Elastic Scattering Using an Artificial Confining Potential

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The discrete energies of a scattering Hamiltonian calculated under the influence of an artificial confining potential of almost arbitrary functional form can be used to determine its phase shifts. The method exploits the result that two short-range Hamiltonians having the same energy will have the same phase shifts upon removal of the confining potential. An initial verification is performed on a simple model problem. Then the stochastic variational method is used to determine the energies of the confined e^--He $^2S^e$ system and thus determine the low energy phase shifts.

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A recurrent theme in the quantum theory of scattering is the desire to develop procedures to take advantage of bound state methods based on square integrable (L^2) wave functions. One reason for this is the wish to adapt existing bound state program packages to the calculation of continuum states. Some of the methods using L^2 functions include the complex absorbing potential approach [1], stabilization approaches [2,3], and the many different types of R-matrix methods [4–6] including the box-variational method [7], which is used for quantum Monte Carlo scattering calculations [8].

The present Letter describes a novel strategy to calculate low energy elastic scattering. An artificial confining potential is added to the scattering Hamiltonian, and the discrete energies of this modified system are determined. We then show that two short-range potentials with the same energies in the confining potential have the same phase shifts when the confining potential is removed. This is similar to the box-variational method [7,9], where the energy inside an infinite-walled box is related to the phase shift. In its simplest form, the box-variational method requires the wave function, and thus the basis functions, to have a zero at the boundary (note that the logarithmic derivative at the boundary can, in principle, be set to any value). The $\ell = 0$ phase shifts for the nth positive energy state with energy E_n are then given by the identity $\delta_n = n\pi - R\sqrt{2E_n}$ [7]. In the present approach, almost any square integrable basis function can be used. Initially, we validate our strategy for scattering with a simple exponential potential. We then determine the low energy phase shifts for e^--He scattering to a higher degree of precision than any previous work [10–12] by using an explicitly correlated basis to generate the e^--He energies inside the confining potential.

The problem is to solve the Schrödinger equation

$$\left(-\frac{\nabla^2}{2} + V(r)\right)\Psi(r) = E\Psi(r) \qquad (1)$$

for $E > 0$. The central potential $V(r)$ will be assumed to be zero beyond some finite radius, say, R_0. Now consider the related equation

$$\left(-\frac{\nabla^2}{2} + V(r) + W_{\rm CP}(r)\right)\Psi(r) = E\Psi(r), \qquad (2)$$

where $W_{\rm CP}$ is a confining potential and E is defined relative to $V(r \to \infty)$. This potential has the property that $W_{\rm CP} \geq E$ as $r \to \infty$. We choose $W_{\rm CP} \sim O(r^n)$ $(n > 1)$ as $r \to \infty$. The potential $W_{\rm CP}(r)$ should have an analytic form which has easy to evaluate matrix elements. Second, $W_{\rm CP}(r)$ should be negligible for $r < R_0$. If these conditions are met, then it can be shown that the discrete energies E_i of the solution of Eq. (2) can be used to determine the phase shifts of Eq. (1) at those energies.

Consider a potential $V_0(r)$ for which Eq. (2) has an eigenvalue E_0. When $r > R_0$, the solution of Eq. (2) will become an exponentially decreasing solution $B\phi_0(r)$ when $E_0 < V_0(r) + W_{\rm CP}(r)$. The amplitude B will depend on the specifics of $V_0(r)$, but the actual radial dependence of $\phi_0(r)$ does not depend on the form of $V_0(r)$. Now consider the behavior of the wave function for $r < R_0$. One simply integrates the Schrödinger equation outward from the origin, and, since $W_{\rm CP}(r)$ is zero here, the functional form of the inner wave function $\Phi_0(r)$ will not be influenced by the form of $W_{\rm CP}(r)$. The eigenstate will then be

$$\Psi(r) = A\Phi_0(r)\ ;\ r < R_0, \qquad \Psi(r) = B\phi_0(r)\ ;\ r > R_0. \qquad (3)$$

The logarithmic derivatives of $\phi_0(r)$ and $\Phi_0(r)$ will agree at the matching radius. The constants A and B are chosen so that the overall normalization of $\Psi(r)$ is unity and that it is continuous at $r = R_0$.

