Ps2$^-$ in a magnetic field: Structure and stability in the M=0 case

B. D. Tregoning, J. A. Salas and K. Varga

Department of Physics and Astronomy,
Vanderbilt University, Nashville, Tennessee 37235, USA

The energy of the Ps2$^-$ (three electrons and two positrons or vice versa) system and all possible fragmentations are calculated in a magnetic field in their M=0 states using the stochastic variational method with a deformed correlated Gaussian basis set. The stability of the system at various field strengths is assessed through comparison of the system's energy to the threshold energy. Examination of the single particle and pairwise densities is also employed for assessment of stability. The structure of the system is examined through calculation of distances between the charged particles. The M=0 state of Ps2$^-$ is found to be stable in fields greater than 0.01 a.u.

I.   INTRODUCTION

Few-body problems in magnetic fields are increasingly popular to study since the recent realization that many high-energy stellar objects are highly magnetized. In order to understand the make-up of these objects, it is helpful to understand what kinds of systems are responsible for their emission spectra. It is likely that positronium-like systems are present in such objects, especially given a magnetic field's ability to stabilize such systems, even when they are made up of increasing numbers of particles.

Given the propensity for constituents in positronium-like systems to annihilate with one another and the extremely strong magnetic fields in question, laboratory studies of positron-electron systems have been rare. Instead, we look to computational studies to understand these systems. Additionally, the study of particle behavior in strong magnetic fields proves difficult because of the challenges associated with the center-of-mass at the system when there is an odd number of particles (Ref. 2). However, this challenge can be bypassed by looking at states where M=0 for the system in question.

In this paper we calculate the energies of positron-electron systems of up to 5 particles in magnetic fields of varying strength using the stochastic variational method with deformed correlated Gaussian basis functions. First, we discuss the some of the formalisms for the Hamiltonian and basis functions. Then, we discuss some of the observables used to assess the stability and structure of the system. Finally, results are presented and discussed.

II.   FORMALISM

A.   Hamiltonian

The Hamiltonian of a Coulombic N-particle system with no nucleus in a magnetic field is given by

$$H = \sum_{i=1}^{N} \left(\frac{1}{2}\Delta_i + \frac{q_i^2}{m_i}\frac{B^2}{8}(x_i^2 + y_i^2) - \frac{q_i}{m_i}\frac{B}{2}L_{iz} \right) + \sum_{i<j}^{N} \frac{q_i q_j}{r_{ij}} + \frac{B}{2}(L_z + 2S_z) \qquad (1)$$

$$= T + V_{ho} + V_L + V_{ep} + \frac{B}{2}(L_z + 2S_z) \qquad (2)$$

where L_z is the z component of the orbital momentum, S_z is the z component of the spin of the system, and the magnetic field B is parallel to the z axis. In the second part of the equation, T represents the kinetic energy term, V_{ho} represents the harmonic-oscillator-like contribution from the magnetic field in the xy plane, V_L represents the contribution of the azimuthal angular momentum in the magnetic field and V_{ep} represents the electron-electron, electron-positron, and positron-positron interactions. The positions of the particles relative to the origin are depicted by $\mathbf{r}_i$ while their relative positions are depicted by $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$. Atomic units are used.

B.   Basis functions

The stochastic variational method makes use of deformed correlated Gaussian basis functions to calculate the energy of the system. The functions take this form:

$$\exp\{-\frac{1}{2}\sum_{i,j=1}^{N}A_{ij}\rho_i\cdot\rho_j-\frac{1}{2}\sum_{i,j=1}^{N}B_{ij}z_i\cdot z_j\}, \tag{3}$$

where the nonlinear parameters are independent in the xy and z directions and $\rho_i=(x_i,y_i)$. This form allows for separate descriptions of the xy plane and z axis. The Hamiltonian does not commute with L^2 but it shares eigenfunctions with L_z. The above form of the basis function is specific to $M=0$. To allow for states in which $M\neq 0$, we multiply the basis by

$$\prod_{i=1}^{N}\xi_{m_i}(\rho_i) \tag{4}$$

where

$$\xi_m(\rho)=(x+iy)^m. \tag{5}$$

Thus, the complete basis function is

$$\Phi_M(\mathbf{r})=\mathcal{A}\left(\prod_{i=1}^{N}\xi_{m_i}(\rho_i)\right)\exp\{-\frac{1}{2}\sum_{i,j=1}^{N}A_{ij}\rho_i\cdot\rho_j-\frac{1}{2}\sum_{i,j=1}^{N}B_{ij}z_i\cdot z_j\}, \tag{6}$$

where m_i are integers and $M=m_1+m_2+...+m_N$. This function is coupled with the spin function to form the complete trial function ($S_z=-S$ is used in the calculations). We restrict ourselves to M=0 states in nonzero magnetic field calculations.

