Relativistic *n*-fermion wave equations in quantum electrodynamics

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The variational method in a reformulated Hamiltonian formalism of quantum electrodynamics is used to derive relativistic wave equations for a system consisting of n fermions and antifermions. Simple Fock-space variational trial states are used to obtain the relativistic n-body equations. The derived kernels of these equations (i.e., momentum-space relativistic potentials) include one-photon exchange and virtual annihilation interactions. The equations are shown to have the Schrödinger nonrelativistic limit. Application to the particular cases of positronium (Ps), positronium negative ion (Ps^-), and positronium molecule (Ps_2, $e^-e^+e^-e^+$) are discussed.

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I. INTRODUCTION

The description of relativistic n-body bound-state systems, including the interactions, by means of equations obtained from an underlying Lagrangian continues to be an object of research. There are various approaches to the relativistic n-body problem with electromagnetic interactions, including those based on the Bethe-Salpeter (BS) equation [1], as well as other methods (see, for example, Refs. [2–8], and references therein). Overviews of applications to n-body nuclear systems are discussed by Serot and Walecka [9], among others, and in presentations on the subject [10]. Early variational approaches are presented, for example, in Refs. [11–14].

An alternative to the BS and other approaches is the variational method within the reformulated Hamiltonian formalism of quantum field theory (QFT), introduced by Darewych [15]. Among the appealing features of this approach is that it can be cast in the form of a relativistic generalization of the Schrödinger description of n-body systems. Furthermore, the method is straightforwardly generalizable to systems of more than two particles.

The simplest few-body problem for a system of fermions and antifermions with electromagnetic interactions is that of positronium (Ps, e^-e^+). In 1934, Mohorovicic [16] postulated the possible existence of Ps following the prediction of antimatter by Dirac in 1930. There have been many theoretical and experimental studies of Ps since 1934. Deutsch [17] was the first person who produced Ps (in gases) in 1951. Since the discovery of Ps, there have been major advances in understanding of the Ps system (see, for example, Rich [18], Pilkuhn [19], and Greiner and Reinhard [20], and references therein) and in the use of Ps to explore the basic structure of quantum electrodynamics (QED). An account of the history of QED has been written by Schweber [21].

Recent theoretical studies of the Ps system are now well advanced. For example, accurate calculations of the positronium hyperfine interval [$O(\alpha^6)$ contributions to ground-state hyperfine splitting in positronium] have been studied by Adkins *et al.* [22]. On a practical level, it has recently become possible to study interactions between Ps atoms by implanting intense pulses of positrons into porous silica films [23]. This leads to the formation of Ps atoms that may become trapped in the internal voids [24,25]. Very recently interactions between pairs of positronium atoms confined in porous silica films have been directly observed for the first time by Cassidy and Mills [26].

The positronium negative ion (Ps^-), consisting of a positron and two electrons ($e^+e^-e^-$), is the simplest system composed of three equal mass fermions, bound only by electromagnetic interactions. The existence of a bound Ps^- system was predicted by Wheeler [27]. Theoretical studies of the Ps^- are now well advanced, including perturbative determinations of relativistic and QED corrections (cf. Drake and Grigorescu [28], and references therein). The Ps^- system was first observed by Mills [29] and recently by Fleischer *et al.* [30]. Measurements are available of the decay rate for the three-body Ps^- system but not as yet of the binding energy. The role of Ps^- in astrophysics and space physics has been discussed by Sivarman and Krishan [31] and in solid state physics by Ferrante [32].

Fundamental fermions antifermions systems with electromagnetic interactions are of interest because they are "pure" QED systems, with pointlike constituents and no nuclear force or size effects. Experiments on such "exotic" atoms, though difficult, are being undertaken not only for positronium and the three-body Ps^- ($e^+e^-e^-$) system, but also for the four-body "positronium molecule" (or "quadronium atom," Ps_2, $e^+e^-e^+e^-$). Recently, in 2005, a team of physicists led by Mills reported the possible creation of positronium molecules [23], and this was supported by Saniz *et al.* [33]. Very recently the positronium molecule was observed by Cassidy and Mills in an outstanding experiment [34].

Positronium molecule [Ps_2, consisting of two electrons and two antielectrons (positrons)] is similar to, but different from the familiar hydrogen molecule H_2. Ps_2 creation [34] heralds a new chapter in the study of matter and antimatter. In addition, as it has been pointed out in Ref. [35], scientists are asking questions about the chemical physics of antimatter, such as the binding of positrons to ordinary atoms [36]. They are also coming closer to fundamental tests of the symmetry of matter and antimatter by comparing the properties of hydrogen and antihydrogen [37,38]. Hence, the investigation of the properties of such exotic systems is of fundamental importance, since not only are we tempted to identify it as a mathematical curiosity, but also as Cassidy and Mills [34] pointed out, it could also help to explain how the observable

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universe ended up with so much more matter than antimatter.

The existence of a bound-state positronium molecule was predicted a long time ago by theoretical calculations of Hylleraas and Ore [39] in 1947. There are many papers on this topic in the literature, for example, Refs. [40–51], and references therein. Recently, an intense pulsed positron source has been developed by Mills and his colleagues, using a buffer gas trap to accumulate a large number of positrons. This creates a dense plasma, which can be used for the formation of positronium molecules and positronium Bose-Einstein condensates [52,53]. Of course, Ps_2 is only a quasibound system because of electron-positron annihilation. However, calculation predicts that its lifetime is almost 2 times as long as that of the positronium atom in the singlet state [40–44].

On a practical level, the role of positronium molecule, Ps_2, is discussed by Mills and his co-workers in [54]. As it has been pointed out in [54], their research paved the way for studying multipositronium interactions, useful for generating coherent gamma radiation, and could help develop fusion power generation as well as annihilation gamma-ray lasers. Cassidy and Mills [34] believe that the production of molecular positronium represents a milestone on the path to produce an annihilation gamma-ray laser.

Moreover, it would be of interest to mention the following points about the gamma-ray laser project of Mills and his co-workers [54]. Their research is mainly focused on dense positronium (Ps) physics, with the long term goal of creating a Bose-Einstein condensate of Ps, and thence an annihilation gamma laser. The positronium laser project may seem to be a very difficult and ambitious project. However, it is also an exciting new area of positron physics, and promises to become more so as progress is made. Furthermore, as it has been pointed out in Ref. [35], if one could increase the density of positronium atoms to 10^{18} cm^{-3}, the system is expected [55] to undergo a transition at a temperature of 15 K to a Bose-Einstein condensate, in which all atoms share the same quantum state. One may expect the material to become a regular, crystalline solid at even higher densities. Also, at densities of 10^{21} cm^{-3}, if one could make a Bose-Einstein condensate of positronium molecules, then there would be the possibility of creating a laser using the gamma-rays from the annihilation process.

To our knowledge there have been no experimental studies of fermion-antifermion "exotic" systems with number of $n>4$, where n is the total number of fermions and antifermions, (e.g., $e^-e^+e^-e^+e^-$, $n=5$), or similar muonic systems. Such exotic atoms or molecules will undoubtedly be investigated in the future. Thus, their theoretical investigation is of interest.

In a recent paper Emami-Razavi [56] has demonstrated the efficacy of the variational method in reformulated Hamiltonian quantum field theory (Darewych [15]) by deriving relativistic n-body equations for spinless bosons in the scalar Yukawa (Wick-Cutkosky) theory. Here, we apply this approach to spin-1/2 fermions in QED. Specifically, we derive relativistic equations for bound-states systems consisting of n_1 electrons (or muons, etc.) and n_2 positrons (or antimuons, etc.), where $n_2=n_1$ or $n_2=n_1-1$ $(n_1+n_2=n)$.

The presentation of the paper is the following. The Lagrangian and Hamiltonian density of reformulated QED are presented in Sec. II. Trial states and resulting n-body wave equations and interaction kernels are given in Sec. III. The two-body (positronium), three-body (Ps^-), and four-body (Ps_2, positronium molecule) examples are presented in Sec. IV. Concluding remarks are given in Sec. V.

II. LAGRANGIAN, HAMILTONIAN, AND VARIATIONAL METHODS

The Lagrangian density obtained in the reformulated version of QED (Darewych [15], Terekidi and Darewych [57]) is given by the following expression $(\hbar=c=1)$:

$$\mathcal{L}_R = \bar{\psi}(x)[i\gamma^\mu\partial_\mu - m - e\gamma_\mu A_0^\mu(x)]\psi(x) - \frac{1}{2}\int d^4x' j^\mu(x')D_{\mu\nu}(x-x')j^\nu(x), \tag{1}$$

where $x=(t,\mathbf{r})$, $A_0^\mu(x)$ is the free photon field,

$$j^\nu(x) = e\bar{\psi}(x)\gamma^\nu\psi(x), \tag{2}$$

and $D_{\mu\nu}(x-x')$ is a symmetric Green function defined by

$$\partial_\alpha\partial^\alpha D_{\mu\nu}(x-x') - \partial_\mu\partial^\alpha D_{\alpha\nu}(x-x') = g_{\mu\nu}\delta^4(x-x'), \tag{3}$$

such that

$$D_{\mu\nu}(x-x') = D_{\mu\nu}(x'-x) \quad \text{and} \quad D_{\mu\nu}(x-x') = D_{\nu\mu}(x-x'). \tag{4}$$

The Hamiltonian density corresponding to the Lagrangian (1) is given by

$$\mathcal{H}(x) = \mathcal{H}_\psi(x) + \mathcal{H}_{I_1}(x) + \mathcal{H}_{I_2}(x), \tag{5}$$

where

$$\mathcal{H}_\psi(x) = \psi^\dagger(x)(-i\vec{\alpha}\cdot\vec{\nabla} + m\beta)\psi(x), \tag{6}$$

$$\mathcal{H}_{I_1}(x) = e\bar{\psi}(x)\gamma_\mu A_0^\mu(x)\psi(x), \tag{7}$$

$$\mathcal{H}_{I_2}(x) = \frac{1}{2}\int d^4x' j^\mu(x')D_{\mu\nu}(x-x')j^\nu(x), \tag{8}$$

where $D_{\mu\nu}(x-x')=\int\frac{1}{(2\pi)^{3+1}}d^{3+1}kD_{\mu\nu}(k)\exp[-ik(x-x')]$ and we suppress the Hamiltonian of the free photon field (since it will not arise in this work).