Now consider the solution of Eq. (1) at $E = E_0$. When $r < R_0$, this will simply be $C\Phi_0(r)$ since the boundary condition at the origin depends only on E_0. At the boundary $r = R_0$, the phase shift δ is determined from the logarithmic derivative Γ:

$$\Gamma_{\Phi}(r) = \frac{1}{\Phi(r)} \frac{d\Phi}{dr}. \tag{4}$$

There is a general functional relation between Γ and δ that can be expressed formally as

$$\delta(E_0) = f(\Gamma_{\Phi}(R_0)). \tag{5}$$

However, the logarithmic derivative of $\phi_0(r)$ is exactly the same as that of $\Phi_0(r)$. The logarithmic derivative of $\phi_0(r)$ at $r = R_0$ is determined by E_0, and its functional dependence $g(E_0)$ does not depend on $V_0(r)$, so

$$\Gamma_{\Phi}(R_0) = \Gamma_{\phi}(R_0) = g(E_0). \tag{6}$$

Combining Eqs. (5) and (6), one can establish a functional relation between the energy E_0 and the phase shift, i.e.,

$$\delta(E_0) = f(g(E_0)). \tag{7}$$

One consequence of Eq. (7) is that Eq. (6) has no explicit functional dependence on the specifics of $V_0(r)$. While $g(E_0)$ depends on R_0, E_0, and the form of $W_{\mathrm{CP}}(r)$, it does not depend on $V_0(r)$. Therefore, if two potentials V_0 and V_1 in Eq. (2) have the same eigenenergy E_0, then their phase shifts (modulo π) will be the same at E_0. Provided the two wave functions have the same logarithmic derivative at $r = R_0$, it does not matter whether bound or continuum boundary conditions are imposed.

The phase shift of the complicated many-body problem can be determined directly from the energy of a bound state calculation. One just constructs a model potential that gives the same confined energy as the real many-body problem, then the confining potential is removed, and the model potential phase shift is computed. We call this approach to determining the scattering wave function the confined variational method (CVM).

This present strategy of using the energies within an artificial confining potential can be regarded as the culmination of a number of related approaches (apart from the box-variational method). For example, a confining potential was used to confine a scattering system, and the stochastic variational method (SVM) was used to optimize a basis of explicitly correlated Gaussians (ECGs) to describe the interaction region [13]. The basis was then used as a foundation for a stabilization calculation. Additionally, the energy shifts of positive energy pseudostates were used to tune a model potential which established the existence of a p-wave shape resonance in e^+-Mg scattering [14]. Finally, Guérout, Jungen, and Jungen [15] used a real confining potential to determine the solution of the Schrödinger equation for the internal region wave function within a multichannel quantum defect theory formalism.

The first test is to verify whether the primary proposition, namely, two short-range potentials with the same energy having the same phase shift, can be achieved in a practical numerical calculation. For this test, we choose

$$V_0(r) = -\exp(-1.4r), \tag{8}$$

$$V_1(r) = B(\exp(-r^2) + r\exp(-2r)). \tag{9}$$

The potential $V_0(r)$ represents the potential for some complicated many-body system, and it will not always be possible to determine its eigenenergies to infinite precision. The potential $V_1(r)$ is the adjustable potential that will be integrated to get the CVM phase shifts. The confining potential was defined as

$$W_{\mathrm{CP}}(r) = 0, \qquad r < R_0, \tag{10}$$

$$W_{\mathrm{CP}}(r) = G(r - R_0)^2, \qquad r > R_0, \tag{11}$$

with G set to 3×10^{-4} and $R_0 = 16$. The first derivative of the confining potential is zero at R_0. The energies of $(V_0 + W_{\mathrm{CP}})$ are determined by diagonalization in a basis of Laguerre-type orbitals (LTOs). The LTOs are defined by

$$\chi_{\alpha}(r) = N_{\alpha} r^{\ell+1} \exp(-\lambda_{\alpha} r) L^{(2\ell+2)}_{n_{\alpha}-\ell-1}(2\lambda_{\alpha} r), \tag{12}$$

and full details are available elsewhere [16]. The exponents λ_{α} were set to 2.0.