The DCG basis functions can be expanded to an equivalent form which emphasizes the distance between particles.

$$\exp\{-\frac{1}{2}\sum_{i,j=1}^{N}A_{ij}\rho_i\cdot\rho_j-\frac{1}{2}\sum_{i,j=1}^{N}B_{ij}z_i\cdot z_j\} \tag{7}$$

$$=\exp\{-\frac{1}{2}\sum_{i,j=1}^{N}\alpha_{ij}(\rho_i-\rho_j)^2-\frac{1}{2}\sum_{i,j=1}^{N}\beta_{ij}(z_i-z_j)^2-\frac{1}{2}\sum_{i=1}^{N}\alpha_i'\rho_i^2-\frac{1}{2}\sum_{i=1}^{N}\beta_i'z_i^2\}. \tag{8}$$

The parameters α_{ij}, β_{ij}, α_i', and β_i' can be defined in terms of A_{ij} and B_{ij}. The parameters α_{ij} and β_{ij} are related to the distances between the charged particles while the parameters α_i' and β_i' are related to the particles' distance from the origin of the system. The results deal only with the distances between particles, as the location of the origin in a system with no nucleus is somewhat arbitrary. We select these parameters from the $[\gamma_{min},\gamma_{max}]$ interval where γ_{min} determines the closest distance between particles and γ_{max} determines the farthest distance.

ECG bases are widely used in atomic physics and quantum chemistry because they come with a number of advantages. First, their matrix elements can be obtained analytically for a general N particle system. Second, they are flexible enough to approximate rapidly changing functions. Third, the permutation symmetry is imposed easily. Fourth, it is simply to make a transformation between the single particle and relative coordinate systems.

The stochastic variational method (SVM) is used to efficiently choose the basis parameters. In this method, the variational parameters A_{ij} and B_{ij} of the deformed correlated Gaussian basis are randomly chosen and the parameters giving the lowest energy are retained as basis states. This procedure can be optimized as described in Refs. 3 and 6.

Despite computational advantages, the ECG basis has a couple of disadvantages compared to the exponential $exp(-\alpha r)$ basis. For one, the ECG basis functions do not have the correct form near the $r_{ij} \rightarrow 0$ coalescence point for interacting Coulombic particles.

C.   Observables

To determine stability, we must compare the energy it takes to move one electron or positron to infinity, called the ionization threshold energy $E_T(M, S_z)$, to the total energy of the Ps2$^-$ system. The system is energetically stable if the total energy is lower than the threshold energy of the system's fragmentations.

$$E_T(M, S_z) = \min\left(E^{Ps2}(M^{Ps2}, S_z^{Ps2}) + E^e(M^e, S_z^e), E^{Ps^-}(M^{Ps^-}, S_z^{Ps^-}) + E^{Ps}(M^{Ps}, S_z^{Ps}), ... \right), \tag{9}$$

where $E^{Ps2}(M^{Ps2}, S_z^{Ps2})$ is the total energy of the Ps2 system, which, along with an electron, is one such fragmentation that makes up Ps2$^-$. The others include Ps$^-$ + Ps, Ps$^-$ + e$^-$ + p$^+$, Ps + 2e$^-$ +p$^+$, and 3e$^-$ + 2p$^+$. The energy of the Ps, Ps$^-$, Ps2, and Ps2$^-$ are calculated via the stochastic variational method while the energy of the single electrons and positrons are given by the Landau energy:

$$E^e(M^e, S_z^e) = (M^e + |M^e| + 2S_z^e + 1)\frac{B}{2} \tag{10}$$

$$E^p(M^p, S_z^p) = (-M^p + |M^p| - 2S_z^p + 1)\frac{B}{2}, \tag{11}$$

whose quantum numbers satisfy

$$M = M^{Ps2} + M^e, M^{Ps^-} + M^p + M^e, ...S_z = S_z^{Ps2} + S_z^e, S_z = S_z^{Ps^-} + S_z^p + S_z^e. \tag{12}$$