In practice, a choice of gauge is needed to specify the Green function. For bound-state problems the Coulomb gauge is a convenient choice. In momentum representation it is

$$D_{00}(q-p)=\frac{1}{|\mathbf{q}-\mathbf{p}|^2},\quad D_{0j}(q-p)=0,$$

$$D_{ij}(q-p)=\frac{1}{(q^\mu-p^\mu)(q_\mu-p_\mu)}\left(\delta_{ij}-\frac{(\mathbf{q}-\mathbf{p})_i(\mathbf{q}-\mathbf{p})_j}{(\mathbf{q}-\mathbf{p})^2}\right). \tag{9}$$

We construct a quantum field theory, based on the reformulated Hamiltonian by replacing the field variables with operators which satisfy the usual anticommutation relations for the fermion fields, commutation rules for the A_0^μ field, and commutation of the A_0^μ field operators with the ψ field operators. For the fermion fields our notation is

$$\psi(x)=\sum_s\int\frac{d^3p}{(2\pi)^{3/2}}\left(\frac{m}{\omega_p}\right)^{1/2}[b_{\mathbf{p}s}u(\mathbf{p},s)e^{-ip\cdot x}+d^\dagger_{\mathbf{p}s}v(\mathbf{p},s)e^{ip\cdot x}], \tag{10}$$

with $p=p^\mu=(\omega_p,\mathbf{p})$, and $\omega_p=\sqrt{m^2+\mathbf{p}^2}$. The mass-$m$ free-particle Dirac spinors u and v, where $(\gamma^\mu p_\mu-m)u(\mathbf{p},s)=0$, $(\gamma^\mu p_\mu+m)v(\mathbf{p},s)=0$, are normalized such that

$$u^\dagger(\mathbf{p},s)u(\mathbf{p},\sigma)=v^\dagger(\mathbf{p},s)v(\mathbf{p},\sigma)=\frac{\omega_p}{m}\delta_{s\sigma}, \tag{11}$$

$$u^\dagger(\mathbf{p},s)v(\mathbf{p},\sigma)=v^\dagger(\mathbf{p},s)u(\mathbf{p},\sigma)=0. \tag{12}$$

The creation and annihilation operators $b^\dagger$, b of the (free) fermions of mass m, and $d^\dagger$, d for the corresponding antiparticles, satisfy the usual anticommutation relations. The nonvanishing ones are

$$\{b_{\mathbf{p}s},b^\dagger_{\mathbf{q}\sigma}\}=\{d_{\mathbf{p}s},d^\dagger_{\mathbf{q}\sigma}\}=\delta_{s\sigma}\delta^3(\mathbf{p}-\mathbf{q}). \tag{13}$$

The vacuum state $|0\rangle$ is defined by $b_{\mathbf{p}}|0\rangle=d_{\mathbf{k}}|0\rangle=0$.

The Hamiltonian operator, $\hat{H}=\int d^3x\hat{\mathcal{H}}(x)$ is expressed in terms of the creation and annihilation operators $b^\dagger,d^\dagger,b,d$ in the usual way. We normal order the entire Hamiltonian (thereby denoting it $:\hat{H}:$); this circumvents the need for mass renormalization and we shall not be concerned with vacuum-energy questions in this work.

In the Hamiltonian formalism of QFT we seek solutions of the eigenvalue equation

$$\hat{P}^\beta|\Psi\rangle=Q^\beta|\Psi\rangle, \tag{14}$$

where $\hat{P}^\beta=(\hat{H},\hat{\mathbf{P}})$ is the energy-momentum operator of the QFT, and $Q^\beta=(E,\mathbf{Q})$ is the energy-momentum eigenvalue. The case $\mathbf{Q}=0$ defines the rest frame of the system. The $\beta=0$ component of (14) is generally not solvable, hence approximation methods, such as the variational method, must be used. The latter amounts to finding approximate solutions by using the variational principle

$$\delta\langle\Psi|:\hat{H}-E:|\Psi\rangle_{t=0}=0, \tag{15}$$

where $|\Psi\rangle$ is a suitably chosen trial state.

III. TRIAL STATE AND RESULTING n-BODY EQUATION AND INTERACTION KERNELS

The simplest trial state for a system of $\frac{n}{2}$ particles and $\frac{n}{2}$ antiparticles $(e^-e^+e^-e^+\cdots e^-e^+)$ is

$$|\psi_n\rangle=\sum_{s_1\cdots s_n}\int d^3p_1\cdots d^3p_nF_{s_1s_2\cdots s_n}(\mathbf{p}_1,\ldots,\mathbf{p}_n)b^\dagger(\mathbf{p}_1,s_1)\times d^\dagger(\mathbf{p}_2,s_2)\cdots b^\dagger(\mathbf{p}_{n-1},s_{n-1})d^\dagger(\mathbf{p}_n,s_n)|0\rangle, \tag{16}$$

where F is a well-behaved, adjustable function (normalizable for bound states). Similarly, for a system of $\frac{n+1}{2}$ particles and $\frac{n-1}{2}$ antiparticles $(e^-e^+e^-e^+\cdots e^-e^+e^-)$,

$$|\psi_n\rangle=\sum_{s_1\cdots s_n}\int d^3p_1\cdots d^3p_nF_{s_1\cdots s_n}(\mathbf{p}_1,\ldots,\mathbf{p}_n)b^\dagger(\mathbf{p}_1,s_1)\times d^\dagger(\mathbf{p}_2,s_2)\cdots b^\dagger(\mathbf{p}_{n-2},s_{n-2})d^\dagger(\mathbf{p}_{n-1},s_{n-1})b^\dagger(\mathbf{p}_n,s_n)|0\rangle. \tag{17}$$

The matrix element corresponding to the rest-plus-kinetic energy of such a n-fermion system is

$$\langle\psi_n|:\hat{H}_\psi-E:|\psi_n\rangle=\sum_{s_1\cdots s_n}\int d^3p_1\cdots d^3p_nF^*_{s_1\cdots s_n}(\mathbf{p}_1,\ldots,\mathbf{p}_n)\times F_{s_1\cdots s_n}(\mathbf{p}_1,\ldots,\mathbf{p}_n)[\omega_{p_1}+\cdots+\omega_{p_n}-E]. \tag{18}$$

The matrix element corresponding to the interactions is a sum of terms corresponding to attractive one-photon exchange plus repulsive virtual annihilation interactions for each particle-antiparticle combination and repulsive one-photon exchange between pairs of fermions of the same sign of charge. Symbolically,

$$\langle\psi_n|:\hat{H}_I:|\psi_n\rangle=[\mathcal{M}^{\text{Attractive}}]+[\mathcal{M}^{\text{Repulsive}}]+[\mathcal{M}^{\text{Annihilation}}]. \tag{19}$$

If n is even (i.e., an equal number of particles and antiparticles), there are $n^2/4$ particle-antiparticle combinations and $(n^2-2n)/4$ two-identical-charge-fermion combinations. For example, for $n=4$ (Ps_2, $e^-e^+e^-e^+$), we have four attractive one-photon exchange terms, two repulsive one-photon exchange terms, and four (repulsive) virtual annihilation interaction terms. If n is odd (i.e., one more particle than antiparticle) there are $(n^2-1)/4$ attractive and virtual annihilation terms, and $(n-1)^2/4$ repulsive terms. For example, for $n=5$ (say $e^-e^+e^-e^+e^-$) we have six attractive, four repulsive, and six virtual annihilation terms.

We note that $\langle\psi_{\text{trial}}|:\hat{H}_{I_1}:|\psi_{\text{trial}}\rangle=0$. That is, the variational trial states (16) or (17) do not sample that part of the interaction Hamiltonian. This means that with such simple trial states only stable bound states and elastic scattering can be described, but not processes that involve the emission or absorption of physical photons.

In any case, for the n-body system described by the trial state (16) or (17), the matrix element corresponding to the interactions is

$$\langle\psi_n|:\hat{H}_I:|\psi_n\rangle = \langle\psi_n|:\hat{H}_{I_2}:|\psi_n\rangle$$
$$= \frac{m^2e^2}{2(2\pi)^3}\sum_{\substack{s_1\cdots s_n\\ s_1'\cdots s_n'}}\int d^3p_1\cdots d^3p_n d^3p_1'\cdots d^3p_n' F^*_{s_1's_2'\cdots s_n'}(\mathbf{p}_1',\ldots\mathbf{p}_n')F_{s_1s_2\cdots s_n}(\mathbf{p}_1,\ldots,\mathbf{p}_n)$$
$$\times\Bigg(\sum_{j=1}^{n-1}\sum_{k=j+1}^{n}{}'\prod_{i=1\ldots n}{}^{(j,k)}\delta_{s_i's_i}\prod_{i=1\cdots n}{}^{(j,k)}\delta^3(\mathbf{p}_i'-\mathbf{p}_i)\frac{\delta^3(\mathbf{p}_j'+\mathbf{p}_k'-\mathbf{p}_j-\mathbf{p}_k)}{\sqrt{\omega_{p_j'}\omega_{p_k'}\omega_{p_j}\omega_{p_k}}}$$
$$\times[-\mathcal{M}^{\text{Attractive}}_{s_js_ks_j's_k'}(\mathbf{p}_j,\mathbf{p}_k,\mathbf{p}_j',\mathbf{p}_k')+\mathcal{M}^{\text{Annihilation}}_{s_js_ks_j's_k'}(\mathbf{p}_j,\mathbf{p}_k,\mathbf{p}_j',\mathbf{p}_k')]$$
$$+\sum_{j=1}^{n-2}\sum_{k=j+2}^{n}{}'\prod_{i=1\cdots n}{}^{(j,k)}\delta_{s_i's_i}\prod_{i=1\cdots n}{}^{(j,k)}\delta^3(\mathbf{p}_i'-\mathbf{p}_i)\frac{\delta^3(\mathbf{p}_j'+\mathbf{p}_k'-\mathbf{p}_j-\mathbf{p}_k)}{\sqrt{\omega_{p_j'}\omega_{p_k'}\omega_{p_j}\omega_{p_k}}}\mathcal{M}^{\text{Repulsive}}_{s_js_ks_j's_k'}(\mathbf{p}_j,\mathbf{p}_k,\mathbf{p}_j',\mathbf{p}_k')\Bigg), \tag{20}$$

where $\Sigma'_{k=a}u_k$ means $u_a+u_{a+2}+u_{a+4}+\cdots$. Our convention is that variables with odd indices correspond to particles (e^-), and those with even indices correspond to antiparticles (e^+).

