Production of Photons in Positronium Decay:

Critique of the Creation-Annihilation Hypothesis:

Part II

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Abstract

The Breit-Pauli Hamiltonian is adjusted through the addition of momentum-dependent exponential damping factors so that it possesses eigenfunctions which correspond to a tightly bound e^+e^- state with $2m_{oe}c^2$ binding energy. The success which the corresponding Schrödinger-type calculations achieves calls into question the creation-annihilation hypothesis on a completely general basis.

Keywords: Breit-Pauli Hamiltonian, Schrödinger equation, Photon, Positronium, Creation-Annihilation, Einstein $E=mc^2$ mass-energy equivalence relation

I. INTRODUCTION

In previous work[1] it has been suggested that there is merit in considering the decay of positronium as an interaction in which an electron and positron are so strongly attracted to one

another that the resulting binding energy is exactly equal to the sum of their rest masses, i.e. $2m_{oe}c^2$ or 1.02 MeV. In the present section, we will focus on the goal of finding a suitable potential which is capable of producing such a relatively large binding energy, while at the same time giving consideration to the possibility that the solution to this problem may have relevance for other types of interactions, particularly those involved in the study of nuclear physics.

II. VARIATIONAL THEORY FOR THE DECAY OF POSITRONIUM

A. A SHORT-RANGE POTENTIAL

The natural point at which to begin this investigation is with the nature of the potential which might be capable of bringing about such a strong attraction between an electron and a positron, although careful consideration must later be given to the manner in which the kinetic energy is treated as well. It is clear from the outset that this must be a distinctly relativistic problem, because the rest mass of the combined e^+e^- system is assumed to be much lower than the sum of those of the separated particles. Both the Schrödinger non-relativistic[2] and Dirac relativistic[3] treatments of positronium tell us that the lowest possible state for this system is analogous to the 1s state of the hydrogen atom. In this case the primary interaction is Coulombic, exclusively so in the non-relativistic treatment and almost exclusively in the relativistic.

A two-component reduction of the Dirac equation leads to the characterization of a number of perturbative terms which are basically magnetic in nature. The most commonly employed such approximation is that of Breit-Pauli theory,[4-6] including the Breit interaction. The perturbations are on the order of $\alpha^2/2 \cong 10^{-5}$ hartree ($\alpha = e^2/2\varepsilon_0 hc = 0.007297 = 137.036^{-1}$, the fine structure constant), and include the spin-orbit (same- and other-orbit), spin-spin, orbit-orbit and Darwin terms, as well as the mass-velocity correction to the non-relativistic kinetic energy.[4] These terms increase as Z^3 or Z^4 (spin-same-orbit) for atoms with nuclear charge Z. For positronium as well as the hydrogen atom they remain quite small, however, and their effects are observed only as fine structure in spectroscopic studies. The potential terms all vary as r^{-3} and thus have relatively short ranges compared to the Coulomb interaction. This point bears further consideration, however, since binding energies of 1.0 MeV and higher are otherwise known only for nuclei, in which case there is clear evidence that short-range forces are involved to a high degree.

We can represent the presumed interaction schematically by plotting the total energy as a function of the average distance r between an electron and positron (Fig. 1). The 1s state of positronium can be thought of as corresponding to a minimum in total energy occurring at r = 2.0 bohr = 1.016 Å, i.e. roughly double the corresponding value for the H atom by virtue of the smaller reduced mass of the e^+e^- system. Toward larger separations the energy gradually increases to zero, *i.e.* the energy of the separated particles. The attractive Coulomb potential varies as r^{-1}, while the kinetic energy varies as $p^2 \approx r^{-2}$, from which it follows that the total energy itself at first *decreases* as the particles approach one another from a large distance. At the location of the energy minimum the shorter range of the kinetic energy term becomes the dominant factor, which explains why the total energy thereafter increases rapidly toward still shorter distances. It can be seen that these arguments are very close to those used by Bohr[7] in arriving at his theory of hydrogenic atoms in 1913.

