

Positronium-positronium scattering using the stochastic variational method

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The stochastic variational method is used in conjunction with stabilization ideas to compute the low-energy *s*-wave phase shifts and scattering lengths for Ps-Ps scattering. The scattering lengths obtained were $8.44a_0$ for the singlet-singlet and $3.00a_0$ for the triplet-triplet states (the spin state refers to the coupling of the two electrons and the coupling of the two positrons in the system). The positive scattering length in the triplet-triplet channel means a stable Bose-Einstein condensate of triplet Ps atoms is physically possible. The large value of the ${}^3\text{Ps}^3\text{Ps} \rightarrow {}^1\text{Ps}^1\text{Ps}$ cross section, $7.41\pi a_0^2$ suggests the use of spin-polarized positrons as advanced by Platzmann and Mills [Phys. Rev. B **49** 454 (1994)].

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I. INTRODUCTION

The Bose-Einstein condensation (BEC) phenomenon has received considerable attention both from theoretical and experimental points of view [1,2] since it is one of a very few known examples of the direct manifestation of quantum effects on the macroscopic scale. Originally, the BEC phenomenon arose in connection with superfluidity and superconductivity phenomena. Later it was recognized that BEC might occur in different areas of physics, e.g., symmetry breaking from the Higgs boson in the guise of a top quark condensate [7].

One of the most startling recent experimental achievements has been the development of gas-phase BECs. The last few years has seen the development of BECs made of a number of alkali atoms and atomic hydrogen [1,2]. These BECs were made possible by the development of experimental techniques, particularly in the area of atomic cooling [3–6].

Just recently, there has been serious interest in the possibility of creating a BEC containing antimatter [8–10]. The first proposals for such a BEC were made about a decade ago [11,12], when it was suggested that it might be feasible to create a BEC from positronium (Ps) atoms. Such system would provide an example of a matter-antimatter condensate. Besides the intrinsic interest, and its importance for BEC physics, study of the BEC of Ps atoms would contribute to the study of Ps atom itself, and eventually to a better understanding of the weak interaction [8,9].

The traditional way to create a BEC in a low-temperature gas involves the trapping and cooling of the atoms inside a region of space illuminated by several lasers. This experiment would be very difficult to perform since positronium has a finite lifetime before electron-positron annihilation takes place. Ground-state positronium in the singlet state,

${}^1\text{Ps}$ annihilates at a rate of $8.0325 \times 10^9 \text{ sec}^{-1}$. The triplet state mainly decays by a process involving the emission of 3 γ quanta at a rate of $7.9852 \times 10^6 \text{ sec}^{-1}$. For this reason, it has been suggested that a Ps condensate might be realized by confining the Ps in a very small cavity in very cold silicon [12]. Basically, the idea is to direct a spin-polarized positron beam into the surrounding silicon with the expectation that some of the positrons will be emitted into the cavity in the form of positronium. The positronium can be expected to cool by colliding with the walls of the cavity. Since Ps is very light, it can be expected to form Ps at much less severe density/temperature regimes than the usual alkali atom condensates. The BEC that is formed will be composed of ${}^3\text{Ps}$ since this has a lifetime that is 1000 times longer than ${}^1\text{Ps}$. Spin-polarized positrons should be used since mutual spin conversion through the ${}^3\text{Ps}^3\text{Ps} \rightarrow {}^1\text{Ps}^1\text{Ps}$ reaction would otherwise lead to the removal of ${}^3\text{Ps}$ even in a gas consisting of 100% ${}^3\text{Ps}$. The use of spin-polarized positrons will eventually lead to a gas of spin-polarized Ps, which does not undergo the mutual spin-conversion reaction. The viability of forming the condensate depends on various factors such as the momentum-transfer cross section with the walls of the cavity, the annihilation rate during collisions with the walls, and the scattering cross sections for Ps-Ps collisions. We also note that there have also been proposals to form a Ps BEC by laser cooling [10].

Knowledge of the Ps-Ps scattering cross sections is useful in designing an experimental configuration to trap Ps and form the BEC. In the first instance, it is vitally important that the scattering lengths for the various Ps-Ps scattering systems be known. After all, the formation of a stable BEC requires a positive scattering length. In the case of a Ps-Ps condensate, it is also useful to know the cross sections for the ${}^3\text{Ps}^3\text{Ps} \rightarrow {}^1\text{Ps}^1\text{Ps}$ process since this determines whether the condensate should be formed using spin-polarized positrons (or electrons) [8,12,13].

From the point of view of scattering theory, an *ab initio* calculation of Ps-Ps scattering presents some serious major technical problems. The source of the difficulty lies in the fact that both the projectile and the target are composite objects with an internal structure. This means that the interaction matrix elements involve multicenter integrals which are

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difficult and time consuming to evaluate [14]. Recently, the stochastic variational method (SVM) [15–19] has been adapted to perform scattering calculations in the kinematic region where only elastic scattering is possible [20]. The method is particularly useful for handling systems containing two composite objects. The SVM uses explicitly correlated Gaussians (ECGs) as basis functions and the multicenter integrals that are normally so difficult to evaluate can be computed relatively easy. The SVM has recently been applied to the calculation of a number of Ps-atom scattering problems [20,21]. Notably, an *ab initio* calculation of the Ps-H scattering, and a series of semiempirical calculations of Ps scattering from the lighter rare gases, He, Ne, and Ar [22].

The scattering of two Ps atoms has received very little attention in the atomic physics literature until very recently [20]. An initial investigation of Ps-Ps scattering was performed using the SVM and phase shifts reported for two spin configurations. These were for the spin configuration with both electrons and both positrons in a singlet state, and the configuration having both electrons and both positrons in a triplet state (this latter configuration corresponds to ^3Ps - ^3Ps scattering with all spins aligned). The singlet-singlet scattering length was $8.4a_0$, while the triplet-scattering length was $2.95a_0$. Oda *et al.* used a semiempirical methods to reliably deduce the Ps-Ps scattering length in the singlet channel [9].