The superscript notation (j,k) in $\Pi_{i=1\cdots n}{}^{(j,k)}\delta^3(\mathbf{p}_i'-\mathbf{p}_i)$ (and in $\Pi_{i=1\cdots n}{}^{(j,k)}\delta s_i's_i$) in Eq. (20) means that the terms with indices j and k are left out. In other words,

$$\prod_{i=1\cdots n}{}^{(j,k)}\delta^3(\mathbf{p}_i'-\mathbf{p}_i)=\prod_{i=1}^{j-1}\delta^3(\mathbf{p}_i'-\mathbf{p}_i)\prod_{i=j+1}^{k-1}\delta^3(\mathbf{p}_i'-\mathbf{p}_i)\times\prod_{i=k+1}^{n}\delta^3(\mathbf{p}_i'-\mathbf{p}_i)$$
$$=\frac{\prod_{i=1}^{n}\delta^3(\mathbf{p}_i'-\mathbf{p}_i)}{\delta^3(\mathbf{p}_j'-\mathbf{p}_j)\delta^3(\mathbf{p}_k'-\mathbf{p}_k)}\quad\text{for } j<k. \tag{21}$$

For the case $n=2$, $\Pi_{i=1\cdots n}{}^{(j,k)}\delta^3(\mathbf{p}_i'-\mathbf{p}_i)=1$ and $\Pi_{i=1\cdots n}{}^{(j,k)}\delta_{s_i's_i}=1$.

The expressions for $\mathcal{M}^{\text{Attractive}}_{s_js_ks_j's_k'}$, $\mathcal{M}^{\text{Repulsive}}_{s_js_ks_j's_k'}$, and $\mathcal{M}^{\text{Annihilation}}_{s_js_ks_j's_k'}$ are as follows:

$$\mathcal{M}^{\text{Attractive}}_{s_js_ks_j's_k'}(\mathbf{p}_j,\mathbf{p}_k,\mathbf{p}_j',\mathbf{p}_k')=\bar{u}(\mathbf{p}_j',s_j')\gamma^\mu u(\mathbf{p}_j,s_j)$$
$$\times[D_{\mu\nu}(\omega_{p_j'}-\omega_{p_j},\mathbf{p}_j'-\mathbf{p}_j)+D_{\mu\nu}(\omega_{p_k'}-\omega_{p_k},\mathbf{p}_k'-\mathbf{p}_k)]$$
$$\times\bar{v}(\mathbf{p}_k,s_k)\gamma^\nu v(\mathbf{p}_k',s_k'), \tag{22}$$

if j is odd (i.e., e^-) and k is even (i.e., e^+), and a similar expression, with u replaced by v, and v replaced by u in Eq. (22) if j is even (i.e., e^+) and k is odd (i.e., e^-). The terms corresponding to one-photon exchange interactions among particles with the same sign of charge are

$$\mathcal{M}^{\text{Repulsive}}_{s_js_ks_j's_k'}(\mathbf{p}_j,\mathbf{p}_k,\mathbf{p}_j',\mathbf{p}_k')=\bar{u}(\mathbf{p}_j',s_j')\gamma^\mu u(\mathbf{p}_j,s_j)$$
$$\times[D_{\mu\nu}(\omega_{p_j'}-\omega_{p_j},\mathbf{p}_j'-\mathbf{p}_j)+D_{\mu\nu}(\omega_{p_k'}-\omega_{p_k},\mathbf{p}_k'-\mathbf{p}_k)]$$
$$\times\bar{u}(\mathbf{p}_k',s_k')\gamma^\nu u(\mathbf{p}_k,s_k), \tag{23}$$

if j and k are both odd (i.e., e^-e^-) and a similar expression, with u replaced by v in Eq. (23) if j and k are both even (i.e., e^+e^+). Last, the terms corresponding to virtual annihilation are

$$\mathcal{M}^{\text{Annihilation}}_{s_js_ks_j's_k'}(\mathbf{p}_j,\mathbf{p}_k,\mathbf{p}_j',\mathbf{p}_k')=\bar{u}(\mathbf{p}_j',s_j')\gamma^\mu v(\mathbf{p}_k',s_k')$$
$$\times[D_{\mu\nu}(\omega_{p_j'}+\omega_{p_k'},\mathbf{p}_j'+\mathbf{p}_k')+D_{\mu\nu}(-\omega_{p_j}-\omega_{p_k},-\mathbf{p}_j-\mathbf{p}_k)]$$
$$\times\bar{v}(\mathbf{p}_k,s_k)\gamma^\nu u(\mathbf{p}_j,s_j), \tag{24}$$

if j is odd (i.e., e^-) and k is even (i.e., e^+), and a similar expression, with u replaced by v, and v replaced by u in Eq. (24) if j is even (i.e., e^+) and k is odd (i.e., e^-). In short, the "virtual annihilation" interactions, as for the "attractive" interactions, occur among terms with odd-even or even-odd indices j and k.

The relativistic n-body wave equation for the coefficient functions $F_{s_1s_2\cdots s_n}(\mathbf{p}_1,\ldots,\mathbf{p}_n)$ of the trial state (16) or (17) that follows from $\delta\langle\Psi|:\hat{H}-E:|\Psi\rangle_{t=0}=0$, is

$$F_{s_1 s_2 \cdots s_n}(\mathbf{p}_1, \ldots, \mathbf{p}_n)[\omega_{p_1} + \cdots + \omega_{p_n} - E]$$
$$= \frac{m^2 e^2}{2(2\pi)^3} \sum_{s_1' \cdots s_n'} \int d^3p_1' \cdots d^3p_n' F_{s_1' s_2' \cdots s_n'}(\mathbf{p}_1', \ldots, \mathbf{p}_n')$$
$$\times \Bigg(\sum_{j=1}^{n-1} \sum_{k=j+1}^{n}{}' \prod_{i=1\ldots n}^{(j,k)} \delta_{s_i' s_i} \prod_{i=1\ldots n}^{(j,k)} \delta^3(\mathbf{p}_i' - \mathbf{p}_i) \frac{\delta^3(\mathbf{p}_j' + \mathbf{p}_k' - \mathbf{p}_j - \mathbf{p}_k)}{\sqrt{\omega_{p_j'} \omega_{p_k'} \omega_{p_j} \omega_{p_k}}}$$
$$\times [\mathcal{M}^{\text{Attractive}}_{s_j s_k s_j' s_k'}(\mathbf{p}_j, \mathbf{p}_k, \mathbf{p}_j', \mathbf{p}_k') - \mathcal{M}^{\text{Annihilation}}_{s_j s_k s_j' s_k'}(\mathbf{p}_j, \mathbf{p}_k, \mathbf{p}_j', \mathbf{p}_k')]$$
$$- \sum_{j=1}^{n-2} \sum_{k=j+2}^{n}{}' \prod_{i=1\cdots n}^{(j,k)} \delta_{s_i' s_i} \prod_{i=1\cdots n}^{(j,k)} \delta^3(\mathbf{p}_i' - \mathbf{p}_i) \frac{\delta^3(\mathbf{p}_j' + \mathbf{p}_k' - \mathbf{p}_j - \mathbf{p}_k)}{\sqrt{\omega_{p_j'} \omega_{p_k'} \omega_{p_j} \omega_{p_k}}} \mathcal{M}^{\text{Repulsive}}_{s_j s_k s_j' s_k'}(\mathbf{p}_j, \mathbf{p}_k, \mathbf{p}_j', \mathbf{p}_k') \Bigg), \tag{25}$$

where $\Sigma'_{k=a} u_k$ means $u_a + u_{a+2} + u_{a+4} + \cdots$, as before.

Equation (25) is our main result. It is a relativistic momentum-space equation for stationary states of a n-fermion system, consisting of either an equal number of fermions and antifermions (if n is even) or with the number of particles one larger than the number of antiparticles (if n is odd). It is Schrödinger-like in structure, with positive-energy solutions only, as can be seen by setting the right-hand side of Eq. (25) to zero (i.e., no interactions). In this respect, Eq. (25) is different from many-fermion Dirac-like equations or the Bethe-Salpeter equation.

The interaction kernels (momentum-space potentials) in Eq. (25) contain all tree-level Feynman diagrams, that is, one-quantum exchange and virtual annihilation interactions, including retardation effects. Thus all physical effects to $O(\alpha^4)$ are contained in Eq. (25), that is, not only relativistic effects but also the field-theoretic virtual annihilation effect. Note that the virtual annihilation interactions follow naturally from the variational derivation of Eq. (25); they are not put in by hand.

Physical effects beyond $O(\alpha^4)$ are not included completely. To do so would require the use of more sophisticated trial states than (16) or (17), as discussed, for example, in Ref. [58]. One could, of course, be less elegant, that is "cheat," by adding by hand higher-order invariant matrix elements (corresponding to one-loop, etc., Feynman diagrams) to the tree-level ones present in (25). However, we shall not pursue these questions further in this paper.

The nonrelativistic limit of Eq. (25) corresponds to $\mathbf{p}^2/m^2 \ll 1$. In this limit $D_{\mu\nu}$ in the expressions for $\mathcal{M}^{\text{Attractive}}_{s_j s_k s_j' s_k'}$, $\mathcal{M}^{\text{Repulsive}}_{s_j s_k s_j' s_k'}$, and $\mathcal{M}^{\text{Annihilation}}_{s_j s_k s_j' s_k'}$ reduce to $D_{00} = 1/|\mathbf{q}-\mathbf{p}|^2$ (and zero otherwise) for the attractive and repulsive terms, and $D_{\mu\nu} = -g_{\mu\nu}/4m^2$ for the annihilation terms. Thus, in the nonrelativistic limit,

$$\tilde{\mathcal{M}}^{\text{Attractive}}_{s_j s_k s_j' s_k'} = 2\bar{u}(0, s_j') \gamma^0 u(0, s_j) \frac{1}{|\mathbf{p}_j' - \mathbf{p}_j|^2} \bar{v}(0, s_k) \gamma^0 v(0, s_k')$$
$$= \frac{2\delta_{s_j s_j'} \delta_{s_k s_k'}}{|\mathbf{p}_j' - \mathbf{p}_j|^2}, \tag{26}$$

$$\tilde{\mathcal{M}}^{\text{Repulsive}}_{s_j s_k s_j' s_k'} = 2\bar{u}(0, s_j') \gamma^0 u(0, s_j) \frac{1}{|\mathbf{p}_j' - \mathbf{p}_j|^2} \bar{u}(0, s_k') \gamma^0 u(0, s_k)$$
$$= \frac{2\delta_{s_j s_j'} \delta_{s_k s_k'}}{|\mathbf{p}_j' - \mathbf{p}_j|^2}, \tag{27}$$

and

$$\tilde{\mathcal{M}}^{\text{Annihilation}}_{s_j s_k s_j' s_k'} = -2\bar{u}(0, s_j') \gamma^\mu v(0, s_k') \frac{g_{\mu\nu}}{4m^2} \bar{v}(0, s_k) \gamma^\nu u(0, s_j)$$
$$= \frac{A_{s_j s_k s_j' s_k'}}{2m^2}, \tag{28}$$

where the nonzero elements of $A_{s_j s_k s_j' s_k'}$ are

$$A_{1111} = A_{2222} = 2$$

and

$$A_{1212} = A_{1221} = A_{2112} = A_{2121} = 1. \tag{29}$$

We use the notation that the subscripts 1 and 2 (or $\uparrow$ and $\downarrow$) correspond to $M_s = 1/2$ and $M_s = -1/2$, respectively. Note that because of the expression $\delta^3(\mathbf{p}_j' + \mathbf{p}_k' - \mathbf{p}_j - \mathbf{p}_k)$ in the wave equation (25), we can use either $1/|\mathbf{p}_j' - \mathbf{p}_j|^2$ or $1/|\mathbf{p}_k' - \mathbf{p}_k|^2$ in $\tilde{\mathcal{M}}^{\text{Attractive}}_{s_j s_k s_j' s_k'}$ and $\tilde{\mathcal{M}}^{\text{Repulsive}}_{s_j s_k s_j' s_k'}$.