The binding energy at the latter e^+e^- minimum is only 6.8 eV, which is quite small compared to the 1.02 MeV given off when positronium decays from the corresponding (1s) state. The possibility we wish to explore in this work is *whether* a *second energy minimum does not occur at* a *much smaller electron-positron separation.* It can be imagined, for example, that at some point the total energy stops increasing toward shorter distances because an attractive short-range potential term begins to overcome the effects of the increasing kinetic energy in this region. Such a potential term would have to vary at a higher inverse power of r than either of the other two terms in the non-relativistic electrostatic Hamiltonian, and would have to be relatively unimportant in the region of the first hydrogenic energy minimum. At the same time, it is evident that some effect with an even shorter range eventually must take over and cause the energy to increase (Fig. 1) once more toward even smaller distances after the assumed 1.02 MeV absolute minimum value is attained. It is also clear that such a second energy minimum must be *totally absent in the corresponding hydrogen atom treatment.* Finally, it is only consistent to assume that an analogous double-minimum curve exists for the proton-antiproton system, but with a binding energy which is 1836 times larger, i.e. 1.85 GeV for its short-range minimum. At least one knows that this much energy is given off when the proton and antiproton interact, whereas no comparable loss of energy is observed for the combination of a proton and an electron.

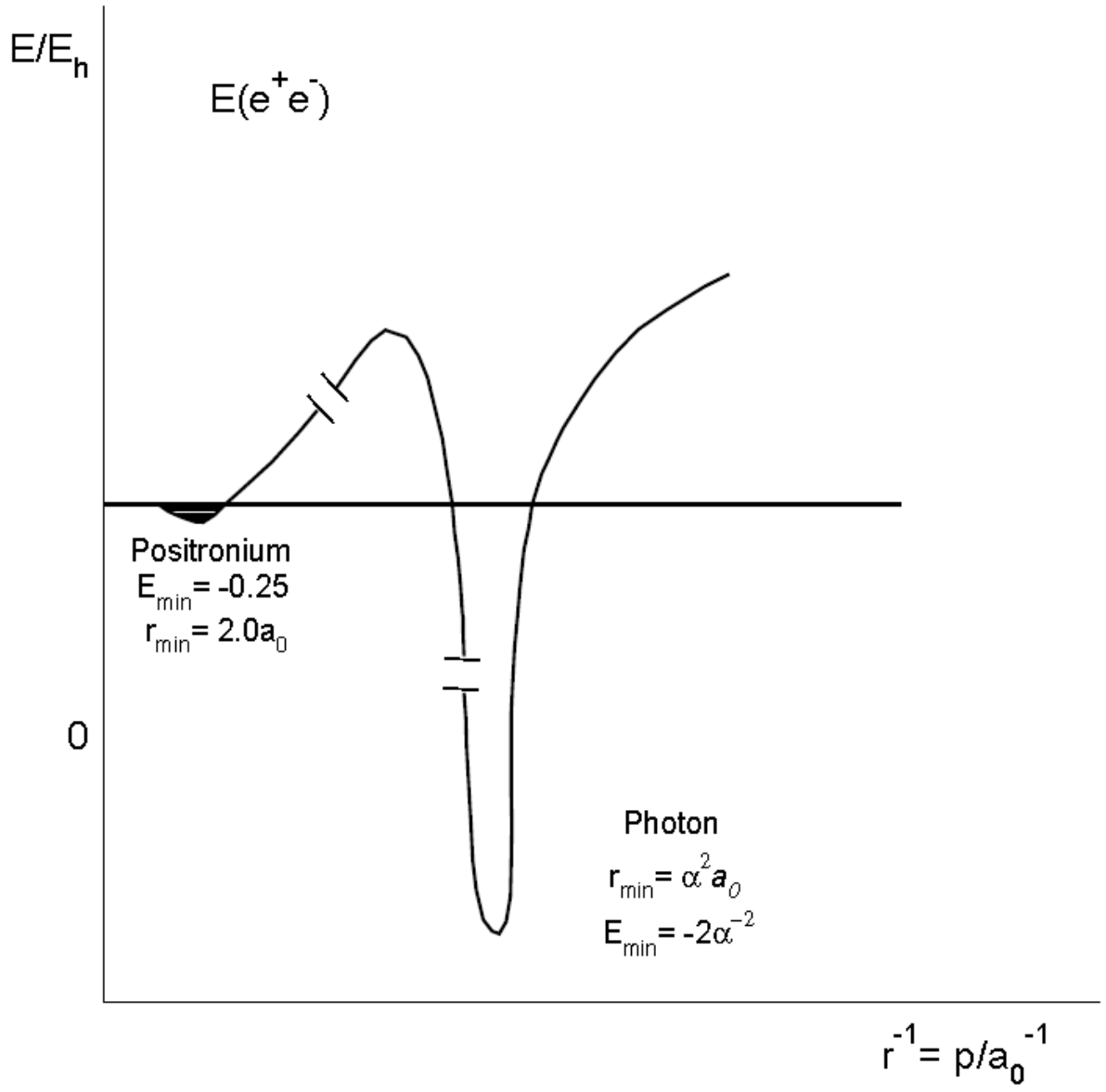

FIG. 1. Schematic diagram showing the variation of the internal energy of the e^+e^- system as a function of the reciprocal of the distance between the two constituent particles. At large separations the Coulomb attractive interaction dominates because of its long-range (r^{-1}) character. A minimum of energy of only -0.25 hartree is eventually reached, corresponding to the familiar hydrogenic ls state of positronium, after which the total energy begins to rise because the shorter-range kinetic energy term begins to dominate. In the present model this trend is eventually reversed again at a much smaller e^+e^- separation, at which point attractive forces of even shorter range ($\approx r^{-3}$) begin to change