However, the positronium atom has a condensed-matter analogue, the exciton which consists of an electron-hole bound state. Exciton-exciton scattering is identical with Ps-Ps when the electron and hole have effective masses the same as the electron and the effective interaction is computed directly from the interparticle Coulomb interactions. The exciton-exciton scattering system has received some attention in the past [23,24], and most recently, a very thorough treatment was performed with the quantum Monte Carlo (QMC) method [25]. The QMC phase shifts for the special case equivalent to Ps-Ps scattering gave a scattering length of $(9.15 \pm 0.04)a_0$ for the singlet-singlet case and $(3.02 \pm 0.06)a_0$ for the triplet-triplet case [25].

In the present paper, a more detailed and thorough study of the Ps-Ps scattering system is reported. The SVM calculation is performed with a larger and more carefully chosen basis, giving an improved description of the phase shifts. The results of the present investigation are largely compatible with our initial calculations and the QMC calculations of Shumway and Ceperley [25]. Knowledge of the phase shifts is important since they give information about the stability and cooling conditions of the condensate and also determine the rate at which the Ps gas will collapse into spin-polarized positronium [8,12,13].

II. CALCULATION SCHEME

A. Determination of the primary phase shifts

The Hamiltonian of the Ps-Ps system is

$$\hat{H} = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{1}{2}\nabla_3^2 - \frac{1}{2}\nabla_4^2 + \frac{1}{r_{13}} + \frac{1}{r_{24}} - \frac{1}{r_{14}} - \frac{1}{r_{12}} - \frac{1}{r_{34}} - \frac{1}{r_{23}}, \quad (1)$$

where $\mathbf{r}_1, \mathbf{r}_3$ are the positrons coordinates and $\mathbf{r}_2, \mathbf{r}_4$ are the electrons coordinates. It is necessary to solve this equation at energies above the Ps($1s$)-Ps($1s$) threshold.

The method used to determine the phase shifts and scattering wave functions uses the stochastic variational method [15–19]. The present method is based upon stabilization ideas which suggest that the positive energy pseudostates resulting from a diagonalization of the interaction Hamiltonian give a reasonable approximation to the exact scattering wave function [26–29]. A complete description has been given elsewhere [20], so only a short summary is presented here.

Configuration space is divided into two regions, an inner or interaction region and an outer or scattering region. In the inner region, the stochastic variational method is used to define an ECG basis (dimension = K) that gives an accurate solution of the Schrödinger equation for the lowest-energy state. The ECG basis functions are written as (properly symmetrized) combinations of the functions

$$\begin{aligned} \Psi &= \sum_i^K C_i \psi_{s^+, m^+, s^-, m^-}(\mathbf{x}, A^i) \\ &= \sum_i^K C_i G(\mathbf{x}, A^i) \chi_{s^+, m^+, s^-, m^-}. \end{aligned} \quad (2)$$

The spatial parts of basis functions were written as explicitly correlated Gaussians (ECGs) [16], i.e.,

$$G(\mathbf{x}, A^i) = \exp\left(-\frac{1}{2} \sum_{\mu, \nu=1}^{N-1} A_{\mu\nu}^i \mathbf{x}_\mu \mathbf{x}_\nu\right) = \exp\left(-\frac{1}{2} \mathbf{x}^T A^i \mathbf{x}\right). \quad (3)$$

The \mathbf{x}_μ are the set of Jacobi coordinates for the Ps₂ system. The matrix $A_{\mu\nu}^i$ must satisfy certain requirements so that the basis functions (3) are square integrable. The details of transformation to the set of Jacobi coordinates, excluding center-of-mass motion, and the detailed form of the requirements imposed upon the matrix $A_{\mu\nu}^i$ have been discussed elsewhere [16]. In cases where the scattering system supports a bound state, the inner wave function is determined by doing a standard SVM calculation to minimize the energy. A slightly different procedure is adopted when the system does not support a bound state. Once again, an energy minimization is done, but in this case the exponents, α_i of the Gaussians containing interparticle distances are restricted to be larger than a certain minimum size, say $\alpha_i > 0.01$. This constrains the particles to be localized reasonably close to each other and results in a SVM iteration procedure that effectively solves the Schrödinger equation in some sort of box. The purpose of the inner basis of dimension K is to give a good representation of the interparticle interactions when the Ps atoms are close together.

Once the inner wave functions have been obtained, a set of ECGs designed to represent the positive energy Ps+Ps breakup was added to the basis. First an eight Gaussian representation of the Ps ground state was constructed (the energy obtained was $-0.249\,997\,23$ hartree). Then a series of

ECGs were constructed by multiplying the Ps Gaussians together with an additional Gaussian with the relative Ps-Ps distance as its argument. Thus, the outer basis functions were constructed from a (properly symmetrized) set of the functions

$$\Psi_{out}^{ijk} = \exp(-\alpha_i R^2) \phi_{Ps}^j(\mathbf{r}_1, \mathbf{r}_2) \phi_{Ps}^k(\mathbf{r}_3, \mathbf{r}_4), \quad (4)$$

where R is the relative distance between the respective Ps centers of mass. The $\phi_{Ps}^i(\mathbf{r}_i, \mathbf{r}_j)$ are individual Gaussians from the superposition used to represent the Ps state. The exponents of the center-of-mass Gaussians, i.e., α_i were chosen to form an even-tempered sequence obeying

$$\alpha_i = \frac{\alpha_1}{T^{i-1}}. \quad (5)$$

The center-of-mass exponents were chosen to span the range of R just outside the interaction region. Experience from the previous calculations [20–22] suggests that sensible values for the ratio T range from 1.3–2, with the smaller values of the ratio generally producing better results. The inner and outer basis are then merged, and the Hamiltonian diagonalized after basis states that could lead to linear dependence and numerical instability were purged from the basis. To extract the phase shifts from the pseudostates, the positron-positron correlation function defined as

$$C(x) = 4\pi x^2 \int d^3x_i \delta(\mathbf{r}_1 - \mathbf{r}_3 - \mathbf{x}) |\Phi(\mathbf{r}_i)|^2 \quad (6)$$

(where the integration is performed over all Jacobi coordinates excluding the center of mass) was computed for a succession of x values and fitted to $B \sin^2(kx + \delta_0)$ over the $x \in [15, 30]a_0$ interval. This region was chosen since it lies outside the charge clouds of the two interacting Ps atoms and the $1/R^6$ van der Waals interaction is also small here.