For arbitrary n, the coordinate-space equation, obtained by Fourier transformation of the nonrelativistic limit of Eq. (25), is the n-body Schrödinger equation,

$$\Bigg(-\frac{1}{2m} \sum_{i=1}^{n} \nabla_i^2 - \epsilon - \sum_{j=1}^{n-1} \sum_{k=j+1}^{n}{}' \frac{\alpha}{|\mathbf{x}_j - \mathbf{x}_k|}$$
$$+ \sum_{j=1}^{n-2} \sum_{k=j+2}^{n}{}' \frac{\alpha}{|\mathbf{x}_j - \mathbf{x}_k|} \Bigg) \Psi_{s_1 \cdots s_n}(\mathbf{x}_1, \ldots, \mathbf{x}_n)$$
$$= -\frac{\alpha\pi}{m^2} \sum_{j=1}^{n-1} \sum_{k=j+1}^{n}{}' \delta(\mathbf{x}_j - \mathbf{x}_k) \sum_{s_1' \ldots s_n'} A_{s_j s_k s_j' s_k'}$$
$$\times \prod_{i=1\cdots n}^{(j,k)} \delta_{s_i' s_i} \Psi_{s_1' \cdots s_n'}(\mathbf{x}_1, \ldots, \mathbf{x}_n), \tag{30}$$

where $\epsilon=E-nm$, $\alpha=e^2/4\pi$, and $\Sigma'_{k=a}u_k$ means $u_a+u_{a+2}+u_{a+4}+\cdots$.

In the strict nonrelativistic limit, the virtual annihilation δ function potentials should be neglected, since they are really relativistic effects that contribute in $O(\alpha)^4$ to the nonrelativistic $[O(\alpha^2)]$ energies. If they are neglected [i.e., $A_{s_j s_k s'_j s'_k}=0$ in Eq. (30)], we see that the same equations are obtained for all $\Psi_{s_1\cdots s_n}$ (or, equivalently, for all $F_{s_1\cdots s_n}$), hence the spin and space parts of the nonrelativistic wave functions separate, and we can write

$$\Psi_{s_1 s_2\cdots s_n}(\mathbf{x}_1,\ldots,\mathbf{x}_n)=\sum_{s_1\cdots s_n}\Lambda_{s_1 s_2\cdots s_n}\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_n). \quad (31)$$

The quantities $\Lambda_{s_1 s_2\cdots s_n}$ are constants needed to specify the (total) spin of the states under consideration. Thus, states of given total spin would be specified by appropriate linear combinations of the form (31) such that the result is an eigenstate of total spin quantum numbers S and M_S.

IV. TWO-BODY (POSITRONIUM), THREE-BODY (Ps^-), AND FOUR-BODY (Ps_2, POSITRONIUM MOLECULE) EXAMPLES

A. Two-body problem (positronium, e^-e^+)

It is instructive to write out the $n=2$, $n=3$, and $n=4$ cases explicitly. Thus, for the two-body problem (e^-e^+), for which the trial state is

$$|\psi_2\rangle=\sum_{s_1 s_2}\int d^3p_1 d^3p_2 F_{s_1 s_2}(\mathbf{p}_1,\mathbf{p}_2)b^\dagger(\mathbf{p}_1,s_1)d^\dagger(\mathbf{p}_2,s_2)|0\rangle, \quad (32)$$

we obtain the following wave equation:

$$\begin{aligned}F_{s_1 s_2}(\mathbf{p}_1,\mathbf{p}_2)[\omega_{p_1}+\omega_{p_2}-E]&=\frac{m^2e^2}{2(2\pi)^3}\sum_{s'_1 s'_2}\int d^3p'_1 d^3p'_2 F_{s'_1 s'_2}(\mathbf{p}'_1,\mathbf{p}'_2)\\&\times\frac{\delta^3(\mathbf{p}'_1+\mathbf{p}'_2-\mathbf{p}_1-\mathbf{p}_2)}{\sqrt{\omega_{p'_1}\omega_{p'_2}\omega_{p_1}\omega_{p2}}}\\&\times[\mathcal{M}^{\text{Attractive}}_{s_1 s_2 s'_1 s'_2}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}'_1,\mathbf{p}'_2)\\&-\mathcal{M}^{\text{Annihilation}}_{s_1 s_2 s'_1 s'_2}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}'_1,\mathbf{p}'_2)],\end{aligned} \quad (33)$$

$$\begin{aligned}\mathcal{M}^{\text{Attractive}}_{s_1 s_2 s'_1 s'_2}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}'_1,\mathbf{p}'_2)&=\bar{u}(\mathbf{p}'_1,s'_1)\gamma^\mu u(\mathbf{p}_1,s_1)\\&\times[D_{\mu\nu}(\omega_{p'_1}-\omega_{p_1},\mathbf{p}'_1-\mathbf{p}_1)\\&+D_{\mu\nu}(\omega_{p'_2}-\omega_{p_2},\mathbf{p}'_2-\mathbf{p}_2)]\\&\times\bar{v}(\mathbf{p}_2,s_2)\gamma^\nu v(\mathbf{p}'_2,s'_2),\end{aligned} \quad (34)$$

$$\begin{aligned}\mathcal{M}^{\text{Annihilation}}_{s_1 s_2 s'_1 s'_2}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}'_1,\mathbf{p}'_2)&=\bar{u}(\mathbf{p}'_1,s'_1)\gamma^\mu v(\mathbf{p}'_2,s'_2)\\&\times[D_{\mu\nu}(\omega_{p'_1}+\omega_{p'_2},\mathbf{p}'_1+\mathbf{p}'_2)\\&+D_{\mu\nu}(-\omega_{p_1}-\omega_{p_2},-\mathbf{p}_1-\mathbf{p}_2)]\\&\times\bar{v}(\mathbf{p}_2,s_2)\gamma^\nu u(\mathbf{p}_1,s_1).\end{aligned} \quad (35)$$

Note that there is no repulsive term for the two-body case.

Equations (33)–(35) were derived previously by Terekidi and Darewych [57] who showed that they yield results for the bound-state energies (including virtual annihilation) agree with earlier calculation to $O(\alpha^4)$ for all states.

In the nonrelativistic limit, the wave equation (33) for the two-body system (e^-e^+) is

$$\begin{aligned}F_{s_1 s_2}(\mathbf{p}_1,\mathbf{p}_2)\left(\frac{\mathbf{p}_1^2}{2m}+\frac{\mathbf{p}_2^2}{2m}-\epsilon\right)&=\frac{e^2}{(2\pi)^3}\sum_{s'_1 s'_2}\int d^3p'_1 d^3p'_2 F_{s'_1 s'_2}(\mathbf{p}'_1,\mathbf{p}'_2)\\&\times\delta^3(\mathbf{p}'_1+\mathbf{p}'_2-\mathbf{p}_1-\mathbf{p}_2)\left(\frac{\delta_{s_1 s'_1}\delta_{s_2 s'_2}}{|\mathbf{p}'_1-\mathbf{p}_1|^2}-\frac{A_{s_1 s_2 s'_1 s'_2}}{4m^2}\right),\end{aligned} \quad (36)$$

where $\epsilon=E-2m$. The coordinate-space form of Eq. (36), obtained via the Fourier transform

$$\begin{aligned}F_{s_1 s_2\cdots s_n}(\mathbf{p}_1,\ldots,\mathbf{p}_n)&=\frac{1}{(2\pi)^{3n/2}}\int d^3x_1\cdots d^3x_n\Psi_{s_1 s_2\cdots s_n}(\mathbf{x}_1,\ldots,\mathbf{x}_n)\\&\times e^{-i(\mathbf{p}_1\cdot\mathbf{x}_1+\cdots+\mathbf{p}_n\cdot\mathbf{x}_n)}\end{aligned} \quad (37)$$

is

$$\begin{aligned}\left(-\frac{1}{2m}\sum_{i=1}^{2}\nabla_i^2-\frac{\alpha}{|\mathbf{x}_1-\mathbf{x}_2|}-\epsilon\right)\Psi_{s_1 s_2}(\mathbf{x}_1,\mathbf{x}_2)&\\+\frac{\pi\alpha}{m^2}\delta(\mathbf{x}_1-\mathbf{x}_2)\sum_{s'_1 s'_2}A_{s_1 s_2 s'_1 s'_2}\Psi_{s'_1 s'_2}(\mathbf{x}_1,\mathbf{x}_2)&=0,\end{aligned} \quad (38)$$

where $\alpha=e^2/4\pi$ is the usual fine-structure constant. We see that the virtual annihilation interaction, in lowest order, is a contact (δ function) potential, which only affects states for which $\Psi_{s_1 s_2}(\mathbf{x}_1,\mathbf{x}_1)\neq 0$ [or $\Psi(0)\neq 0$ in the rest frame], that is states with $\ell=0$ only.