more rapidly than the kinetic energy. Finally, a second potential minimum, much deeper than the first, is reached which corresponds to a binding energy exactly equal to the sum of the rest energies of the electron and positron. At still smaller inter-particle distances the total energy rises again, reflecting the effect of some momentum-dependent damping of the short-range potential in this region. A form for the potential is sought for which only the Coulomb energy minimum survives when the positron is replaced by a proton

Concentrating on the comparison of e^+e^- with p^+e^-, the obvious question is how can the differences in the properties of the proton and positron lead to such an enormous distinction in their respective attractions to the electron. The traditional view embodied in the Schrödinger[2] and Dirac[3] equations for one-electron atoms holds that the large difference in mass of the two positively charged particles only plays a minor role in this connection, simply affecting the reduced mass of the electron. The magnetic moments (which have the charge-to-mass ratios as a factor) of e^+ and p^+ differ by a far greater amount because of the difference in rest masses, but this distinction is found to be of only minor importance in the Dirac equation treatment, in which effects such as the spin-orbit and spin-spin interactions depending on this quantity are accounted for explicitly.

Yet one knows from the outset that if there is indeed a much lower-lying state of the e^+e^- system than the familiar 1s species, it cannot be found among the solutions of the hydrogen atom Dirac or Schrödinger equations. *To progress further in this regard it is necessary to do something differently.*[1] Especially since the effect that might cause such a novel tight-binding e^+e^- state seems almost certainly short-range in nature (Fig. 1), there is reason to give closer consideration to the above magnetic-type interactions. As noted previously, there are numerous Breit-Pauli terms which fall in this category, varying as the inverse cube of the distance between interacting particles. They are all of order $\alpha^2/2 \cong 10^{-5}$ hartree for typical *atomic* electron-nucleus separations, so this characteristic fulfills another requirement from Fig. 1, namely that such a short-range effect be relatively insignificant at these distances.