There are a number of possible spin states to be considered. When it comes to diagonalizing the Hamiltonian, the most convenient representation is to write the spin states as

$$\chi_{s^+, m^+, s^-, m^-} = |e_1^+ e_3^+ [s^+, m^+] e_2^- e_4^- [s^-, m^-]\rangle, \quad (7)$$

where $e_{1,3}^+$ and $e_{2,4}^-$ refer to the positron and electron spins, and $[s^{\pm+}, m^{\pm+}]$ refers to the total spin of the two-lepton pair. The Hamiltonian itself is invariant with respect to the values of m^- and m^+ and so the phase shift in this representation only depends on the value of s^+ and s^- . A complete description of s -wave scattering only requires that the Hamiltonian be diagonalized in the representations corresponding to the singlet-singlet ($s^+ = 0, s^- = 0$) and triplet-triplet ($s^+ = 1, s^- = 1$) spin combinations. The ($s^+ = 0, s^- = 1$) and ($s^+ = 1, s^- = 0$) spin combinations would mean the total spin wave function was symmetric for electron-electron or positron-positron interchange. Therefore, the spatial part of the wave function would be antisymmetric with respect to electron-electron interchange or positron-positron interchange. This antisymmetric spatial wave function would

mean the spatial part of the total wave function was also antisymmetric under the 1,2→3,4 interchange. Such a wave function would have a nodal surface and therefore would not describe s -wave scattering. The phase shift corresponding to the ($s^+ = 0, s^- = 0$) configuration is designated δ_0 and the phase shift corresponding to the ($s^+ = 1, s^- = 1$) configuration denoted as δ_1 . The ($s^+ = 1, s^- = 1$) configuration can be coupled to a total spin of 0, 1, or 2 and all of these couplings can contribute to s -wave scattering.

B. Transformation to the scattering representation

The representation used to diagonalize the Hamiltonian and extract the phase shifts is not the same as the spin-coupling representation describing the scattering states. The scattering states consist of two outgoing (incoming) positronium states. The electrons and positrons in the scattering states are first coupled to each other, to form either ^1Ps or ^3Ps , and then the two Ps atoms are coupled to determine the total spin of the scattering system. The physical scattering states are written as $|\text{Ps}[S_1]\text{Ps}[S_2]; SM_S\rangle$ and constructed in terms of the linear combinations of different spin substates, e.g., $|e_1^+ e_2^- [S_1] e_3^+ e_4^- [S_2]; SM_S\rangle$. The state vectors corresponding to the SVM coupling scheme and the scattering states are connected by the standard recoupling formula

$$\begin{aligned} & |e_1^+ e_3^+ [s^+] e_2^- e_4^- [s^-] S\rangle \\ &= \sum_{S_3, S_4} \sqrt{(2s^+ + 1)(2s^- + 1)(2S_3 + 1)(2S_4 + 1)} \\ & \times \begin{Bmatrix} 1/2 & 1/2 & S_3 \\ 1/2 & 1/2 & S_4 \\ s^+ & s^- & S \end{Bmatrix} |e_1^+ e_2^- [S_3] e_3^+ e_4^- [S_4] S\rangle. \quad (8) \end{aligned}$$

The T -matrix elements for the scattering states are linear combinations of the T -matrix elements that arise from the diagonalization of the Hamiltonian in the $|e_1^+ e_3^+ [s^+, m^+] e_2^- e_4^- [s^-, m^-]\rangle$ representation. The T -matrix in the $|e_1^+ e_3^+ [s^+, m^+] e_2^- e_4^- [s^-, m^-]\rangle$ representation does not depend on m^+ or m^- and this certainly simplifies the analysis.

The statistics of the scattering states means that only certain spin combinations can occur for s -wave scattering. The spin part of the wave functions should be symmetric with respect to the transformation interchanging coordinates of both electrons and both positrons (this is physically equivalent to interchanging the two Ps atoms). If this is not the case, then the coordinate part of the wave function would be antisymmetric with respect to this transformation. An antisymmetric orbital wave would then have a nodal surface and could not therefore correspond to s -wave scattering.

The $|\text{Ps}[0]\text{Ps}[0]\rangle$ and $|\text{Ps}[1]\text{Ps}[1]\rangle$ systems involve the collision of two identical bosons. Therefore, they can undergo s -wave scattering through the $S=0$ and $S=2$ channels, viz.

$$\begin{aligned}
|\text{Ps}[0]\text{Ps}[0];0\rangle &= |e_1^+ e_2^- [1] e_3^+ e_4^- [1];0\rangle \\
&= \frac{1}{2} |e_1^+ e_3^+ [0] e_2^- e_4^- [0];0\rangle \\
&\quad + \sqrt{\frac{3}{2}} |e_1^+ e_3^+ [1] e_2^- e_4^- [1];0\rangle, \\
|\text{Ps}[1]\text{Ps}[1];0\rangle &= |e_1^+ e_2^- [1] e_3^+ e_4^- [1];0\rangle \\
&= \sqrt{\frac{3}{2}} |e_1^+ e_3^+ [0] e_2^- e_4^- [0];0\rangle \\
&\quad - \frac{1}{2} |e_1^+ e_3^+ [1] e_2^- e_4^- [1];0\rangle, \quad (9)
\end{aligned}$$

$$\begin{aligned}
|\text{Ps}[1]\text{Ps}[1];2\rangle &= |e_1^+ e_3^- [1] e_2^+ e_4^- [1];2\rangle \\
&= |e_1^+ e_3^+ [1] e_2^- e_4^- [1];2\rangle.
\end{aligned}$$

Scattering of identical bosons through the $S=1$ total spin channel can only occur through the p and other odd partial waves.