An important consequence of these equations is that negative (positive) M states are energetically degenerate with the M=0 state for electrons (positrons). Meanwhile, positive (negative) M states increase the energy of the electrons. This allows us to make the generalization that the electron and positron energy is minimized at the M=0 state.

Aside from the energy, we also calculate the probability density and average distances between particles. Separate calculations were done for distances and probabilities between electrons and electrons, electrons and positrons, and positrons and positrons. The probability density averaged over the radial coordinate is given by

$$C_{sp}(z) = \langle\Psi| \sum_i \delta(z - z_i)|\Psi\rangle, \tag{13}$$

where Ψ is the variational wave function and the bra-ket notation stands for integration over all the single-particle coordinates. The probability density averaged over the z coordinate is given by

$$C_{sp}(\rho) = \langle\Psi| \sum_i \delta(\rho - \rho_i)|\Psi\rangle \tag{14}$$

With these in mind, the square distances for single particles are given by

$$\rho_{sp}^2 = \int_0^\infty \rho^2 C(\rho) d\rho \tag{15}$$

and

$$z_{sp}^2 = \int_{-\infty}^\infty z^2 C(z) dz. \tag{16}$$

The probability density for pairs of particles are given by

$$C_{pair}(z) = \langle \Psi | \sum_i < j \delta(z_j - z_i) | \Psi \rangle, \tag{17}$$

and

$$C_{pair}(\rho) = \langle \Psi | \sum_i < j \delta(\rho_j - \rho_i) | \Psi \rangle \tag{18}$$

The average distances are defined similarly for pairs of particles. In unbound systems, these distances diverge to infinity. Thus, the average distances of the wave functions are important in assessing the stability of the system.

D. Virial Theorem

If the wave function is an exact eigenstate of the Hamiltonian, then it will satisfy

$$\langle \Psi | [H, O] | \Psi \rangle = 0, \tag{19}$$

where O is any operator. We will use

$$O = \frac{i}{\hbar} \sum_i \mathbf{r_i p_i} = \sum_\mathbf{i} \mathbf{r_i} \frac{\partial}{\partial \mathbf{r_i}}, \tag{20}$$

in which case, the virial theorem for our Hamiltonian is

$$- 2\langle \Psi | T | \Psi \rangle = \langle \Psi | V_{ep} | \Psi \rangle - 2\langle \Psi | V_{ho} | \Psi \rangle \tag{21}$$

and we can define

$$\eta = -2 \frac{\langle \Psi | T | \Psi \rangle}{\langle \Psi | V_{ep} | \Psi \rangle - 2\langle \Psi | V_{ho} | \Psi \rangle}. \tag{22}$$

The virial theorem is satisfied when $\eta = 1$. It is very rare to satisfy the theorem exactly when using the variational principle, however the proximity of η to the desired value provides a useful measure of the quality of the calculation. Note, however, that this is a necessary but insufficient condition for a good wave function. A bad wave function can still be used to obtain a good virial value through scaling.

III.   RESULTS

A.   Method

Using the DCG basis functions, we achieved results comparable to results obtained using Hylleraas-type basis functions (Wunner et al. 1981), however our basis set does provide a value quite as low as the Hylleraas-type set. Given that energies always approach the lower limit when using the variational method, we can say that this basis set is not as effective as the Hylleraas basis at very high magnetic fields.

In the absence of a magnetic field, the analytic ground state energy of Ps is approximated from the hydrogen case and has a value of -0.25 a.u. Our calculations approach this closely from above with a value of -0.24995 a.u. at basis size $N = 400$. We also reproduce the results for the ground state of Ps2 in zero magnetic field found using SVM with a correlated Gaussian basis (Usukura et al. 1998).

