-wave phase shift at different energies which illustrate the resonance pattern obtained with different values of $C$. The resonance position shifts monotonically towards lower energies with decreasing of $C$ from unity. We have shown it in steps where the value of $C$ is varied from unity to 0.785. The resonance position matches with the accurate prediction of 4.01 eV [18] for $C = 0.785$. In Fig. 2, we plot $k \cot \delta$ versus $k^2$ for the corresponding low-energy S-wave phase shifts $\delta$. Figure 2 demonstrates how the improvement in the resonance position simultaneously improves the Ps-H binding energy. For $C = 1.0$ the resonance and binding energies are 4.715 eV and 0.165 eV, respectively; for $C = 0.9$ the corresponding energies are 4.470 eV and 0.445 eV, respectively. At $C = 0.785$, while the resonance position is correctly fitted to 4.01 eV (Fig. 1), we obtain an approximate binding energy of 1.02 eV from a linear extrapolation as in Fig. 2, and 0.99 eV with more precise fitting considering second order corrections, compared to the accurate prediction of $1.0598 - 1.067$ eV [19]. This behavior of the low-energy phase shifts, which yields simultaneously the Ps-H resonance and binding energies, indicates that the use of the model potential (4) in a coupled-channel scheme can lead to a good description of Ps-H scattering.

We exhibit in Figs. 3 (a), (b), and (c) the present elastic cross sections, for Ps scattering by He, (three-Ps-state [4]) Ne and Ar (static-exchange), respectively, for $C = 1$, 0.85, and 0.785. The value $C = 0.785$ yielded the good agreement in the case of Ps-H. For the closed-shell atoms, a typical $C$ close to 0.85 works well for the 3-Ps-state model in Ps-He and for

the static-exchange model in Ps-Ar and Ps-Ne. Although the present cross sections differ from other theoretical [10, 11] and experimental [20] works at low energies for Ps-He (See, Fig. 6 of Ref. [4]), they agree well with the recent measurements of Skalsey et al. [3] and unpublished work of G. Peach as quoted in Ref. [2].

Table I: Low-energy S-wave phase shifts in radians for Ps-He, Ps-Ne, and Ps-Ar for different $k$ in au. The entries for $k = 0$ correspond to the scattering lengths in units of $a_0$, incident positronium energy $E = 6.8k^2$ eV.

| $k$ | Ar(SE) | Ne(SE) | He(SE) | He(3st) |
|-----|--------|--------|--------|---------|
| 0.0 | 1.65 | 1.41 | 1.03 | 0.90 |
| 0.1 | $-0.164$ | $-0.141$ | $-0.103$ | $-0.088$ |
| 0.2 | $-0.319$ | $-0.277$ | $-0.202$ | $-0.172$ |
| 0.3 | $-0.457$ | $-0.404$ | $-0.294$ | $-0.249$ |
| 0.4 | $-0.572$ | $-0.518$ | $-0.375$ | $-0.315$ |
| 0.5 | $-0.656$ | $-0.615$ | $-0.444$ | $-0.368$ |
| 0.6 | $-0.706$ | $-0.694$ | $-0.500$ | $-0.408$ |
| 0.7 | $-0.720$ | $-0.754$ | $-0.541$ | $-0.433$ |
| 0.8 | $-0.699$ | $-0.792$ | $-0.569$ | $-0.445$ |

Table II: Low-energy P-wave phase shifts in radians for Ps-He, Ps-Ne, and Ps-Ar for different $k$ in au. The incident positronium energy $E = 6.8k^2$ eV. The numbers in parenthesis denote powers of ten.

| $k$ | Ar(SE) | Ne(SE) | He(SE) | He(3st) |
|-----|--------|--------|--------|---------|
| 0.1 | $-2.71(-3)$ | $-1.63(-3)$ | $-8.19(-4)$ | $-6.24(-4)$ |
| 0.2 | $-1.94(-2)$ | $-1.20(-2)$ | $-6.11(-3)$ | $-4.63(-3)$ |
| 0.3 | $-5.51(-2)$ | $-3.55(-2)$ | $-1.85(-2)$ | $-1.38(-2)$ |
| 0.4 | $-1.06(-1)$ | $-7.17(-2)$ | $-3.81(-2)$ | $-2.80(-2)$ |
| 0.5 | $-1.65(-1)$ | $-1.17(-1)$ | $-6.33(-2)$ | $-4.53(-2)$ |
| 0.6 | $-2.23(-1)$ | $-1.66(-1)$ | $-9.15(-2)$ | $-6.26(-2)$ |
| 0.7 | $-2.75(-1)$ | $-2.15(-1)$ | $-1.20(-1)$ | $-7.63(-2)$ |
| 0.8 | $-3.17(-1)$ | $-2.60(-1)$ | $-1.47(-1)$ | $-7.89(-2)$ |