The $|\text{Ps}[1]\text{Ps}[0]\rangle$ collision is best analyzed by writing the wave function as a symmetric or antisymmetric collision system:

$$\begin{aligned}
|\text{Ps}[0]\text{Ps}[1];1\rangle_{\text{Sym}} &= \frac{1}{\sqrt{2}} (|e_1^+ e_2^- [1] e_3^+ e_4^- [0];1\rangle \\
&\quad + |e_1^+ e_2^- [0] e_3^+ e_4^- [1];1\rangle) \\
&= |e_1^+ e_3^+ [1] e_2^- e_4^- [1];1\rangle, \\
|\text{Ps}[0]\text{Ps}[1];1\rangle_{\text{Antisym}} &= \frac{1}{\sqrt{2}} (|e_1^+ e_2^- [1] e_3^+ e_4^- [0];1\rangle \\
&\quad - |e_1^+ e_2^- [0] e_3^+ e_4^- [1];1\rangle). \quad (10)
\end{aligned}$$

Only the symmetric combination corresponds to s -wave scattering. A table expressing information equivalent to Eqs. (9) and (10) has been given previously [25].

The partial cross sections for the s -wave scattering of identical Ps atoms in terms of the phase-shifts δ_0 and δ_1 are

$$\begin{aligned}
\sigma_{00\rightarrow00}^{S=0} &= \frac{8\pi}{k^2} \left[\frac{1}{4} \sin^2(\delta_0) + \frac{3}{4} \sin^2(\delta_1) - \frac{3}{16} \sin^2(\delta_0 - \delta_1) \right], \\
\sigma_{11\rightarrow11}^{S=0} &= \frac{8\pi}{k^2} \left[\frac{3}{4} \sin^2(\delta_0) + \frac{1}{4} \sin^2(\delta_1) - \frac{3}{16} \sin^2(\delta_0 - \delta_1) \right], \\
\sigma_{11\rightarrow00}^{S=0} &= \frac{8\pi}{k^2} \left[\frac{3}{16} \sin^2(\delta_0 - \delta_1) \right], \\
\sigma_{11\rightarrow11}^{S=2} &= \frac{8\pi}{k^2} \sin^2(\delta_1). \quad (11)
\end{aligned}$$

In these expressions, the total spin is given as the superscript

while the subscripts denote the spin of the incoming Ps pair and the outgoing Ps pair. The factor of 8π (instead of the usual 4π) arises because it is not possible to distinguish projectile and target when two identical bosons scatter [2,31,32].

The case of ^1Ps and ^3Ps involves distinguishable particle scattering and the cross section is written as

$$\sigma_{01\rightarrow01}^{S=1} = \frac{4\pi}{k^2} \sin^2(\delta_1). \quad (12)$$

The multiplying factor of 4π for $\sigma_{01\rightarrow01}^{S=1}$ is the result of two factors. First, the multiplying factor should be 4π since the scattering particles are distinguishable. Second, although the physical scattering state is written in terms of a linear combination of symmetric and antisymmetric states, there are two possible exit states, $|e_1^+ e_2^- [1] e_3^+ e_4^- [0];1\rangle$ and $|e_1^+ e_2^- [0] e_3^+ e_4^- [1];1\rangle$ so this aspect has no impact on the cross section.

Although the present analysis was done independently of Shumway and Ceperley [25], the expressions in Eq. (11) are essentially the same as those given in Table II of Shumway and Ceperley (their table entries for $\sigma_{01\rightarrow01}^{S=1}$ are a bit confusing and it is not clear whether they calculated this cross section correctly).

The total elastic s -wave cross section for ^3Ps - ^3Ps scattering and the total cross section for ^3Ps - ^1Ps spin conversion are

$$\begin{aligned}
\sigma_{11\rightarrow11} &= \frac{8\pi}{k^2} \left[\frac{1}{8} \sin^2(\delta_0) + \frac{7}{8} \sin^2(\delta_1) - \frac{1}{32} \sin^2(\delta_0 - \delta_1) \right], \\
\sigma_{11\rightarrow00} &= \frac{\pi}{4k^2} \sin^2(\delta_0 - \delta_1). \quad (13)
\end{aligned}$$

These represent the spin average of the $\sigma^{S=0}$ and $\sigma^{S=2}$ partial cross sections (the spin conversion reaction has no flux through the $\sigma^{S=2}$ channel). In the limit of zero momenta, Eqs. (11) and (13) simplify to

$$\begin{aligned}
\sigma_{00\rightarrow00}^{S=0} &= 8\pi \left(\frac{1}{4} A_0 + \frac{3}{4} A_1 \right)^2, \\
\sigma_{11\rightarrow11}^{S=0} &= 8\pi \left(\frac{3}{4} A_0 + \frac{1}{4} A_1 \right)^2, \\
\sigma_{11\rightarrow00}^{S=0} &= 8\pi \frac{3}{16} (A_0 - A_1)^2, \\
\sigma_{01\rightarrow01}^{S=1} &= 4\pi A_1^2, \\
\sigma_{11\rightarrow11}^{S=2} &= 8\pi A_1^2, \\
\sigma_{11\rightarrow11} &= 8\pi \left(\frac{3}{32} A_0^2 + \frac{27}{32} A_1^2 + \frac{1}{16} A_0 A_1 \right), \quad (14)
\end{aligned}$$

$$\sigma_{11 \rightarrow 00} = \frac{\pi}{4} (A_0 - A_1)^2,$$

where A_0 , A_1 are the singlet-singlet and triplet-triplet scattering lengths defined in the usual way. The effective range relation used to determine scattering lengths is described in the next section.