The energies of the diagonalization of the lowest state of V_0 are listed in Table I. The energy for the ith eigenstate for a basis of dimension N is denoted by $E_{i,N}$. The exact energy of the ith eigenstate is for all practical purposes given by $E_{\mathrm{exact},i} = E_{i,50}$. Integrating the Schrödinger equation for V_0 at $E_{1,N}$ gives $\delta_{\mathrm{exact},1,N}$.

The CVM phase shifts extracted from the energy of the ith state are denoted by $\delta_{\mathrm{CVM},i,N}$. The potential V_1 was diagonalized in the same LTO basis and B adjusted until the energy was equal to $E_{1,N}$. The phase shift $\delta_{\mathrm{CVM},i,N}$ was obtained by integrating V_1 with the tuned value of B. The phase shifts were also determined by evaluating the logarithmic derivative (at $r = R_0$) of the wave function resulting from the diagonalization of V_0 under W_{CP}. This approach is called the boundary condition (BC) method (the phase shifts are denoted by $\delta_{\mathrm{BC},i,N}$) and is essentially the approach adopted by Guérout, Jungen, and Jungen [15].

A striking result from Table I is the high accuracy of the CVM phase shifts. They are in agreement with the phase shifts obtained by integrating the Schrödinger equation for $V_0(r)$ to seven significant digits for $N > 30$. This accuracy was maintained for the phase shift extracted from the second lowest state.

TABLE I. The convergence of the energy and derived phase shift with respect to the dimension of the LTO basis set. A description of the phase shift entries can be found in the text.

N	$E_{1,N}$	$\delta_{\mathrm{exact},1,N}$	$\delta_{\mathrm{BC},1,N}$	$\delta_{\mathrm{CVM},1,N}$
20	0.008 105 924 660 3	0.477 396 5	0.530 962 7	0.477 394 5
25	0.006 045 691 902 6	0.431 086 4	0.493 142 2	0.431 085 8
30	0.005 629 924 168 6	0.419 939 5	0.414 794 1	0.419 939 5
40	0.005 607 701 459 6	0.419 323 0	0.419 474 8	0.419 323 0
50	0.005 607 701 142 2	0.419 323 0	0.419 357 2	0.419 323 0

The extreme accuracy is a consequence of the variational theorem. The energy of any variational wave function is accurate to the square of the error in the wave function, i.e., $\delta E \sim (\delta\Psi)^2$. The BC phase shifts in Table I are much less accurate than the CVM phase shifts. The BC method (and the approach of Guérout, Jungen, and Jungen [15]) relies on the precision of the local properties of the variational wave function and these are much less accurate than their global properties [17].

The CVM was then applied to e^--He scattering in the $^2S^e$ symmetry. The confining potential was chosen as $W_{\rm CP}(r) = 1.059\,942 \times 10^{-4}(r-18)^2$. This confining potential was chosen in order to keep the energy of the second eigenstate, i.e., E_2, close to $E_0 + 0.020$ a.u., where E_0 is the He ground state energy. This corresponds to $k = 0.2a_0^{-1}$ and made it easier to compare with previous calculations [10–12]. The imposition of the confining potential would increase the He energy of $-2.903\,724\,377\,0$ a.u. [18] by less than 10^{-15} a.u. The energies of the two lowest states were generated with the SVM which solves the Schrödinger equation in a basis of ECGs [13,19,20]. The energy being optimized was the mean of the two lowest energies, i.e., $E_{\rm opt} = (E_1 + E_2)/2$. Table II gives the energies of the second lowest state at various stages of the energy optimization.