In Table I we present the S-wave phase shifts for Ps-Ar (static exchange model denoted SE), Ps-Ne (SE), and Ps-He (SE and three-Ps-state models) scattering for $C = 0.85$. In Table

II we present the same for the P wave. The magnitude of the scattering lengths, low-energy cross sections and phase shifts (well below Ps-excitation threshold) increase monotonically as we move from He to Ne and from Ne to Ar. As the effective potential for elastic scattering in these cases is repulsive in nature, this indicates an increase in repulsion from He to Ne and from Ne to Ar.

We find from Figs. 3 that the energy-dependences of the elastic cross sections are similar for all the closed-shell atoms studied here. The cross section has a monotonic slow decrease with increasing energy. This trend is consistently found in all previous theoretical calculations in Ps-He. Also, this is expected as the underlying effective potential for elastic scattering is repulsive in nature.

In conclusion, we have reinvestigated the problem of low-energy elastic Ps scattering by H, and He (three-Ps-state) using a symmetric nonlocal electron-exchange potential with a parameter $C$. We further apply this potential to Ps scattering by Ne, and Ar (static-exchange). Although the value $C = 1$ was originally suggested, a slightly lower value $C \approx 0.8$ leads to good agreement with accurate experiment [3] and accurate calculations [18, 19] in the present cases. Although, a non-symmetric form of the model potential provides a fairly good account of the cross section [7], we have found that the symmetric form is able to provide a more precise description of scattering. The Ref. [4] we have demonstrated the effectiveness of the present exchange potential in electron-impact scattering. Simplicity of the present exchange potential and the reliability of the present results calculated with it from a two- (Ps-H) to a 19-electron (Ps-Ar) system reveals the effectiveness of the exchange model and warrants further study with it.

# References

[1] N. Zafar, G. Laricchia, M. Charlton, and A. Garner, Phys. Rev. Lett. 76 (1996) 1595.

[2] A. J. Garner, G. Laricchia, and A. Ozen, J. Phys. B 29 (1996) 5961.

[3] M. Skalsey, J. J. Engbrecht, R. K. Bithell, R. S. Vallery, and D. W. Gidley, Phys. Rev. Lett. 80 (1998) 3727.

[4] P. K. Biswas and S. K. Adhikari, Phys. Rev. A 59 (1999) 363.

[5] S. K. Adhikari and P. K. Biswas, Phys. Rev. A 59 (1999) 2058.

[6] C. P. Campbell, M. T. McAlinden, F. G. R. S. MacDonald, and H. R. J. Walters, Phys. Rev. Lett. 80 (1998) 5097.

[7] P. K. Biswas and S. K. Adhikari, J. Phys. B 31 (1998) 3147; 31 (1998) 5403.

[8] P. K. Biswas and S. K. Adhikari, J. Phys. B 31 (1998) L737.

[9] S. K. Adhikari, P. K. Biswas, and R. A. Sultanov, Phys. Rev. A 59 (1999) 4828.

[10] M. I. Barker, B. H. Bransden, J. Phys. B 1 (1968) 1109; 2 (1969) 730.

[11] N. K. Sarkar and A. S. Ghosh, J. Phys. B 30 (1997) 4591.

[12] P. K. Sinha, P. Chaudhury, and A. S. Ghosh, J. Phys. B 30 (1997) 4643.

[13] M. E. Riley and D. G. Truhlar, J. Chem. Phys. 63 (1975) 2182; see, especially, its Eq. (1) and related discussion below it.

[14] M. A. Morrison, A. N. Feldt, and D. Austin, Phys. Rev. A 29 (1984) 2518.

[15] T. L. Gibson and M. A. Morrison, J. Phys. B 15 (1982) L221.

[16] J. R. Oppenheimer, Phys. Rev. 32 (1928) 361.