An experiment to form the Ps BEC will probably be done with polarized electrons with the goal of obtaining a gas of spin-aligned Ps. Therefore, for reasons of completeness, the cross sections are also given in a representation in which the states are labeled by the individual spins and spin projections of the two Ps atoms S_1, M_1, S_2, M_2 . The manifold of states with $M_S = M_1 + M_2 = 0$ is the most important since the mutual spin conversion of ^3Ps to ^1Ps goes through this channel. The scattering channels, in the $|\text{Ps}[S_1 M_1]\text{Ps}[S_2 M_2]\rangle$ representation can be written using obvious notation as

$$\begin{aligned} |\text{Ps}[1,1]\text{Ps}[1,-1]\rangle &= \frac{1}{\sqrt{2}} (|e_1^+ e_2^- [1,1] e_3^+ e_4^- [1,-1]\rangle \\ &\quad + |e_1^+ e_2^- [1,-1] e_3^+ e_4^- [1,1]\rangle) \\ &= \frac{1}{\sqrt{2}} |e_1^+ e_3^+ [0] e_2^- e_4^- [0]; 00\rangle \\ &\quad - \frac{1}{\sqrt{6}} |e_1^+ e_3^+ [1] e_2^- e_4^- [1]; 00\rangle \\ &\quad + \frac{1}{\sqrt{3}} |e_1^+ e_3^+ [1] e_2^- e_4^- [1]; 20\rangle, \\ |\text{Ps}[00]\text{Ps}[10]\rangle &= \frac{1}{\sqrt{2}} (|e_1^+ e_2^- [0,0] e_3^+ e_4^- [1,0]\rangle \\ &\quad + |e_1^+ e_2^- [1,0] e_3^+ e_4^- [0,0]\rangle) \\ &= |e_1^+ e_3^+ [1] e_2^- e_4^- [1]; 10\rangle, \\ |\text{Ps}[00]\text{Ps}[00]\rangle &= |e_1^+ e_2^- [0,0] e_3^+ e_4^- [0,0]\rangle \\ &= \frac{1}{2} |e_1^+ e_3^+ [0] e_2^- e_4^- [0]; 00\rangle \\ &\quad + \sqrt{\frac{3}{2}} |e_1^+ e_3^+ [1] e_2^- e_4^- [1]; 00\rangle, \\ |\text{Ps}[10]\text{Ps}[10]\rangle &= |e_1^+ e_2^- [1,0] e_3^+ e_4^- [1,0]\rangle \\ &= -\frac{1}{2} |e_1^+ e_3^+ [0] e_2^- e_4^- [0]; 00\rangle \\ &\quad + \frac{1}{\sqrt{12}} |e_1^+ e_3^+ [1] e_2^- e_4^- [1]; 00\rangle \\ &\quad + \sqrt{\frac{2}{3}} |e_1^+ e_3^+ [1] e_2^- e_4^- [1]; 20\rangle. \end{aligned} \tag{15}$$

The transformations implied by these formulas gives the set of cross sections $\sigma_{S_1 M_1, S_2 M_2 \rightarrow S'_1 M'_1 S'_2 M'_2}$. These cross sections are labeled with $M_1 \leq M_2$ and $M'_1 \leq M'_2$ since the state vectors $|\text{Ps}[S_1 M_1]\text{Ps}[S_2 M_2]\rangle$ and $|\text{Ps}[S_2 M_2]\text{Ps}[S_1 M_1]\rangle$ represent the same physical states.

$$\begin{aligned} \sigma_{00,00 \rightarrow 00,00} &= \frac{8\pi}{k^2} \left[\frac{1}{4} \sin^2(\delta_0) + \frac{3}{4} \sin^2(\delta_1) - \frac{3}{16} \sin^2(\delta_0 - \delta_1) \right], \\ \sigma_{10,10 \rightarrow 10,10} &= \frac{8\pi}{k^2} \left[\frac{1}{4} \sin^2(\delta_0) + \frac{3}{4} \sin^2(\delta_1) - \frac{3}{16} \sin^2(\delta_0 - \delta_1) \right], \\ \sigma_{1-1,11 \rightarrow 1-1,11} &= \frac{8\pi}{k^2} \left[\frac{1}{2} \sin^2(\delta_0) + \frac{1}{2} \sin^2(\delta_1) \right. \\ &\quad \left. - \frac{1}{4} \sin^2(\delta_0 - \delta_1) \right], \\ \sigma_{00,10 \rightarrow 00,10} &= \frac{4\pi}{k^2} \sin^2(\delta_1), \\ \sigma_{10,10 \rightarrow 00,00} &= \frac{\pi}{k^2} \frac{1}{2} \sin^2(\delta_1 - \delta_0), \\ \sigma_{1-1,11 \rightarrow 00,00} &= \frac{\pi}{k^2} \sin^2(\delta_1 - \delta_0), \\ \sigma_{1-1,11 \rightarrow 10,10} &= \frac{\pi}{k^2} \sin^2(\delta_1 - \delta_0). \end{aligned} \tag{16}$$

One of the equations (16) (the fourth) involves Ps atoms in different spin states and therefore the multiplying factor in this case is 4π . Cross sections for the forward and backward reactions are the same since all initial and final states have the same multiplicity. Cross sections for processes that are trivially the same as those presented above, e.g., $\sigma_{1-1,1-1 \rightarrow 00,00}$ are not listed.