Case	Our calculation	Reference calculation	Reference
Ps ground state $\beta = 0$	-0.24995	-0.25	Analytic
Ps ground state $\beta = 50$	-2.779	-2.91130	Wunner et al. 1981
Ps2 ground state $\beta = 0$	-0.51514	-0.51600	Usukura et al. 1998

B.   Stability of Ps2$^-$

While the DCG basis may not fully account for the energy, we can still make use of it to make predictions about the stability of Ps2$^-$ because the variational method guarantees that all the calculated energy values are overestimations. We predict that Ps2$^-$ becomes stable between magnetic fields of $\beta = 0$ and $\beta = 0.005$ against decays into constituents in the M=0 state. The table that compares the energy of Ps2$^-$ with the threshold energy at various magnetic fields takes the threshold energy for decays into this state. All the systems that give the threshold energy are in the $M = 0$ state.

| β	Ps2-	Threshold	Threshold system
0.0	-0.4974330	-0.5151445	Ps$^-$ + Ps
0.005	-0.5236842	-0.5213326	Ps$^-$ + Ps
0.01	-0.5363207	-0.5298523	Ps$^-$ + Ps
0.1	-0.7027896	-0.6108035	Ps$^-$ + Ps
0.2	-0.8358979	-0.5573477	Ps$^-$ + Ps
1.0	-1.3560716	0.6258706	Ps2 + e$^-$
2.0	-1.7117848	2.2720147	Ps2 + e$^-$
3.0	-1.9673873	4.018780971	Ps2 + e$^-$
4.0	-2.1677849	5.8158273	Ps2 + e$^-$
5.0	-2.3375918	7.6438768	Ps2 + e$^-$
6.0	-2.4931030	9.4933668	Ps2 + e$^-$
7.0	-2.6256301	11.3588853	Ps2 + e$^-$
8.0	-2.7472093	13.2390526	Ps2 + e$^-$
9.0	-2.8534868	15.1268289	Ps2 + e$^-$
10.0	-2.9582851	17.0223008	Ps2 + e$^-$
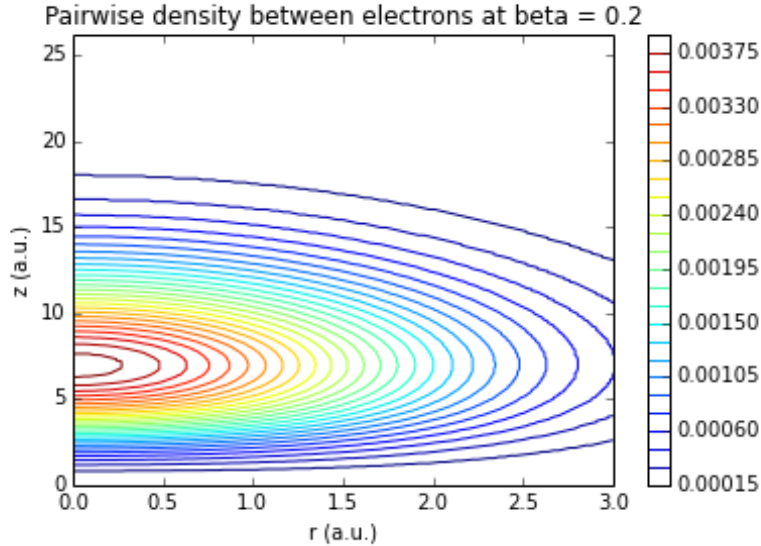
FIG. 1: Contour plot of probability densities of average distances between like particles in Ps2$^-$ at beta = 0.2

The two most energetically favorable decay modes for Ps2$^-$ are Ps2 + e$^-$ and Ps$^-$ + Ps as these systems minimize the number of free particles which tend to be high energy in these magnetic fields. We know from equations 10 and 11 that we must only consider electrons and positrons in the M=0 state to determine stability as other M states will be at least as energetic as the M=0. For Ps, Ps$^-$, and Ps2, we confirm that nonzero M states have higher energy that the M=0 in the magnetic fields from the values given in the above table. Thus, if a decay mode is energetically unfavorable in the M=0 state, it will remain unfavorable in states where $M_{total} \neq 0$. Note that $M_{total} = M_+ + M_-$ with M_+ representing the state of the positrons' angular momenta in the system and M_- representing the state of the electrons' angular momenta. With these considerations, we conclude that the M=0 state of Ps2$^-$ stable. The $M_- \neq 0$ and $M_+ \neq 0$ states were taken by setting the angular momenta of all the electrons and positrons in the system to 1, respectively. Except for the Ps2 $\beta = 0.2$ case of $M_+ \neq 0$, where the positron angular momenta were set to -1 in order to look at a slightly different case.