In fact, from Eq. (36) it is evident that the virtual annihilation contribution is negligible in the nonrelativistic limit ($\mathbf{p}^2\ll m^2$), hence only the Coulomb potential remains. Thus, the strict nonrelativistic limit of (33) corresponds to the usual Schrödinger equation with a Coulomb potential only [i.e., Eqs. (36) and (38) with $A_{s_1 s_2 s'_1 s'_2}=0$], for which the spin dependence separates, $\Psi_{s_1 s_2}(\mathbf{r})=\Lambda_{s_1 s_2}\psi(\mathbf{r})$ (in the rest frame). Therefore, we have the usual hydrogenlike positronium solutions $\psi_{n\ell m_\ell}(\mathbf{r})$ with $\epsilon_n=-\frac{1}{4}m\alpha^2\frac{1}{n^2}$ (here n is the principal quantum number).

Multiplying both sides of Eq. (38) by $\psi^*(\mathbf{r})$, integrating over $\mathbf{r}$, with $\int\psi^*(\mathbf{r})\psi(\mathbf{r})d^3r=1$, and summing over $\Sigma_{s_1 s_2}\Lambda_{s_1 s_2}$ with $\Sigma_{s_1 s_2}\Lambda^*_{s_1 s_2}\Lambda_{s_1 s_2}=1$, we obtain, in the rest frame,

$$(\epsilon_n - \epsilon) + \frac{\pi\alpha}{m^2}\int d^3r|\psi(\mathbf{r})|^2\delta(\mathbf{r})\left(\sum_{s_1s_2s_1's_2'}\Lambda^S_{s_1s_2}A_{s_1s_2s_1's_2'}\Lambda^S_{s_1's_2'}\right) = 0. \tag{39}$$

Recall that the two-body nonrelativistic solutions are grouped into singlets, corresponding to total spin quantum number $S=0$, and triplets with $S=1$. They are $\psi^S(\mathbf{r}) = \psi(\mathbf{r})\Sigma_{s_1s_2}\Lambda^S_{s_1s_2}$, where the nonzero elements of the coefficients $\Lambda^S_{s_1s_2}$ are $\Lambda^{S=0}_{12}=-\Lambda^{S=0}_{21}=1/\sqrt{2}$ and $\Lambda^{S=1}_{11}=1$ for $M_S=+1$, $\Lambda^{S=1}_{12}=\Lambda^{S=1}_{21}=1/\sqrt{2}$ for $M_S=0$ and $\Lambda^{S=1}_{22}=1$ for $M_S=-1$. It follows straightforwardly from Eq. (39) that the perturbative correction to the nonrelativistic energy of a fermion-antifermion system, due to the virtual annihilation interaction, is given by

$$\Delta E^{\text{Annihilation}}_S = \frac{\pi\alpha}{m^2}|\psi(0)|^2\Lambda_S = \frac{\pi\alpha}{m^2}|\psi(0)|^2 2\delta_{S1} = m\alpha^4\frac{1}{4n^3}\delta_{\ell 0}\delta_{S1}, \tag{40}$$

where $\Lambda_S=\Sigma_{s_1s_2s_1's_2'}\Lambda^S_{s_1s_2}A_{s_1s_2s_1's_2'}\Lambda^S_{s_1's_2'}$. This is a well-known result [18].

B. Three-body problem (positronium negative ion, Ps^-, $e^-e^+e^-$)

For the Ps^- case ($e^-e^+e^-$), with the trial state [cf. Eq. (17)]

$$|\psi_3\rangle = \sum_{s_1s_2s_3}\int d^3p_1d^3p_2d^3p_3F_{s_1s_2s_3}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3) \times b^\dagger(\mathbf{p}_1,s_1)d^\dagger(\mathbf{p}_2,s_2)b^\dagger(\mathbf{p}_3,s_3)|0\rangle, \tag{41}$$

the three-body wave equation is the following:

$$\begin{aligned}
&F_{s_1s_2s_3}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3)(\omega_{p_1}+\omega_{p_2}+\omega_{p_3}-E)\\
&\quad=\frac{m^2e^2}{2(2\pi)^3}\sum_{s_1's_2's_3'}\int d^3p_1'd^3p_2'd^3p_3'F_{s_1's_2's_3'}(\mathbf{p}_1',\mathbf{p}_2',\mathbf{p}_3')\\
&\quad\times\Bigg(\left[\mathcal{M}^{\text{Attractive}}_{s_1s_2s_1's_2'}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_1',\mathbf{p}_2')-\mathcal{M}^{\text{Annihilation}}_{s_1s_2s_1's_2'}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_1',\mathbf{p}_2')\right]\delta_{s_3's_3}\delta^3(\mathbf{p}_3'-\mathbf{p}_3)\frac{\delta^3(\mathbf{p}_1'+\mathbf{p}_2'-\mathbf{p}_1-\mathbf{p}_2)}{\sqrt{\omega_{p_1'}\omega_{p_2'}\omega_{p_1}\omega_{p_2}}}\\
&\quad+\left[\mathcal{M}^{\text{Attractive}}_{s_2s_3s_2's_3'}(\mathbf{p}_2,\mathbf{p}_3,\mathbf{p}_2',\mathbf{p}_3')-\mathcal{M}^{\text{Annihilation}}_{s_2s_3s_2's_3'}(\mathbf{p}_2,\mathbf{p}_3,\mathbf{p}_2',\mathbf{p}_3')\right]\delta_{s_1's_1}\delta^3(\mathbf{p}_1'-\mathbf{p}_1)\frac{\delta^3(\mathbf{p}_2'+\mathbf{p}_3'-\mathbf{p}_2-\mathbf{p}_3)}{\sqrt{\omega_{p_2'}\omega_{p_3'}\omega_{p_2}\omega_{p_3}}}\\
&\quad-\mathcal{M}^{\text{Repulsive}}_{s_1s_3s_1's_3'}(\mathbf{p}_1,\mathbf{p}_3,\mathbf{p}_1',\mathbf{p}_3')\delta_{s_2's_2}\delta^3(\mathbf{p}_2'-\mathbf{p}_2)\frac{\delta^3(\mathbf{p}_1'+\mathbf{p}_3'-\mathbf{p}_1-\mathbf{p}_3)}{\sqrt{\omega_{p_1'}\omega_{p_3'}\omega_{p_1}\omega_{p_3}}}\Bigg).
\end{aligned} \tag{42}$$

The expressions for $\mathcal{M}^{\text{Attractive}}_{s_js_ks_j's_k'}$, $\mathcal{M}^{\text{Repulsive}}_{s_js_ks_j's_k'}$, and $\mathcal{M}^{\text{Annihilation}}_{s_js_ks_j's_k'}$ are given in Eqs. (22)–(24), respectively.

Equation (42) was derived earlier by Barham [59] (see also Barham and Darewych [60]), who used it to calculate perturbatively relativistic corrections for Ps^- ground-state energy in the present formalism. These were found to be in reasonable agreement with calculations of relativistic corrections by Drake and Grigorescu [28], Frolov [61], and Bhatia and Drachman [62].

In the nonrelativistic limit, Eq. (42) reduces to the following:

$$\begin{aligned}
F_{s_1s_2s_3}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3)\left(\frac{\mathbf{p}_1^2}{2m}+\frac{\mathbf{p}_2^2}{2m}+\frac{\mathbf{p}_3^2}{2m}-\epsilon_3\right) &= \frac{e^2}{(2\pi)^3}\sum_{s_1's_2's_3'}\int d^3p_1'd^3p_2'd^3p_3'F_{s_1's_2's_3'}(\mathbf{p}_1',\mathbf{p}_2',\mathbf{p}_3')\\
&\times\Bigg[\left(\frac{\delta_{s_1s_1'}\delta_{s_2s_2'}\delta_{s_3's_3}}{|\mathbf{p}_1'-\mathbf{p}_1|^2}-\frac{1}{4m^2}A_{s_1s_2s_1's_2'}\delta_{s_3's_3}\right)\delta^3(\mathbf{p}_3'-\mathbf{p}_3)\delta^3(\mathbf{p}_1'+\mathbf{p}_2'-\mathbf{p}_1-\mathbf{p}_2)\\
&+\left(\frac{\delta_{s_1's_1}\delta_{s_2s_2'}\delta_{s_3's_3}}{|\mathbf{p}_2'-\mathbf{p}_2|^2}-\frac{1}{4m^2}A_{s_2s_3s_2's_3'}\delta_{s_1's_1}\right)\delta^3(\mathbf{p}_1'-\mathbf{p}_1)\delta^3(\mathbf{p}_2'+\mathbf{p}_3'-\mathbf{p}_2-\mathbf{p}_3)\\
&-\frac{1}{|\mathbf{p}_1'-\mathbf{p}_1|^2}\delta_{s_1's_1}\delta_{s_2s_2'}\delta_{s_3's_3}\delta^3(\mathbf{p}_2'-\mathbf{p}_2)\delta^3(\mathbf{p}_1'+\mathbf{p}_3'-\mathbf{p}_1-\mathbf{p}_3)\Bigg],
\end{aligned} \tag{43}$$

where $\epsilon_3=E-3m$. In the coordinate space, this becomes the following expression:

$$\left[-\frac{1}{2m}\left(\sum_{i=1}^{3}\nabla_i^2\right)-\epsilon_3-\frac{\alpha}{|\mathbf{x}_1-\mathbf{x}_2|}-\frac{\alpha}{|\mathbf{x}_2-\mathbf{x}_3|}+\frac{\alpha}{|\mathbf{x}_1-\mathbf{x}_3|}\right]\times\Psi_{s_1s_2s_3}(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)$$
$$=-\frac{\alpha\pi}{m^2}\delta(\mathbf{x}_1-\mathbf{x}_2)\sum_{s_1's_2's_3'}A_{s_1s_2s_1's_2'}\delta_{s_3's_3}\Psi_{s_1's_2's_3'}(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)$$
$$-\frac{\alpha\pi}{m^2}\delta(\mathbf{x}_2-\mathbf{x}_3)\sum_{s_1's_2's_3'}A_{s_2s_3s_2's_3'}\delta_{s_1's_1}\Psi_{s_1's_2's_3'}(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3), \tag{44}$$

where $\alpha=e^2/4\pi$. On the right-hand side of Eq. (44) we have the virtual annihilation terms for the Ps^- system. As noted in the Ps case, in the strict nonrelativistic limit, the virtual annihilation δ function potentials should be neglected, since they are really relativistic effects that contribute in $O(\alpha)^4$ to the nonrelativistic $[O(\alpha^2)]$ energies.

The virtual annihilation terms are generally not discussed for the Ps^- system in the literature. We show below that for the ground-state energy of the Ps^-, the contribution of virtual annihilation interaction is zero to the order $O(\alpha)^4$. Of course, for (virtual) excited bound states of Ps^- (that is, the position of resonances in e^--Ps scattering) the order $O(\alpha)^4$ contribution of virtual annihilation interaction terms is not necessarily zero.