The manifold of $M_S = 1$ s -wave states consists of two members

$$\begin{aligned} |\text{Ps}[00]\text{Ps}[11]\rangle &= \frac{1}{\sqrt{2}} (|e_1^+ e_2^- [0,0] e_3^+ e_4^- [1,1]\rangle \\ &\quad + |e_1^+ e_2^- [1,1] e_3^+ e_4^- [0,0]\rangle) \\ &= |e_1^+ e_3^+ [1] e_2^- e_4^- [1]; 11\rangle, \\ |\text{Ps}[10]\text{Ps}[11]\rangle &= \frac{1}{\sqrt{2}} (|e_1^+ e_2^- [1,0] e_3^+ e_4^- [1,1]\rangle \\ &\quad + |e_1^+ e_2^- [1,1] e_3^+ e_4^- [1,0]\rangle) \\ &= |e_1^+ e_3^+ [1] e_2^- e_4^- [1]; 21\rangle, \end{aligned} \tag{17}$$

with cross sections given by

$$\sigma_{00,11 \rightarrow 00,11} = \frac{4\pi}{k^2} \sin^2(\delta_1),$$

$$\sigma_{10,11 \rightarrow 10,11} = \frac{8\pi}{k^2} \sin^2(\delta_1). \quad (18)$$

The manifold of $M_S=2$ s -wave channels is trivial since it consists of only one member, $|\text{Ps}[11]\text{Ps}[11]\rangle$. The cross section of the only possible elastic-scattering process is

$$\sigma_{11,11 \rightarrow 11,11} = \frac{8\pi}{k^2} \sin^2(\delta_1). \quad (19)$$

It is easy to verify that total triplet-triplet scattering cross section, which is defined as

$$\begin{aligned} \sigma_{11 \rightarrow 11} &= \frac{1}{N} \sum_{M_1 \leq M_2, M_3 \leq M_4} \sigma_{1, M_1, 1, M_2 \rightarrow 1, M_3, 1, M_4} \\ &= \frac{1}{6} (\sigma_{10,10 \rightarrow 10,10} + \sigma_{10,10 \rightarrow 11,1-1} + \sigma_{10,11 \rightarrow 10,11} \\ &\quad + \sigma_{1-1,10 \rightarrow 1-1,10} \sigma_{1-1,11 \rightarrow 1-1,11} + \sigma_{1-1,11 \rightarrow 10,10} \\ &\quad + \sigma_{11,11 \rightarrow 11,11} + \sigma_{1-1,1-1 \rightarrow 1-1,1-1}), \end{aligned} \quad (20)$$

reproduces Eq. (13) if the expressions in Eqs. (16), (18), and (19) are substituted for the cross sections. Similarly, the triplet-singlet spin conversion reaction defined as

$$\begin{aligned} \sigma_{11 \rightarrow 00} &= \frac{1}{N} \sum_{M_1 \leq M_2} \sigma_{1, M_1, 1, M_2 \rightarrow 0,0,0,0} \\ &= \frac{1}{6} (\sigma_{10,10 \rightarrow 00,00} + \sigma_{1-1,11 \rightarrow 00,00}) \end{aligned} \quad (21)$$

also reproduces Eq. (13) if expressions from Eqs. (16) are substituted into Eq. (21).

III. PHASE SHIFTS AND CROSS SECTIONS

One of the problems with the present L^2 approach to Ps-H scattering is that the phase shifts δ_0 and δ_1 are computed at different energies that cannot be determined in advance. This means that the L^2 phase shifts cannot be combined directly to compute the cross sections. In order to compute cross sections it is necessary to fit δ_0 and δ_1 to an effective range expansion [32,33]. For Ps-Ps scattering, this expansion can be written

$$k \cot \delta_i(k) = -\frac{1}{A_i} + \frac{1}{2} r_i k^2 + O(k^3), \quad (22)$$

where $i=0,1$ for singlet-singlet and triplet-triplet cases, respectively. The cross sections are then computed directly from the effective range expansion.

The scattering lengths reported in [20] only included the $-1/A_i$ term in the fit. The scattering lengths reported in the present paper can be regarded as superseding those published in [20] since the basis sets were larger and the effective range was also included in the fitting procedure.

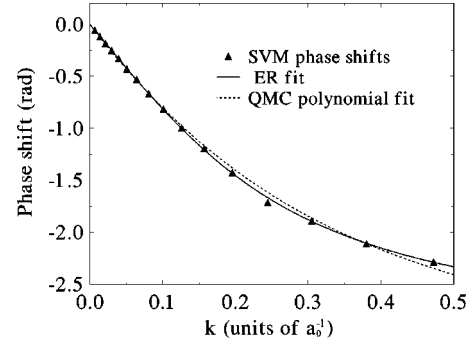


FIG. 1. The singlet-singlet phase shift δ_0 as a function of k (modulo π). The up triangles are the explicitly calculated phase shifts and the solid line is the effective range fit to those phase shifts using the values given in Table I. The dashed line gives the QMC phase shifts from the polynomial fit given by Eq. (23) [25].

A. Singlet-singlet scattering

The Hamiltonian for the singlet-singlet spin combination supports a bound state, the well-known Ps_2 molecule. An optimized basis of dimension $K=350$ gave a Ps_2 binding energy of 0.016 003 4 hartree. This is in very good agreement with the current best estimate of the binding energy, namely, 0.016 003 7 hartree [16]. The outer basis had the following specifications, $\alpha_1=1.0$, $T=1.5$, the smallest value of exponent was $\alpha_{25}=5.94 \times 10^{-5}$, giving a total of 900 additional basis functions. The final basis had a dimension of $M=1230$ once functions leading to possible linear dependence were removed.

The phase shifts derived from these calculations are shown in Fig. 1 as is the effective range fit to the phase shifts. The effective ranges parameters were $A_0=8.44a_0$ and $r_0=4.76a_0$. These values were obtained by fitting all phase shifts in the range $k \in [0, 0.5]a_0^{-1}$ to Eq. (22). It can be seen from Fig. 1 that the effective range formula gives an excellent fit to the directly computed phase shifts.

The scattering length obtained from the fit appears to be highly reliable. The stability of the scattering length was tested by performing additional fits using different subsets of the phase shifts in the $k \in [0, 0.5]a_0^{-1}$ range. For example, using the points in the $k \in [0, 0.3]a_0^{-1}$ interval gave $A_0=8.41a_0$ and $r_0=4.82a_0$. Other variations of the calculation have been done, such as changing the specifications of the inner and outer basis, and changing the range over which the phase shifts were extracted from the correlation functions. The variations of the scattering length for these different calculations was less than 1%. Accordingly, conservative estimates of the uncertainties in the scattering length and effective range would be 2 and 10%, respectively.