System	β	$M = 0$	$M_- \neq 0$	$M_+ \neq 0$
Ps	0.01	-0.259797099	-0.255251373	-0.235221431
Ps	0.1	-0.332299176	-0.292573204	-0.092645493
Ps$^-$	0.01	-0.270055370	-0.262170232	-0.241215604
Ps$^-$	0.1	-0.278504363	-0.230663742	-0.1781148854
Ps2	0.01	-0.544061662	-0.532652285	-0.543998106
Ps2	0.2	-0.851511152	-0.706864925	-0.742058025

Figures 1-4 represent the probability densities of the distances between particles of Ps2$^-$ at two different magnetic field values. The x-axis represents the radial distance between particles in the plane perpendicular to the magnetic field, while the y-axis represents their distance in the direction of the magnetic field. It can be seen that at higher magnetic fields (figures 3 and 4), the particles are squeezed closer to together, which corresponds to our prediction of increased stability of the system in higher fields.
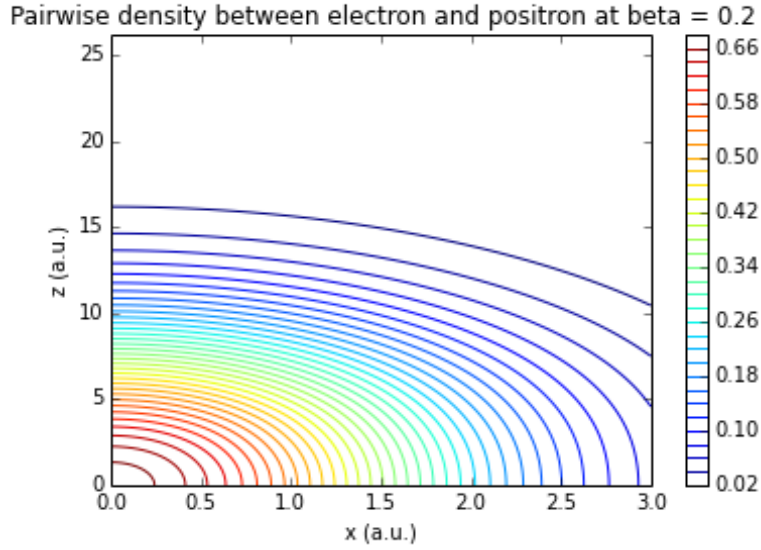
FIG. 2: Contour plot of probability densities of average distances between electrons and positrons in Ps2$^-$ at beta = 0.2
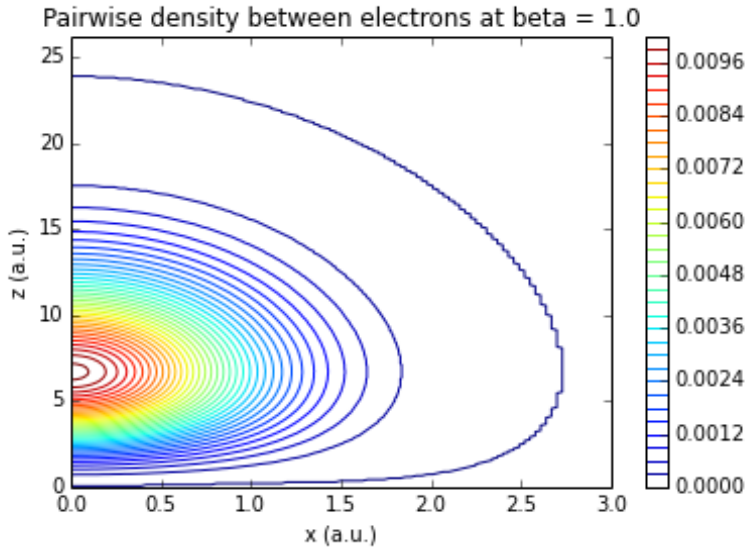

FIG. 3: Contour plot of probability densities of average distances between like particles in Ps2$^-$ at beta = 1.0

IV. CONCLUSION

Using the stochastic variational method we have calculated the energies and inter-particle distances of positron-electron systems in the M=0 state of up to five particles. We compared the results of this method using deformed correlated Gaussian basis functions to other findings in the literature to assess the efficacy of the basis set. We find that these functions approximate the systems well in zero magnetic field. At very high magnetic fields, we find that these functions do not fully account for the energy of the system.