[17] E. Clementi and C. Roetti, At. Data and Nucl. Data Tables 14 (1974) 177.

[18] Y. K. Ho, Phys. Rev. A 17 (1978) 1675.

[19] A. M. Frolov and V. H. Smith, Jr., Phys. Rev. A 55 (1997) 2662 and references therein.

[20] Y. Nagashima, T. Hyodo, K. Fujiwara, and A. Ichimura, J. Phys. B 31 (1998) 329 and private communication.

Figure Caption

1. S-wave singlet Ps-H phase shifts in radian showing the variation of the resonance position with the variation of $C$ in (5) using present three-Ps-state model.

2. $k \cot \delta$ and $ik$ versus $k^2$ plot showing the change in Ps-H binding energy with the variation in $C$ as in figure 1 (Energy = $6.8k^2$ eV). The crossing of the $k \cot \delta$ and $ik$ curves give the energy of the bound state.

3. Cross section of Ps scattering by (a) He, (three-Ps-state model) (b) Ne, and (c) Ar (static-exchange model) for different $C$: $C = 1$ (full line), $C = 0.85$ (dashed-dotted) line, $C = 0.785$ (dashed line), experiment (box, Ref. [3]).
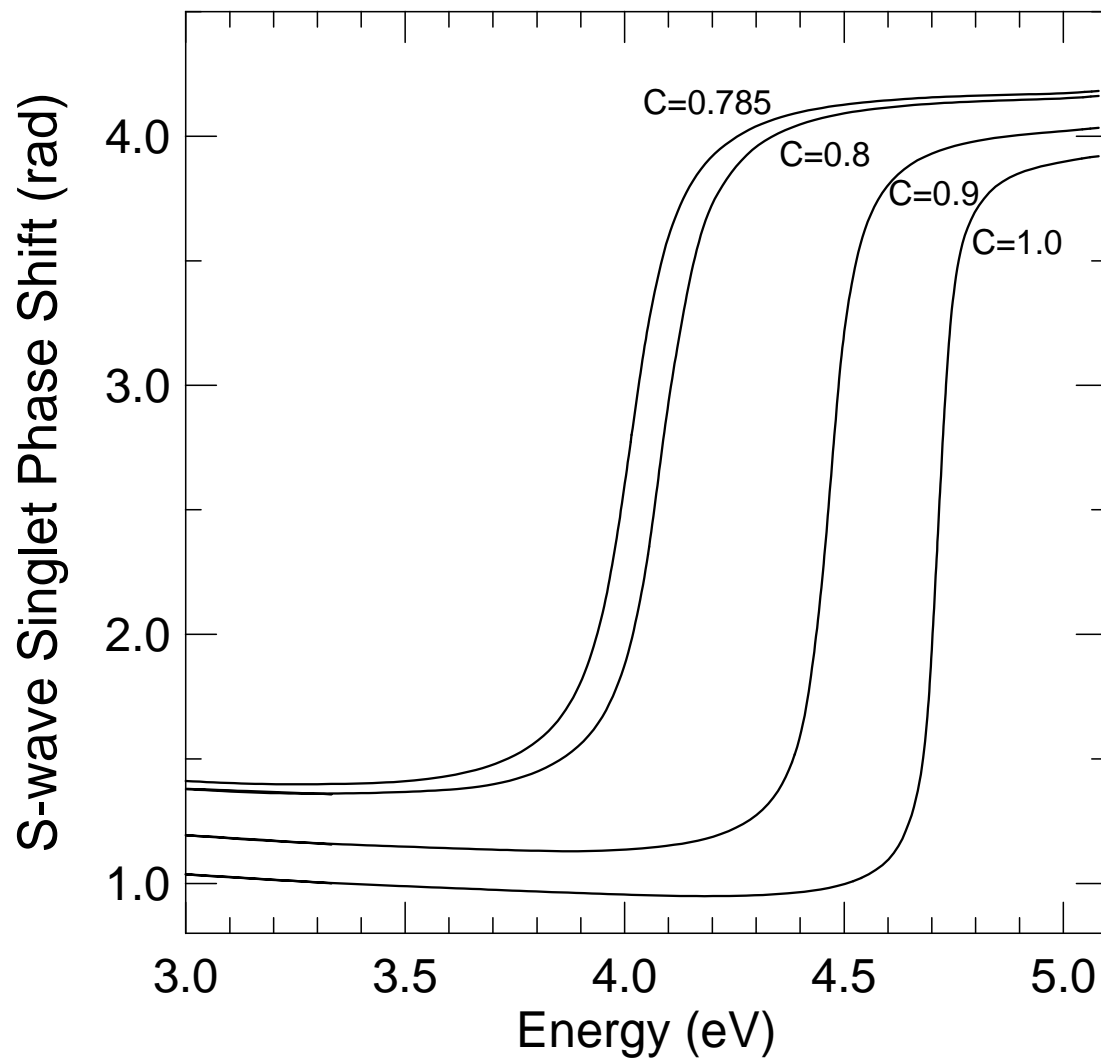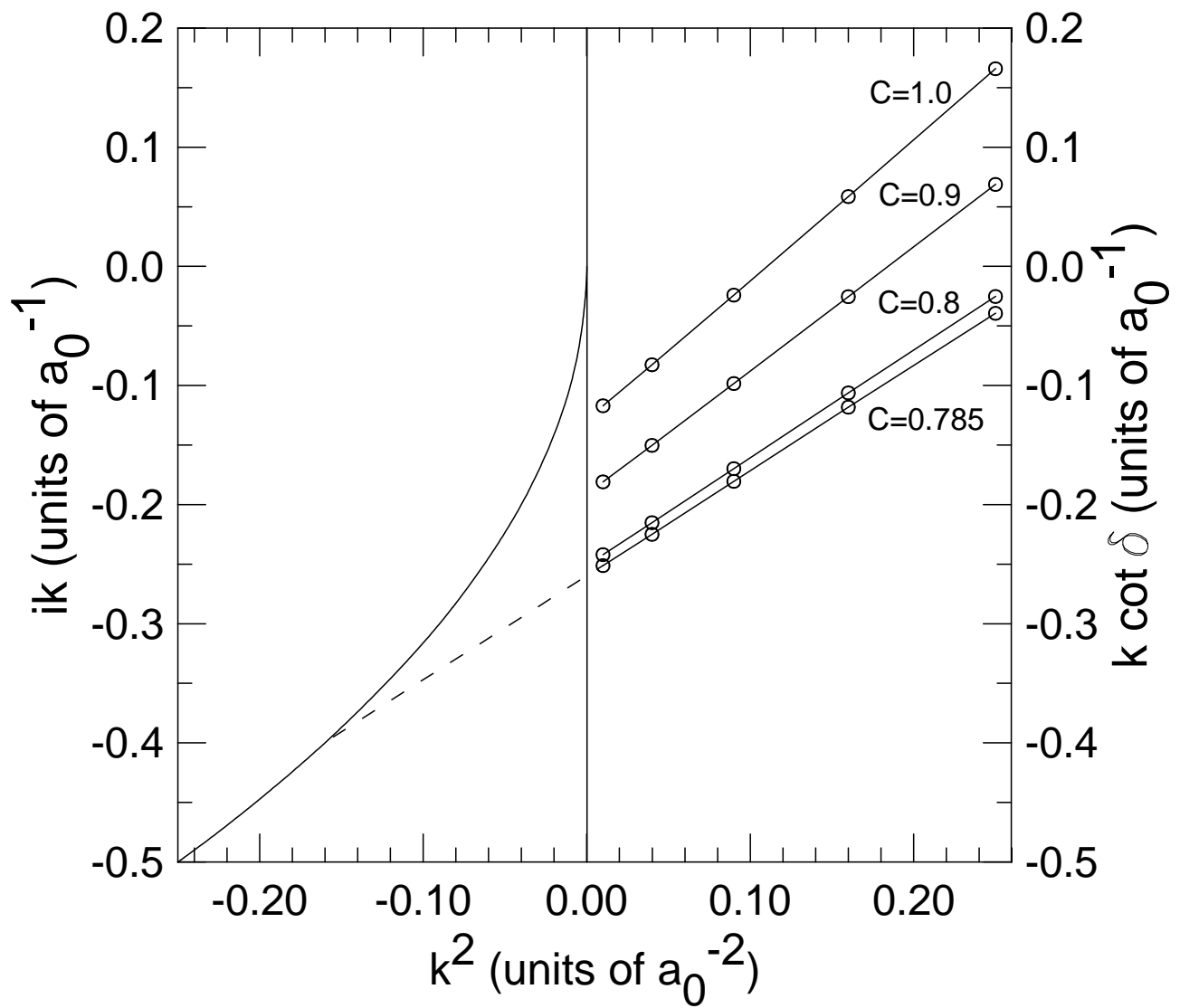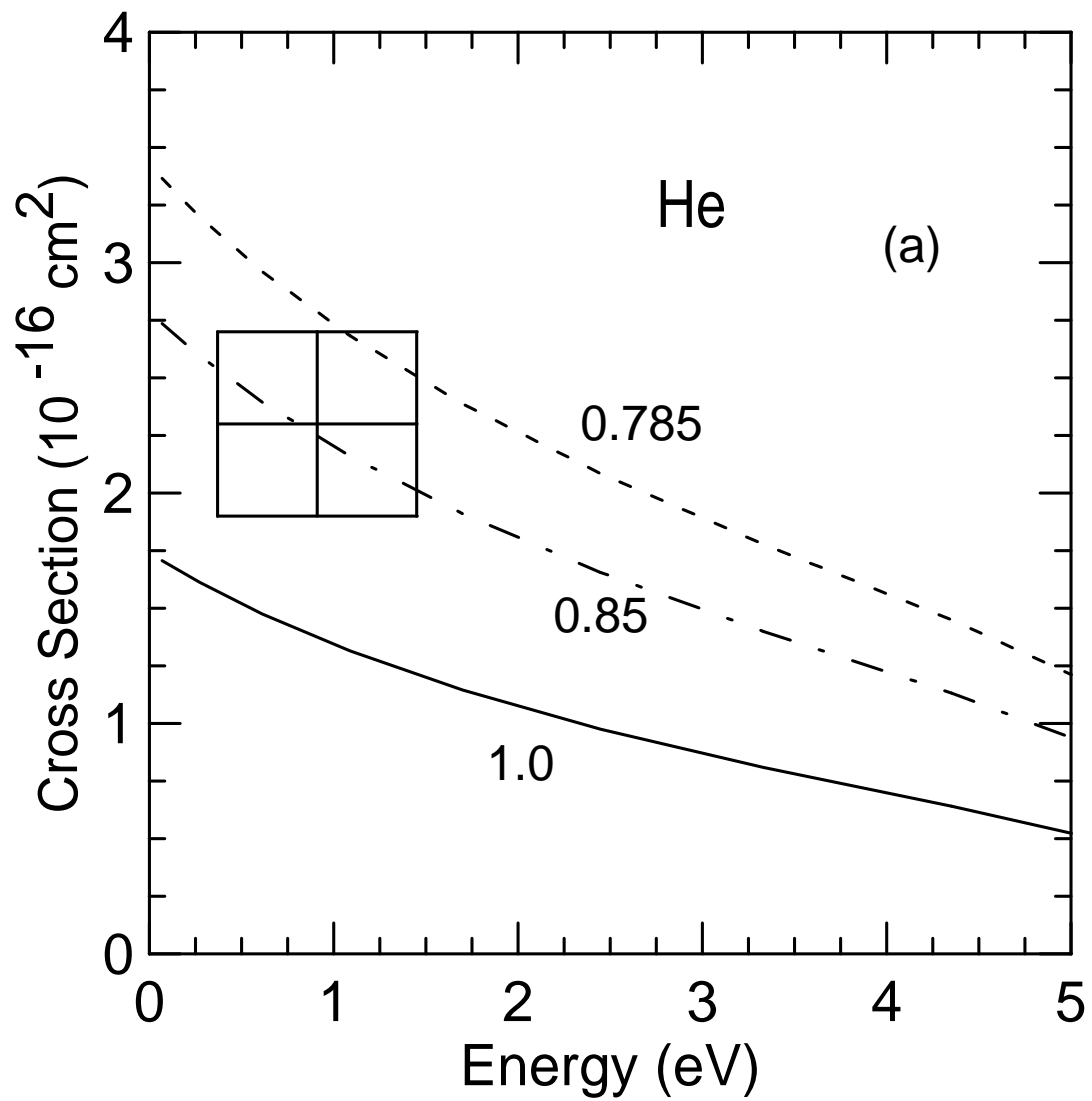
Figure 1

Figure 2

Figure 3

Figure 3