Figure 1 also shows phase shifts of the quantum Monte Carlo calculation performed by Shumway and Ceperley [25]. The phase shifts that are shown are not the directly computed phase shifts, rather, they were taken from their polynomial representation of δ_0 ,

$$\delta_0(k) = \pi - 9.148k + 11.98k^2 - 6.632k^3. \quad (23)$$

TABLE I. The scattering length and effective range (in a_0) for some calculations of Ps-Ps scattering. The present results are given to three significant figures after the decimal point purely for plotting purposes.

Method	Singlet		Triplet	
	A_0	r_0	A_1	r_1
Estimate from Ps_2 energy	5.59			
^a Platzmann and Mills [12]	≈ 5.7		≈ 1.9	
^a Oda <i>et al.</i> [9]	8.26	3.84	3.02	
Superseded SVM [20]	8.4		2.95	
Present SVM	8.443	4.761	2.998	2.247
QMC [25]	9.148 ± 0.042	-6.632	3.024 ± 0.058	1.729

^aThe triplet values are not the result of any calculation, but rather estimates based on physical insight about the nature of the collision.

[Note, the coefficients of Eq. (23) are not those published in [25]. They have been rescaled to take into account the different length scale used in [25].] Their curve follows the present effective range phase shift rather closely. The value they report for the scattering length, namely $(9.148 \pm 0.042)a_0$ is about 8% larger than the present value of $8.44a_0$. The reason for the discrepancy lies in the fact that Eq. (23) for δ_0 has a term proportional to k^2 , which is incompatible with effective range theory [30]. The coefficient of the k^2 term, $c_2 \approx 12$ is rather large and was probably responsible for the inaccuracy in their scattering length. We hasten to add that the explicitly calculated phase shifts of Shumway and Ceperley, which span the $k \in [0.1, 0.5]a_0^{-1}$ interval seem to be compatible with the present L^2 phase shifts.

Table I gives a summary of scattering lengths for the two spin configurations. The model of Oda *et al.* [9] using a semiempirical van der Waals potential tuned to the Ps_2 binding energy gave reasonably reliable estimates of the scattering length and effective range, namely, $8.26a_0$ and $3.84a_0$, respectively. Such semiempirical calculations can often give reliable results and provide a useful adjunct to large scale *ab initio* calculations.

B. Triplet-triplet states

The inner basis for the triplet-triplet channel was defined with $K=350$. This basis should be large enough to represent

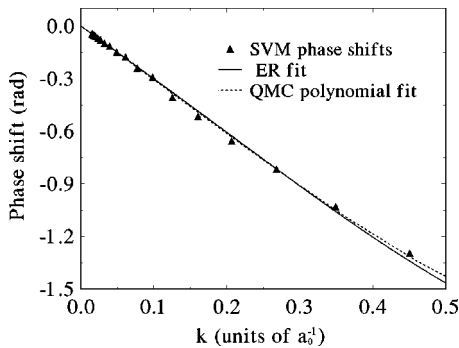


FIG. 2. The triplet-triplet phase shift δ_1 as a function of k (in a_0^{-1}). The up triangles are the explicitly calculated phase shifts and the solid line is the effective range fit to those phase shifts using the values given in Table I. The dashed line gives the QMC phase shifts from the polynomial fit given by Eq. (24) [25].

the particle interactions in the inner regions since the repulsive exchange interactions tends to keep particles apart and lessens the importance of electron-electron and positron-positron correlations. The outer basis was constructed with the exponents defined according to a Fibonacci as opposed to geometric series. Briefly, $\alpha_i = 7.0/T_{i+1}$ where the T_i are elements of the Fibonacci sequence with $T_1, T_2, T_3, T_4, T_5 = 1, 1, 2, 3, 5$ and so on. The Fibonacci scaling was chosen after some numerical experimentation revealed that the outer basis had better linear dependence properties and the random fluctuations of the phases shifts was smaller than for geometric scaling. The smallest value of the set α_i was $\alpha_{30} = 5.2 \times 10^{-6}$ giving a total of 840 additional basis functions. The final basis had a dimension of $M=1148$.

The phase shifts and effective range fit are shown in Fig. 2. All the phase shifts in the $k \in [0, 0.5]a_0^{-1}$ interval were used in the fit to Eq. (22) which gave $A_1 = 3.00a_0$ and $r_1 = 2.25a_0$ for the scattering length and the effective range, respectively. The stability of the effective range parameters were tested by some numerical experiments in which the size and construction of the inner and outer basis were altered. These calculations gave scattering lengths ranging from $2.95a_0$ to $3.08a_0$. Accordingly, it was estimated that the error in the scattering length was (conservatively) $\pm 3\%$. The uncertainty in the effective range was larger and here an uncertainty of $\pm 20\%$ is indicated.

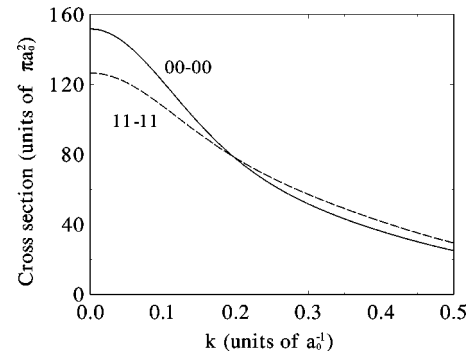


FIG. 3. The s -wave cross sections for $^1\text{Ps}-^1\text{Ps}$ elastic scattering ($\sigma_{00 \rightarrow 00}$) and $^3\text{Ps}-^3\text{Ps}$ elastic scattering ($\sigma_{11 \rightarrow 11}$) in units of πa_0^2 as a function of k (in units of a_0^{-1}). The cross sections were computed from the effective range parameters as described in the text.