The e^--He potential has a long-range polarization potential of the form $V_{\rm pol} \approx -\alpha_d/(2r^4)$. Helium has a dipole polarizability of $1.3832a_0^3$ [21]. The phase shift obtained from the CVM process strictly gives the phase shift at R_0. The value of $V_{\rm pol}(r = R_0)$ is -6.6×10^{-6} a.u. This can affect the derived phase shift at $k \approx 0.2a_0^{-1}$ at the 0.1% level. Polarization effects were included by using a tuning potential with the correct long-range form, specifically,

$$V_{\rm He}(r) = B\exp(-2r) - \frac{\alpha_d}{2r^4}[1-\exp(-r^6/\rho^6)], \tag{13}$$

where the parameter ρ was set to $\rho = 3a_0$. The formal justification presented earlier relies only on $W_{\rm CP}(r)$ being zero for $r < R_0$. The actual scattering potential can have a long-range component provided this component is also present in the tuning potential.

TABLE II. The convergence of the second lowest eigenstate of the confined e^--He system for the $^2S^e$ symmetry as a function of the number of ECGs N. The asymptotic momentum of the system k and derived phase shifts are also listed.

N	$E_{2,N}$ (a.u.)	$k_{2,N}$ (a_0^{-1})	$\delta_{{\rm CVM},2,N}$
600	−2.883 716 39	0.200 039 9	−0.266 58
800	−2.883 720 89	0.200 017 4	−0.265 72
1000	−2.883 722 51	0.200 009 3	−0.265 40
1200	−2.883 723 23	0.200 005 7	−0.265 26
With augmented basis			
640	−2.883 723 28	0.200 005 5	−0.265 25
840	−2.883 723 92	0.200 002 3	−0.265 13
1040	−2.883 724 14	0.200 001 2	−0.265 09
1240	−2.883 724 22	0.200 000 8	−0.265 07
KV [10]		0.20	−0.2655(6)
MCHF [11]		0.20	−0.2630
RM [12]		0.20	−0.265(1)

Table II also gives the phase shifts of the second lowest state. The parameter B of Eq. (13) was adjusted until the energy of $V_{\rm He}$ under $W_{\rm CP}$ was equal to $(E_{i,N} + E_0)$, where E_0 is the energy of the He ground state. The continuum Schrödinger equation for Eq. (13) was integrated to $500a_0$ to give the phase shift $\delta_{{\rm CVM},2,N}$.

Additional ECGs designed to represent an electron moving in the static potential of the He ground state were used to augment the basis and thus accelerate convergence. These basis functions were

$$\Psi^i_{\rm out} = \psi^{\rm He}(\mathbf{r}_1, \mathbf{r}_2)\exp(-\tfrac{1}{2}\alpha_i r_3^2), \tag{14}$$

$$\psi^{\rm He}(\mathbf{r}_1, \mathbf{r}_2) = \sum_k d_k F_k^{\rm He}(\mathbf{r}_1, \mathbf{r}_2). \tag{15}$$

The He ground wave function was written as a linear combination of 90 ECGs ($F_k^{\rm He}$). This basis gave $-2.903\,724\,33$ a.u. for the He ground state energy. A total of 40 electron Gaussians, defined by the relation $\alpha_i = 19.54/1.45^{i-1}$, multiplying the He ground state wave function were included. The energies $E'_{2,N}$ and derived phase shifts ($\delta'_{{\rm CVM},2,N}$) for the augmented basis are given in Table II.

The usefulness of the augmented basis is seen in Fig. 1, where the phase shifts $\delta_{\rm CVM}$ and $\delta'_{\rm CVM}$ for the different-sized basis sets are plotted. The horizontal axis gives the difference $\Delta E = |E'_{2,N} - E_{2,N}|$. This difference ΔE will tend to zero as the basis size increases. Continuation of the series of calculations would result in $\delta_{\rm CVM}$ and $\delta'_{\rm CVM}$ tending to a common intercept. The best phase shift from an explicit calculation was $\delta'_{\rm CVM}$ for the $N = 1240$ basis, which gave $-0.265\,07$ rad. The convergence pattern exhibited in Fig. 1 suggests that this phase shift is converged