For perturbative $O(\alpha)^4$ calculations we can take the eight adjustable functions of the trial state (41) to be of the following separable form:

$$F_{s_1s_2s_3}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3)=\sum_{s_1,s_2,s_3}\Lambda_{s_1s_2s_3}f(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3), \tag{45}$$

where $f(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3)$ is an adjustable function and $\Lambda_{s_1s_2s_3}$ are a set of constants specifying the spin configuration. Correspondingly, in configuration space

$$\Psi_{s_1s_2s_3}(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)=\sum_{s_1,s_2,s_3}\Lambda_{s_1s_2s_3}\Psi(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3). \tag{46}$$

For the ground-state energy of the Ps^- we shall consider the following two specific cases:

$$(1)\quad \Lambda_{121}=-\Lambda_{211}=\frac{1}{\sqrt{2}},\ \text{and otherwise } 0, \tag{47}$$

for all s_1, s_2, $S=1/2$, $M_s=1/2$, and

$$(2)\quad \Lambda_{122}=-\Lambda_{212}=\frac{1}{\sqrt{2}},\ \text{and otherwise } 0, \tag{48}$$

for all s_1, s_2, $S=1/2$, $M_s=-1/2$, where S is the total spin and M_s is the spin projection quantum number of the state. For both cases, the spin part of the adjustable function is normalized such that $\Sigma_{s_1s_2s_3}\Lambda^*_{s_1s_2s_3}\Lambda_{s_1s_2s_3}=1$. Recall that we use the notation that the subscripts 1 and 2 (or $\uparrow$ and $\downarrow$) correspond to $M_s=1/2$ and $M_s=-1/2$, respectively. Note that the trial state takes a form in which particles 1 and 2 are described by a spin singlet state; for the first case, particle 3 is in a spin-up state and for the second case, particle 3 is in a spin-down state. The nonzero elements of $A_{s_js_ks_j's_k'}$ are given in Eq. (29).

We multiply both sides of Eq. (44) by $\Psi^*(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)\Lambda^*_{s_1s_2s_3}$ and integrate over the spatial coordinates. The wave functions are taken to be normalized, i.e.,

$$\int\Psi^*(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)\Psi(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)d^3\mathbf{x}_1d^3\mathbf{x}_2d^3\mathbf{x}_3=1, \tag{49}$$

and we sum over $s_1s_2s_3$, $\Sigma_{s_1s_2s_3}\Lambda^*_{s_1s_2s_3}\Lambda_{s_1s_2s_3}=1$. The resulting contribution to the energy of the virtual annihilation interaction is

$$\Delta E^{\text{virtual annihilation}}=\frac{\alpha\pi}{m^2}\int d^3\mathbf{x}_1d^3\mathbf{x}_2d^3\mathbf{x}_3|\Psi(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)|^2\delta(\mathbf{x}_1-\mathbf{x}_2)\times\sum_{\substack{s_1s_2s_3\\s_1's_2's_3'}}\Lambda^s_{s_1s_2s_3}A_{s_1s_2s_1's_2'}\Lambda^s_{s_1's_2's_3'}\delta_{s_3's_3}$$
$$+\frac{\alpha\pi}{m^2}\int d^3\mathbf{x}_1d^3\mathbf{x}_2d^3\mathbf{x}_3|\Psi(\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3)|^2\delta(\mathbf{x}_2-\mathbf{x}_3)\times\sum_{\substack{s_1s_2s_3\\s_1's_2's_3'}}\Lambda^s_{s_1s_2s_3}A_{s_2s_3s_2's_3'}\Lambda^s_{s_1's_2's_3'}\delta_{s_1's_1}. \tag{50}$$

There are two virtual annihilation terms on the right-hand side of Eq. (50); one annihilation term between electron with index (1) and positron with index (2), and the second term is between electron with index (3) and positron with index (2). The calculations of the contribution of these two terms are similar. For example, for the first term on the right-hand side of (50), if we let

$$\Lambda^s_1=\sum_{\substack{s_1s_2s_3\\s_1's_2's_3'}}\Lambda^s_{s_1s_2s_3}A_{s_1s_2s_1's_2'}\Lambda^s_{s_1's_2's_3'}\delta_{s_3's_3}, \tag{51}$$

using the numbers given in Eqs. (47), (48), and (29), we obtain

$$\Lambda^s_1=\left(\frac{1}{\sqrt{2}}\ \ 1\ \ \frac{1}{\sqrt{2}}\right)+\left(\frac{1}{\sqrt{2}}\ \ 1\ \ \frac{-1}{\sqrt{2}}\right)+\left(\frac{-1}{\sqrt{2}}\ \ 1\ \ \frac{-1}{\sqrt{2}}\right)+\left(\frac{-1}{\sqrt{2}}\ \ 1\ \ \frac{1}{\sqrt{2}}\right)=0, \tag{52}$$

for both $S=1/2$, $M_s=+1/2$ and $S=1/2$, $M_s=-1/2$. For the second virtual annihilation term in Eq. (50), similarly (we call it Λ^s_2), we obtain $\Lambda^s_2=0$. Therefore, the total virtual annihilation interaction for the ground state of Ps^- $(e^-e^+e^-)$ is zero to order $O(\alpha)^4$.

Even though the virtual excited states of Ps^- $(e^-e^+e^-)$ have not been observed as yet, it is worthwhile to note that, for example, for the case where the two electrons and the positron have spin up $(S=3/2,\ M_s=3/2)$, we have $\Lambda^{s=3/2}_{111}=1$ and otherwise zero, and hence considering the numbers in Eq. (29), we obtain Λ^s_1 and $\Lambda^s_2\neq 0$. This means that the

contribution of the virtual annihilation interaction in this case is not zero.

C. Four-body problem (positronium molecule, Ps_2, $e^-e^+e^-e^+$)

For the four-body case ($e^-e^+e^-e^+$), with the trial state [cf. Eq. (16)],

$$|\psi_4\rangle = \sum_{s_1\cdots s_4} \int d^3p_1 \cdots d^3p_4 F_{s_1\cdots s_4}(\mathbf{p}_1, \ldots, \mathbf{p}_4) b^\dagger(\mathbf{p}_1, s_1) \times d^\dagger(\mathbf{p}_2, s_2) b^\dagger(\mathbf{p}_3, s_3) d^\dagger(\mathbf{p}_4, s_4)|0\rangle, \tag{53}$$

we obtain the following wave equation:

$$\begin{aligned}
&F_{s_1s_2s_3s_4}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3,\mathbf{p}_4)(\omega_{p_1}+\omega_{p_2}+\omega_{p_3}+\omega_{p_4}-E)\\
&\quad=\frac{m^2e^2}{2(2\pi)^3}\sum_{s_1's_2's_3's_4'}\int d^3p_1'd^3p_2'd^3p_3'd^3p_4' F_{s_1's_2's_3's_4'}(\mathbf{p}_1',\mathbf{p}_2',\mathbf{p}_3',\mathbf{p}_4')\\
&\qquad\times\Bigg(\mathcal{M}^A_{s_1s_2s_1's_2'}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_1',\mathbf{p}_2')\delta_{s_3's_3}\delta_{s_4's_4}\delta^3(\mathbf{p}_3'-\mathbf{p}_3)\delta^3(\mathbf{p}_4'-\mathbf{p}_4)\frac{\delta^3(\mathbf{p}_1'+\mathbf{p}_2'-\mathbf{p}_1-\mathbf{p}_2)}{\sqrt{\omega_{p_1'}\omega_{p_2'}\omega_{p_1}\omega_{p_2}}}\\
&\qquad+\mathcal{M}^A_{s_2s_3s_2's_3'}(\mathbf{p}_2,\mathbf{p}_3,\mathbf{p}_2',\mathbf{p}_3')\delta_{s_1's_1}\delta_{s_4's_4}\delta^3(\mathbf{p}_1'-\mathbf{p}_1)\delta^3(\mathbf{p}_4'-\mathbf{p}_4)\frac{\delta^3(\mathbf{p}_2'+\mathbf{p}_3'-\mathbf{p}_2-\mathbf{p}_3)}{\sqrt{\omega_{p_2'}\omega_{p_3'}\omega_{p_2}\omega_{p_3}}}\\
&\qquad+\mathcal{M}^A_{s_3s_4s_3's_4'}(\mathbf{p}_3,\mathbf{p}_4,\mathbf{p}_3',\mathbf{p}_4')\delta_{s_1's_1}\delta_{s_2's_2}\delta^3(\mathbf{p}_1'-\mathbf{p}_1)\delta^3(\mathbf{p}_2'-\mathbf{p}_2)\frac{\delta^3(\mathbf{p}_3'+\mathbf{p}_4'-\mathbf{p}_3-\mathbf{p}_4)}{\sqrt{\omega_{p_3'}\omega_{p_4'}\omega_{p_3}\omega_{p_4}}}\\
&\qquad+\mathcal{M}^A_{s_1s_4s_1's_4'}(\mathbf{p}_1,\mathbf{p}_4,\mathbf{p}_1',\mathbf{p}_4')\delta_{s_2's_2}\delta_{s_3's_3}\delta^3(\mathbf{p}_2'-\mathbf{p}_2)\delta^3(\mathbf{p}_3'-\mathbf{p}_3)\frac{\delta^3(\mathbf{p}_1'+\mathbf{p}_4'-\mathbf{p}_1-\mathbf{p}_4)}{\sqrt{\omega_{p_1'}\omega_{p_4'}\omega_{p_1}\omega_{p_4}}}\\
&\qquad-\mathcal{M}^{\text{Repulsive}}_{s_1s_3s_1's_3'}(\mathbf{p}_1,\mathbf{p}_3,\mathbf{p}_1',\mathbf{p}_3')\delta_{s_2's_2}\delta_{s_4's_4}\delta^3(\mathbf{p}_2'-\mathbf{p}_2)\delta^3(\mathbf{p}_4'-\mathbf{p}_4)\frac{\delta^3(\mathbf{p}_1'+\mathbf{p}_3'-\mathbf{p}_1-\mathbf{p}_3)}{\sqrt{\omega_{p_1'}\omega_{p_3'}\omega_{p_1}\omega_{p_3}}}\\
&\qquad-\mathcal{M}^{\text{Repulsive}}_{s_2s_4s_2's_4'}(\mathbf{p}_2,\mathbf{p}_4,\mathbf{p}_2',\mathbf{p}_4')\delta_{s_1's_1}\delta_{s_3's_3}\delta^3(\mathbf{p}_1'-\mathbf{p}_1)\delta^3(\mathbf{p}_3'-\mathbf{p}_3)\frac{\delta^3(\mathbf{p}_2'+\mathbf{p}_4'-\mathbf{p}_2-\mathbf{p}_4)}{\sqrt{\omega_{p_2'}\omega_{p_4'}\omega_{p_2}\omega_{p_4}}}\Bigg),
\end{aligned}\tag{54}$$

where $\mathcal{M}^A_{s_1s_2s_1's_2'}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_1',\mathbf{p}_2')=\mathcal{M}^{\text{Attractive}}_{s_1s_2s_1's_2'}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_1',\mathbf{p}_2')-\mathcal{M}^{\text{Annihilation}}_{s_1s_2s_1's_2'}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_1',\mathbf{p}_2')$, etc. The expressions for $\mathcal{M}^{\text{Attractive}}_{s_js_ks_j's_k'}$, $\mathcal{M}^{\text{Repulsive}}_{s_js_ks_j's_k'}$, and $\mathcal{M}^{\text{Annihilation}}_{s_js_ks_j's_k'}$ are given in Eqs. (22)–(24).