Most importantly, however, all these Breit-Pauli terms[6] depend on the product of the magnetic moments (or charge-to-mass ratios) of the interacting particles. For the spin-other-orbit, spin-spin and orbit-orbit terms each of these quantities appears once in the corresponding product. Thus these terms are weighted by a factor of 1836 (the ratio of the rest masses of proton and positron) larger for e^+e^- than for p^+e^-. For the spin-same-orbit and Darwin terms the distinction is less important because in these cases the square of the mass of one of the constituent particles is involved rather than the product of both. As a result, there is an extra factor of two for these interactions for e^+e^- than for the hydrogen atom, by virtue of the fact that the square of the charge-to-mass ratio of the proton is negligible compared to that of the positron. At atomic distances these distinctions are still relatively unimportant because in this range the

Coulomb interaction dominates, but it is not difficult to imagine the situation could be far different at shorter range.

Before considering this possibility further, however, it is well to note that the Breit-Pauli Hamiltonian terms as such also have some undesirable properties which make them unsuitable for a variational calculation, that is, one in which the charge distributions of the particles involved are allowed to assume optimal forms so as to minimize the total energy. Since these terms vary as r^{-3}, there is nothing to keep the total energy from decreasing beyond any limit. They do not therefore provide a possibility of a second energy minimum of the type indicated in Fig. 1, rather only the attractive branch to the long-distance side of it. This fact has long deterred giving serious consideration to the Breit-Pauli terms as having any truly dominant role to play in quantum mechanical calculations. Nonetheless, there are other higher-order terms in a power-series expansion of the Dirac equation which need to be considered to properly understand their role in determining atomic fine structure. Specifically, the next terms in such expansions are of the order of $\alpha^4 r^{-4}$, and these higher-order effects prevent variational collapse in Dirac-equation solutions that would otherwise occur if only the $\alpha^2 r^{-3}$ terms were included.

A similar situation exists for the Lorentz force in classical electromagnetic theory. There one has a term of the form $|\mathbf{p} + e\,\mathbf{A}/c|^2$, where $\mathbf{A}$ is the vector potential. The cross term involving $\mathbf{p} \cdot \mathbf{A}$ is typically[1,8] also of the form $\alpha^2\, r^{-3}$ ($c = \alpha^{-1}$ in atomic units) for the interaction of a charged particle with an electromagnetic field, but it is damped at short range by the $|\mathbf{A}|^2$ term, which varies as $\alpha^4 r^{-4}$. An interesting possibility is nonetheless opened up by the fact that such repulsive terms *are of even shorter range and higher order in* α^2 than their Breit-Pauli counterparts. Including such terms might not keep the total energy in Fig. 1 from turning downward at short distances because of the attractive $\alpha^2 r^{-3}$ interactions, but they would insure that this trend not continue indefinitely toward still smaller inter-particle separations, *with the result that the proposed non-hydrogenic second minimum of energy could be formed.*

If one simply assumes a potential which is the difference of these short-range terms, $-\alpha^2 r^{-3} + \alpha^4 r^{-4}$, it is easily shown that it possesses a minimum near $r \cong 4\alpha^2/3$. Such a distance corresponds to roughly 10^{-5} bohr, which is a typical separation for bound nucleons ($r = \alpha^2/2$ is normally given for the range of the nuclear force, for example). The possible connection between an e^+e^- tight-binding state and the nuclear force is thus reinforced by these considerations as well.

There are basically three arguments for pursuing this line of reasoning further. First, the theory of quantum electrodynamics has a very precisely defined range of applicability. Despite its ability to make extremely accurate predictions for interactions involving electrons and photons in an atomic environment, it is generally accepted that the theory in its established form is not capable[9] of describing high-energy interactions such as those involved in nuclear bonding. Any indication as to how *the framework of quantum electrodynamics could be adapted so as to become relevant to the description of short-range forces* therefore merits serious consideration.

Secondly, the analysis of the positronium decay process has provided a basis for associating the assumed e^+e^- tight-binding state with the photon itself. Given the prominent role of the photon in quantum electrodynamics, it seems likely that its internal structure would also have an important relationship to the electromagnetic force.