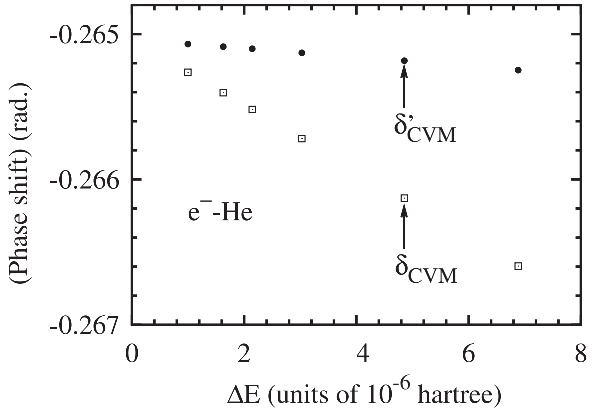

FIG. 1. The s-wave phase shifts for e^--He scattering at $k \approx 0.2a_0^{-1}$ plotted as function of ΔE for different-sized basis sets.

to better than 10^{-4} rad, and a conservative estimate of the $\Delta E \rightarrow 0$ limit would be $-0.265\,03(5)$ rad. This assumes no great deviation from the apparently linear behavior of $\delta_{\rm CVM}$ and $\delta'_{\rm CVM}$ with ΔE.

The variability in the energy at which the phase shifts are determined has only a small impact on the derived values of the phase shifts. The effective range expression $\tan(\delta) = -Ak$ suggests that the change in phase shift due to a momentum offset is $\Delta\delta \approx -A\Delta k$. The scattering length for e^--He scattering is about $-1.184(6)a_0$ [10]. A momentum offset of $10^{-5}a_0^{-1}$ leads to a change in phase shift of only 1.2×10^{-5} rad.

The present phase shift at $k = 0.2a_0^{-1}$, namely, $-0.265\,03$ rad, is the best estimate of the He phase shift yet determined. The long-range polarization potential that is based on second-order perturbation theory is a source of uncertainty. The usage of the polarization potential for $r > R_0$ increases the phase shift by about 0.000 19 rad. This correction should be reliable to better than 0.000 01 rad since the r^{-6} term in the polarization expansion involving the quadrupole (2.445 a.u.) and nonadiabatic dipole (0.7076 a.u.) polarizabilities is less than 0.5% of the magnitude of the r^{-4} dipole term at $r = 18a_0$.

There have been three large scale calculations aimed at giving definitive values for the low energy helium cross section. The Kohn variational (KV) calculations of Nesbet [10] used a basis of single particle orbitals centered on the nucleus to represent the target and scattering electrons. This is also true of the multiconfiguration Hartree-Fock (MCHF) calculation [11]. Another notable calculation was the R-matrix calculation (RM) by O'Malley, Burke, and Berrington [12]. The KV helium elastic cross section of Nesbet is often adopted as the theoretical benchmark cross section [22,23]. There is a 1% scatter among these three calculations with the KV phase shifts being the most negative. The present phase shift is 0.2% more positive than the KV phase shift. This is within the uncertainty of 0.24% estimated by Nesbet [10]. It is probably not coincidental that the KV elastic cross section is about 1% larger than experiment at $k = 0.2a_0^{-1}$ [23].

One source of uncertainty with our strategy is the value of the confining potential inner radius, namely, R_0. The present approach treats polarization effects for $r > R_0$ using second-order perturbation theory. The e^--H phase shift in the ${}^3S^e$ channel at $k = 0.20a_0^{-1}$ has been computed with two different confining potentials: one with $R_0 = 18a_0$ (using the second lowest energy) and the other with $R_0 = 22a_0$ (using the third lowest energy). The phase shifts were $-0.424\,09(1)$ and $-0.424\,10(4)$ rad, respectively. Although convergence in the wider confining potential was inhibited by linear dependency effects, the phase shifts are stable to better than 0.000 05 rad against a variation in R_0. The best previous determination of this phase shift was $-0.4242(2)$ rad [24].

In summary, a strategy for extracting phase shifts from bound state calculations is presented. The phase shift for the e^--He system is an order of magnitude more precise than those reported previously [10–12]. The strategy can be adapted to almost any method that diagonalizes the Schrödinger equation in a square integrable basis, and it can be applied to target systems which are themselves many-body systems.

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