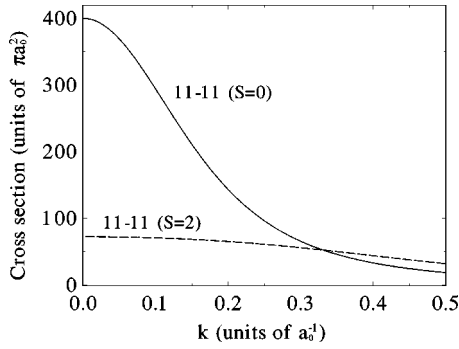


FIG. 4. The s -wave partial cross sections for ${}^3\text{Ps}$ - ${}^3\text{Ps}$ elastic scattering $\sigma_{11\rightarrow 11}^{S=0}$ and $\sigma_{11\rightarrow 11}^{S=2}$ (in units of πa_0^2) as a function of k (in units of a_0^{-1}).

The phase shifts of Shumway and Ceperley [25], as represented by the fit

$$\delta_1(k) = -3.024k - 0.552k^2 + 1.7282k^3, \quad (24)$$

are also shown in Fig. 2. Once again, the polynomial fit of Shumway and Ceperley largely reproduces the present set of phase shifts. Moreover, their scattering length, $A_1 = (3.024 \pm 0.058)a_0$, and even their effective range $r_1 = (1.728 \pm 0.512)a_0$, are compatible with the present values. In this case, the coefficient of the k^2 term, namely, -0.552 was much smaller and therefore did not have such an impact on the derived scattering length.

The estimates of the triplet-triplet scattering length by Platzmann and Mills [12] and Oda *et al.* (listed in Table I) are little more than estimates based upon physical insight. However, their estimates were amazingly good.

C. Cross sections for Ps-Ps scattering

The different cross sections for elastic scattering are shown in Figs. 3, 4, and 5. Figure 3 shows the $\sigma_{00\rightarrow 00}(k)$ and the $\sigma_{11\rightarrow 11}(k)$ cross sections. Figure 4 shows the $\sigma_{11\rightarrow 11}^{S=0}(k)$ and $\sigma_{11\rightarrow 11}^{S=2}(k)$ cross sections. The $\sigma_{01\rightarrow 01}^{S=0}(k)$ cross section is not shown since at low energies it is the same as $\sigma_{11\rightarrow 11}^{S=2}(k)$ apart from the multiplying factor of $1/4$. The $\sigma_{11\rightarrow 11}^{S=2}(k)$ cross section is the same as the cross section for spin-polarized scattering, i.e., $\sigma_{11,11\rightarrow 11,11}^{S=2}(k)$ and therefore defines the stability conditions of the ${}^3\text{Ps}$ condensate. The cross sections for all the possible reactions in the $|\text{Ps}[S_1M_1]\text{Ps}[S_2M_2]\rangle$ representation are not given since they can easily be constructed from the effective range expansions in Table I.

The existence of the spin-conversion reaction, i.e., ${}^3\text{Ps}^3\text{Ps} \rightarrow {}^1\text{Ps}^1\text{Ps}$ means that any practical approach to the creation of a Ps BEC should use spin-polarized positrons. Although ${}^3\text{Ps}$ has a lifetime of $0.142 \mu\text{s}$, collisions between two ${}^3\text{Ps}$ atoms can produce ${}^1\text{Ps}$, which rapidly decays. The use of spin-polarized positrons can be used to prevent complete collisional quenching of the ${}^3\text{Ps}$ atoms. The ${}^3\text{Ps}$ gas will decay into a spin-polarized ${}^3\text{Ps}$ gas with the same polarization as the positrons at a rate which is largely deter-

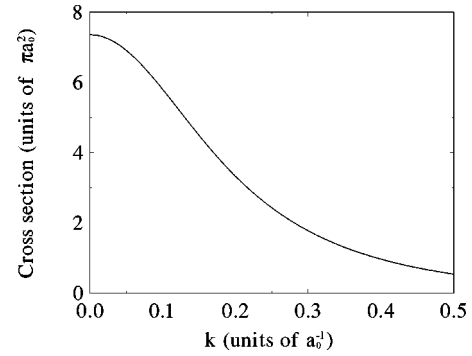


FIG. 5. The s -wave cross section for the ${}^3\text{Ps}^3\text{Ps} \rightarrow {}^1\text{Ps}^1\text{Ps}$ spin conversion reaction ($\sigma_{11\rightarrow 00}$ in units of πa_0^2) as a function of k (in units of a_0^{-1}).

mined by $\sigma_{11\rightarrow 00}(k)$. The cross section for $\sigma_{11\rightarrow 00}(k)$ is shown in Fig. 5, and at zero energy it is $7.41\pi a_0^2$. The large size of cross section emphasizes the need to use a source of spin-polarized positrons in any experimental attempt to realize a Ps BEC. For example, Saito and Hyodo [13] concluded that a spin-polarized beam was essential after using a postulated spin-conversion cross section that was more than two orders of magnitude smaller than the current estimate. Platzmann and Mills [12] had previously made that conclusion after using a spin-conversion cross section that was closer in size to the present value.

IV. SUMMARY

The stochastic variational method has been adapted to the calculation of the s -wave phase shifts for Ps-Ps scattering in both the singlet-singlet and triplet-triplet spin configurations. The present set of phase shifts is largely compatible with an earlier set of phase shifts computed using the same method [20], and also compatible with a QMC calculation of the phase shifts [25]. The evidence suggests that the description of low-energy (i.e., $E < 1$ eV) Ps-Ps scattering is accurate at the level of a few percent.

The present scattering lengths can be reliably used to determine the stability regime of the ${}^3\text{Ps}$ BEC. Just recently, the Gross-Pitaevskii (GP) equation for spin-aligned ${}^3\text{Ps}$ atoms was solved using a scattering length obtained by a process best described as an educated guess [9]. However, the scattering length they used, $3.02a_0$ is practically the same as the present explicit calculation and so their solution of the GP equation should be reliable.

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