For the four-body system (Ps_2, $e^-e^+e^-e^+$), in the nonrelativistic limit $\mathbf{p}^2/m^2 \ll 1$, keeping lowest order nontrivial terms, Eq. (54) reduces to the following equation:

$$\begin{aligned}
&F_{s_1s_2s_3s_4}(\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3,\mathbf{p}_4)\left(\frac{\mathbf{p}_1^2}{2m}+\frac{\mathbf{p}_2^2}{2m}+\frac{\mathbf{p}_3^2}{2m}+\frac{\mathbf{p}_4^2}{2m}-\epsilon_4\right)\\
&\quad=\frac{e^2}{(2\pi)^3}\sum_{s_1's_2's_3's_4'}\int d^3p_1'd^3p_2'd^3p_3'd^3p_4' F_{s_1's_2's_3's_4'}(\mathbf{p}_1',\mathbf{p}_2',\mathbf{p}_3',\mathbf{p}_4')\\
&\qquad\times\Bigg[\left(\frac{\delta_{s_1s_1'}\delta_{s_2s_2'}}{|\mathbf{p}_1'-\mathbf{p}_1|^2}-\frac{A_{s_1s_2s_1's_2'}}{4m^2}\right)\delta_{s_3's_3}\delta_{s_4's_4}\delta^3(\mathbf{p}_3'-\mathbf{p}_3)\delta^3(\mathbf{p}_4'-\mathbf{p}_4)\delta^3(\mathbf{p}_1'+\mathbf{p}_2'-\mathbf{p}_1-\mathbf{p}_2)\\
&\qquad+\left(\frac{\delta_{s_2s_2'}\delta_{s_3's_3}}{|\mathbf{p}_2'-\mathbf{p}_2|^2}-\frac{A_{s_2s_3s_2's_3'}}{4m^2}\right)\delta_{s_1s_1'}\delta_{s_4's_4}\delta^3(\mathbf{p}_1'-\mathbf{p}_1)\delta^3(\mathbf{p}_4'-\mathbf{p}_4)\delta^3(\mathbf{p}_2'+\mathbf{p}_3'-\mathbf{p}_2-\mathbf{p}_3)\\
&\qquad+\left(\frac{\delta_{s_3's_3}\delta_{s_4's_4}}{|\mathbf{p}_3'-\mathbf{p}_3|^2}-\frac{A_{s_3s_4s_3's_4'}}{4m^2}\right)\delta_{s_1s_1'}\delta_{s_2's_2}\delta^3(\mathbf{p}_1'-\mathbf{p}_1)\delta^3(\mathbf{p}_2'-\mathbf{p}_2)\delta^3(\mathbf{p}_3'+\mathbf{p}_4'-\mathbf{p}_3-\mathbf{p}_4)\\
&\qquad+\left(\frac{\delta_{s_1s_1'}\delta_{s_4's_4}}{|\mathbf{p}_1'-\mathbf{p}_1|^2}-\frac{A_{s_1s_4s_1's_4'}}{4m^2}\right)\delta_{s_2's_2}\delta_{s_3's_3}\delta^3(\mathbf{p}_2'-\mathbf{p}_2)\delta^3(\mathbf{p}_3'-\mathbf{p}_3)\delta^3(\mathbf{p}_1'+\mathbf{p}_4'-\mathbf{p}_1-\mathbf{p}_4)
\end{aligned}$$

$$- \delta_{s_1 s_1'} \delta_{s_2' s_2} \delta_{s_3' s_3} \delta_{s_4' s_4} \delta^3(\mathbf{p}_2' - \mathbf{p}_2) \delta^3(\mathbf{p}_4' - \mathbf{p}_4) \frac{\delta^3(\mathbf{p}_1' + \mathbf{p}_3' - \mathbf{p}_1 - \mathbf{p}_3)}{|\mathbf{p}_1' - \mathbf{p}_1|^2}$$

$$- \delta_{s_1 s_1'} \delta_{s_2' s_2} \delta_{s_3' s_3} \delta_{s_4' s_4} \delta^3(\mathbf{p}_1' - \mathbf{p}_1) \delta^3(\mathbf{p}_3' - \mathbf{p}_3) \frac{\delta^3(\mathbf{p}_2' + \mathbf{p}_4' - \mathbf{p}_2 - \mathbf{p}_4)}{|\mathbf{p}_2' - \mathbf{p}_2|^2} \Bigg], \tag{55}$$

where $\epsilon_4 = E - 4m$. Its coordinate-space version is the four-body Schrödinger equation, Eq. (30) with $n=4$. The interactions are described by attractive or repulsive Coulomb potentials and the repulsive contact (δ function) virtual annihilation potentials.

As mentioned in the Introduction, there are many calculations of the ground-state binding energy of the positronium molecule based on the nonrelativistic Schrödinger equation (see, for example, Refs. [40–51], and references therein). The majority of recent calculated values of the nonrelativistic binding energy of the positronium molecule are around 0.435 eV (for example, in [42]).

In a very recent work, Bubin *et al.* [51] reported that they have obtained a very accurate variational wave function for nonrelativistic binding energy of the positronium molecule (Ps_2), which they used to calculate the relativistic corrections. Their calculations were performed within the framework of the Breit-Pauli formalism. In this formalism, a quantum system is described by the Hamiltonian, $\hat{H}_{\text{tot}} = \hat{H}_{\text{nonrel}} + \alpha^2 \hat{H}_{\text{rel}}$, where $\hat{H}_{\text{nonrel}}$ is the Schrödinger Hamiltonian, and $\alpha^2 \hat{H}_{\text{rel}}$ is the relativistic corrections (α is the fine structure constant). Bubin *et al.* [51] solved the nonrelativistic problem variationally and used their solutions to calculate the relativistic corrections in first-order perturbation theory. Their result for the ground-state binding energy of Ps_2 is 0.015 954 25 hartree (i.e., 0.434 137 3 eV). This includes the $O(\alpha^2)$ relativistic corrections to the nonrelativistic ground-state energy of Ps_2.

In this paper we shall use Eq. (30) with $n=4$ to calculate perturbatively the $O(\alpha^4)$ virtual annihilation contribution to the Ps_2 ground-state energy in a manner analogous to that obtained for Ps earlier in Sec. IV, Eqs. (38) and (40). Our wave function is taken to be of the form

$$\Psi_{s_1 s_2 s_3 s_4}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4) = \sum_{s_1 \ldots s_4} \Lambda_{s_1 s_2 s_3 s_4} \Psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4). \tag{56}$$

For the ground state of the positronium molecule, with $S=0$ and $M_s=0$, the spin part of the wave function is given by the following expression [42]:

$$\chi_{00} = \frac{1}{2}(|\uparrow_1 \uparrow_2 \downarrow_3 \downarrow_4\rangle - |\uparrow_1 \downarrow_2 \downarrow_3 \uparrow_4\rangle - |\downarrow_1 \uparrow_2 \uparrow_3 \downarrow_4\rangle + |\downarrow_1 \downarrow_2 \uparrow_3 \uparrow_4\rangle), \tag{57}$$

where, for example, the notation $\downarrow_3$ means: particle 3 and spin down. Note that particles 1 and 3 are electrons and particles 2 and 4 are positrons. We recall that we use the notation that the subscript 1 corresponds to spin up ($\uparrow$), and the subscript 2 corresponds to spin down ($\downarrow$). Thus, the nonzero values of $\Lambda_{s_1 s_2 s_3 s_4}$ are

$$\Lambda_{1122} = \frac{1}{2}, \quad \Lambda_{1221} = -\frac{1}{2}, \quad \Lambda_{2112} = -\frac{1}{2}, \quad \Lambda_{2211} = \frac{1}{2}. \tag{58}$$

Multiplying Eq. (30) with $n=4$, by Ψ^*, integrating over the spatial coordinates and summing over the spin indices (the wave functions are taken to be normalized), gives the virtual annihilation contribution to the Ps_2 energy to be

$$\Delta E^{\text{virtual annihilation}} = \frac{\alpha\pi}{m^2} \int d^3\mathbf{x}_1 \cdots d^3\mathbf{x}_4 |\Psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4)|^2 \delta(\mathbf{x}_1 - \mathbf{x}_2) \sum_{\substack{s_1 s_2 s_3 s_4 \\ s_1' s_2' s_3' s_4'}} \Lambda^s_{s_1 s_2 s_3 s_4} A_{s_1 s_2 s_1' s_2'} \Lambda^s_{s_1' s_2' s_3' s_4'} \delta_{s_3' s_3} \delta_{s_4' s_4}$$

$$+ \frac{\alpha\pi}{m^2} \int d^3\mathbf{x}_1 \cdots d^3\mathbf{x}_4 |\Psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4)|^2 \delta(\mathbf{x}_2 - \mathbf{x}_3) \sum_{\substack{s_1 s_2 s_3 s_4 \\ s_1' s_2' s_3' s_4'}} \Lambda^s_{s_1 s_2 s_3 s_4} A_{s_2 s_3 s_2' s_3'} \Lambda^s_{s_1' s_2' s_3' s_4'} \delta_{s_1' s_1} \delta_{s_4' s_4}$$

$$+ \frac{\alpha\pi}{m^2} \int d^3\mathbf{x}_1 \cdots d^3\mathbf{x}_4 |\Psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4)|^2 \delta(\mathbf{x}_3 - \mathbf{x}_4) \sum_{\substack{s_1 s_2 s_3 s_4 \\ s_1' s_2' s_3' s_4'}} \Lambda^s_{s_1 s_2 s_3 s_4} A_{s_3 s_4 s_3' s_4'} \Lambda^s_{s_1' s_2' s_3' s_4'} \delta_{s_1' s_1} \delta_{s_2' s_2}$$

$$+ \frac{\alpha\pi}{m^2} \int d^3\mathbf{x}_1 \cdots d^3\mathbf{x}_4 |\Psi(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4)|^2 \delta(\mathbf{x}_1 - \mathbf{x}_4) \sum_{\substack{s_1 s_2 s_3 s_4 \\ s_1' s_2' s_3' s_4'}} \Lambda^s_{s_1 s_2 s_3 s_4} A_{s_1 s_4 s_1' s_4'} \Lambda^s_{s_1' s_2' s_3' s_4'} \delta_{s_2' s_2} \delta_{s_3' s_3}. \tag{59}$$