Given the nature of the variational method, though, we could still use the DCG basis to make predictions about the stability and structure of Ps2$^-$. We predict that Ps2$^-$ becomes energetically stable in fields between $\beta = 0$ and $\beta = 0.005$. We also offer the probability
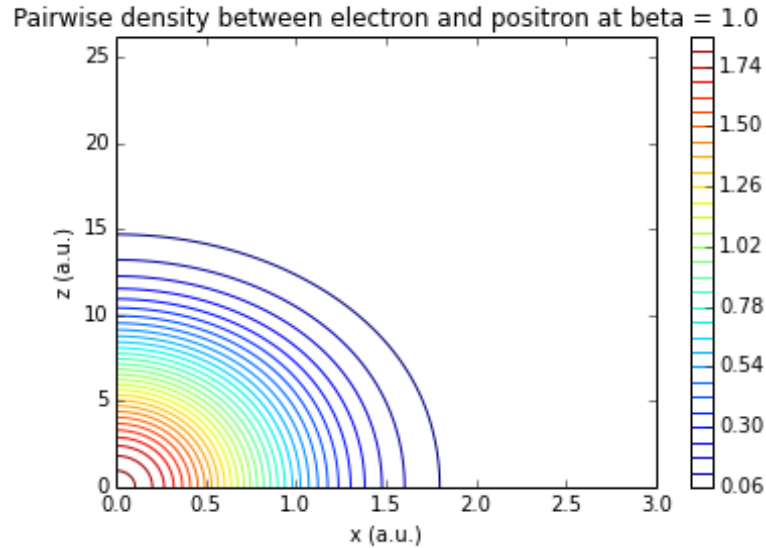
FIG. 4: Contour plot of probability densities of average distances between electrons and positrons in Ps2$^-$ at beta = 1.0

densities of the various inter-particle distances for Ps2$^-$ at $\beta = 0.2$ in figures 1 and 2 and $\beta = 1.0$ in figures 3 and 4.

Ps2$^-$ has seen very little computational study. As far as we have seen, this is the first statement that has been made regarding the stability of Ps2$^-$ in magnetic fields. Hopefully other labs will begin to study this system in magnetic fields using different basis functions or other methods.

V. REFERENCES

1. Salas, J. A., & Varga, K. (2014). He in a magnetic field: Structure and stability. Physical Review A, 89(5), 052501. http://doi.org/10.1103/PhysRevA.89.052501

2. Baye, D., & Vincke, M. (1988). Spontaneous dissociation of m0 positronium states in strong magnetic fields. Physics Letters A, 129(2), 109112. http://doi.org/10.1016/0375-9601(88)90079-5

3. Varga, K., & Suzuki, Y. (1995). Precise solution of few-body problems with the stochastic variational method on a correlated Gaussian basis. Physical Review C, 52(6).

4. Wunner, G., Ruder, H., & Herold, H. (1981). Energy levels, electromagnetic transitions and annihilation of positronium in strong magnetic fields. Journal of Physics B: Atomic and Molecular Physics, 14(4), 765772. http://doi.org/10.1088/0022-3700/14/4/023

5. Ho, Y. K. (1986). Binding energy of positronium molecules. Physical Review A, 33(5), 35843587. http://doi.org/10.1103/PhysRevA.33.3584

6. Mitroy, J., Bubin, S., Horiuchi, W., Suzuki, Y., Adamowicz, L., Cencek, W., Varga, K. (2013). Theory and application of explicitly correlated Gaussians. Reviews of Modern Physics, 85(2), 693749. http://doi.org/10.1103/RevModPhys.85.693