We see that in the above equation we have four virtual interaction terms for the Ps_2 system. The calculation of those four terms are similar. For example, for the first term on the right-hand side of Eq. (59), we let

$$\Lambda_1^s = \sum_{\substack{s_1 s_2 s_3 s_4 \\ s_1' s_2' s_3' s_4'}} \Lambda^s_{s_1 s_2 s_3 s_4} A_{s_1 s_2 s_1' s_2'} \Lambda^s_{s_1' s_2' s_3' s_4'} \delta_{s_3' s_3} \delta_{s_4' s_4}. \tag{60}$$

Using the numbers given in Eqs. (29) and (58), we obtain the following:

$$\Lambda_1^s = \left(\frac{1}{2}\ \ 2\ \ \frac{1}{2}\right) + \left(\frac{-1}{2}\ \ 1\ \ \frac{-1}{2}\right) + \left(\frac{-1}{2}\ \ 1\ \ \frac{-1}{2}\right) + \left(\frac{1}{2}\ \ 2\ \ \frac{1}{2}\right) = \frac{3}{2} \neq 0. \tag{61}$$

The contribution of the four virtual annihilation interaction terms for the ground-state energy of the positronium molecule Ps_2 is not zero to order $O(\alpha)^4$.

We estimate the order of magnitude of the virtual annihilation effects in the Ps_2 ground-state system, using the simple trial wave function of Hylleraas and Ore [39]. Although the Hylleraas and Ore wave function is rather crude (it gives the value of 0.115 eV for Ps_2 ground-state binding energy versus the accurate recent value of 0.434 eV [51]), it is sufficient for our illustrative purposes. The Hylleraas-Ore wave function is [39]

$$2\Psi = \exp\left[-\frac{1}{2}(1+b)(r_{12}+r_{34}) - \frac{1}{2}(1-b)(r_{14}+r_{23})\right] + \exp\left[-\frac{1}{2}(1-b)(r_{12}+r_{34}) - \frac{1}{2}(1+b)(r_{14}+r_{23})\right]. \tag{62}$$

Here the indices 1,3 refer to the two electrons, and 2,4 to the positrons, i.e., r_{12} represents the distance of positron 2 to electron 1, etc. b is a variational parameter. The above wave function is constructed so that it can describe the Ps_2 molecule in which each electron is strongly bound to one of the two positrons and only loosely bound to the second one. The case $b=1$ corresponds to two separate positronium atoms, whereas for $b=0$ we have the case of equal binding within all electron-positron pairs. Hylleraas and Ore [39] found the value of 0.115 eV for the Ps_2 ground-state binding energy with the variational parameter $b \simeq 0.70$ a.u. ($b^2=0.50$). Note also that the wave function in Eq. (62) is presented in atomic units (a.u.). The wave function (62) can equivalently be written in the following form:

$$\Psi = \exp\left(-\frac{1}{2}(w_1+w_2)\right)\cosh\frac{b(t_1-t_2)}{2}, \tag{63}$$

where

$$w_1 = r_{12}+r_{14}, \quad w_2 = r_{23}+r_{34}, \quad t_1 = r_{12}-r_{14}, \quad t_2 = r_{23}-r_{34}. \tag{64}$$

The corresponding volume element is

$$d\tau = dv\frac{1}{4}(w_1^2 - t_1^2)dw_1 dt_1 \frac{1}{4}(w_2^2 - t_2^2)dw_2 dt_2, \tag{65}$$

the limits of integration being $v \leq w_1, w_2 \leq +\infty$; $-v \leq t_1, t_2 \leq v$; and $0 \leq v \leq +\infty$.

The expression of virtual annihilation interactions contribution to the Ps_2 is [Eq. (59)]

$$\Delta E^{\text{virtual annihilation}} = \frac{\langle\Psi|:H^{\text{virtual annihilation}}:|\Psi\rangle}{C}, \tag{66}$$

where C is a constant which is equal to the norm of the wave function (63). Its expression is the following:

$$C = \int \Psi^2 d\tau = \frac{1}{2}\left(\frac{33}{8} + \frac{33/8 - 11b^2/4 + 5b^4/8}{(1-b^2)^3}\right). \tag{67}$$

As mentioned before, the computations of the four virtual annihilation terms of Eq. (59) are similar. Thus, for the first term on the right-hand side of Eq. (59), because of the term $\delta(\mathbf{x}_1 - \mathbf{x}_2)$ inside the integral, the position of particle 1 (e^-) will be the same position as particle 2 (e^+). Hence, Eq. (64) becomes the following expression:

$$w_1 = -t_1 = r_{14}, \quad w_2 = r_{23}+r_{34}, \quad t_2 = r_{23}-r_{34}. \tag{68}$$

Note that, now we have only three independent variables for the relative coordinates. We call them u, w, and t instead of w_1, w_2, and t_2, respectively. This means that Eq. (68) becomes

$$u = r_{14}, \quad w = r_{23}+r_{34}, \quad t = r_{23}-r_{34}. \tag{69}$$

The wave function in Eq. (63) for the first term of the virtual annihilation interaction in Eq. (59), using the variables of Eq. (69), can be written as follows:

$$\Psi = \exp\left(-\frac{1}{2}(w+u)\right)\cosh\frac{b(-u-t)}{2}. \tag{70}$$

The volume element corresponding to Eq. (69) is

$$d\tau' = \frac{1}{16}u(w^2 - t^2)dwdudt, \tag{71}$$

the limits of integration being $u \leq w \leq +\infty$, $-u \leq t \leq u$, and $0 \leq u \leq +\infty$.

The calculations of the four virtual annihilation terms of the positronium molecule and the computations of the multidimensional integrals inside those terms, though tedious, are similar and they can be done using, for example, Maple software. The numerical result for the contribution of virtual annihilation terms for the ground-state energy of the positronium molecule is (with $b \simeq 0.70$ a.u.) $\Delta E^{\text{virtual annihilation}} \simeq 10^{-4}$ eV. To our knowledge there is only the recent paper of Bubin *et al.* [51] in which the relativistic corrections to the nonrelativistic ground-state energy of the positronium molecule are worked out. For the virtual annihilation contribution Bubin *et al.* [51] found the value of 6.044×10^{-4} eV or 2.221×10^{-5} a.u. (from Table I of [51]; virtual annihilation term is $\alpha^2 H_A$ with $\alpha \simeq 1/137$ and $H_A \simeq 0.4169$ a.u. or hartree). Our result is only in order-of-magnitude agreement with the Bubin *et al.* value. This is not surprising given the

relative inaccuracy of the Hylleraas and Ore wave function as already pointed out.

V. CONCLUDING REMARKS

We have used the variational method within the Hamiltonian formalism of reformulated QED, with a simple Fock-space trial state, to derive relativistic momentum-space wave equations and the corresponding kernels (relativistic momentum-space potentials) for n-fermion systems. These include the familiar case of positronium (Ps, $n=2$), the positronium negative ion (Ps^-) system ($n=3$), the positronium molecule or Ps_2 (i.e., $e^+e^-e^+e^-$, $n=4$), and similar "exotic" neutral and negative-ion systems with $n>4$. Of course, the equations are applicable also to exotic systems in which e is replaced by μ.

The relativistic kinematics are included exactly in these equations, but the interactions contain tree-level interactions only (one-photon exchange and virtual annihilation), that is they are incomplete beyond $O(\alpha^4)$. The equations have positive-energy solutions only so that they are amenable to variational solution with no negative-energy-dissolution difficulties. There are no relative-time coordinates so that the equations yield wave functions in the usual Schrödinger sense. Indeed the equations are similar to relativistic generalizations of the n-body Schrödinger equations (to which they reduce in the nonrelativistic limit).

Since the method of deriving the equations (including the interactions) is variational, the description of the interactions can be improved systematically by using more elaborate n-body trial states than (16) and (17). This has been demonstrated recently for the well-known case of positronium ($n=2$) [58]. Doing so for higher n systems, such as Ps^- or Ps_2 is straightforward, though increasingly more tedious.

The recent observation of positronium molecule by Cassidy and Mills [34] raises interest in other exotic systems and polyelectrons with $n>4$ such as $e^-e^+e^-e^+e^-$, $n=5$ or $e^-e^+e^-e^+e^-e^+$, $n=6$. In 2001, a calculation of the five-body system ($e^-e^+e^-e^+e^-$, $n=5$) was reported by Mezei *et al.*, but a bound state was not found [63]. Mezei *et al.* used the stochastic variational method (SVM) for their calculations. The SVM and quantum Monte Carlo methods are popular among other methods for the computation of complicated systems [64].

It is not possible to solve the relativistic n-body equations (25) derived in the paper analytically, even in the nonrelativistic limit for $n>2$. Therefore, approximate (i.e., numerical, variational or perturbative) solutions must be sought for various cases of interest. Since n-body fermion-antifermion systems with electromagnetic interactions (such as Ps_2) are weakly bound and relativistic effects are small, perturbative solutions are generally sufficient. Nevertheless, approximate variational solutions of the n-body system can be obtained by replacing $F_{s_1 s_2 \cdots s_n}(\mathbf{p}_1, \ldots, \mathbf{p}_n)$ with analytical functions containing adjustable features (functions, parameters) to compute and minimize the expectation value of the Hamiltonian. For $n>2$ the evaluation of the multidimensional integrals that arise in the computation of the matrix elements is a challenging problem, requiring the use of methods such as Monte Carlo simulations [65]. We note that the relativistic equation (25) has solutions of positive energy only, hence no negative-energy difficulties would be encountered in variational approximations.

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