Finally, examination of the multiplet structures and other properties exhibited by nuclei has already led to the conclusion[10-11] in the nuclear-shell model that spin-orbit or related terms[12] are almost certainly involved in this type of high-energy interaction. Taken together these observations suggest that a solution to the proposed problem may lie in an adaptation of the Dirac equation which does not detract from the reliability of the original theory's predictions for quantum-electrodynamics phenomena, but which at the same time enables an accurate treatment of interactions of much shorter range and higher binding energy. This eventuality would amount to an extension of the Bohr correspondence principle,[13] which proved so effective in making the transition from classical to quantum mechanics at the beginning of this century.

B. KINETIC ENERGY CONSIDERATIONS

As remarked above, it is not satisfactory to use a non-relativistic form for the kinetic energy of the positron and electron if a large binding energy is assumed. In this respect the problem is significantly different than in the conventional treatment of nuclear binding, because there the kinetic energies of the nucleons are still relatively small compared to the energy equivalent of their rest masses.

As Einstein showed[14] on the basis of his special theory of relativity, the non-relativistic $p^2/2m_o$ term is actually just an element in the power series of the square-root quantity $(p^2c^2 + m_o^2c^4)^{1/2} - m_oc^2$. The Breit-Pauli approximation includes[6] a term of order p^4 to account for relativistic kinetic energy contributions, but just as for the corresponding potential terms, it is

known that this correction leads to variational collapse when the electronic charge distribution is allowed to vary freely so as to minimize the total energy. It is possible to circumvent this difficulty,[15] however, by employing the Einstein square-root expression directly in the Hamiltonian instead of relying on a truncated power-series expansion for it. The inconvenience of employing a square-root operator can be dealt with for general atomic and molecular systems by means of a standard matrix procedure.[15] Each particle has its own kinetic energy and thus the square-root terms are treated as one-electron operators, exactly as their non-relativistic $p_i^2/2m_i$ counterparts in conventional quantum mechanical treatments.

This procedure brings with it another difficulty, however, namely how to separate the total kinetic energy into its internal and translational (center-of-mass) components. In the non-relativistic case it is well known that the $p_1^2/2m_1 + p_2^2/2m_2$ term can be replaced exactly[16] by $p^2/2\mu + P^2/2M$ by employing a linear coordinate transformation (p is the internal and P, the center-of-mass, momentum respectively, $M= m_1+m_2$ is the sum of the individual particle masses and μ is the reduced mass). The new coordinates are defined as $x = x_1 - x_2$ and $X = (m_1x_1 + m_2x_2)/M$, where x_1 and x_2 are Cartesian coordinates of the two particles, with analogous expressions for the y and z directions. Since the Coulomb potential only depends on the internal coordinates, it is thus possible to effect a separation of coordinates which leads to the familiar situation that the solutions of the corresponding Schrödinger equation can always be formed as simple products of the type Ψ (r) χ (R), i.e. as a product of a function of the internal coordinates with one involving only those of the center of mass.

This procedure can be generalized for any number of particles, but there is an important assumption to be noted. The derivation generally used[17] comes from classical mechanics and relies on the fact that $\mathbf{p} \cdot \mathbf{P}$ cross-terms cancel out as a result of the coordinate transformation. The cancellation is perfect for the non-relativistic kinetic energy, but *use of the relativistic one-particle form,* in which p_1^2 and p_2^2 appear in separate square-root expressions, *does not lend itself to the same simplification.* If one of the particle's masses is much larger than the other, it is not difficult to find approximations from which the desired coordinate separation effectively results even in the relativistic case. Since the nuclear masses are so much larger than the electron's, it is therefore easy to justify this approach for atomic calculations, both for the Dirac equation itself and in the Breit-Pauli approximation.

The difficulty is not so easily circumvented when both masses are equal, however, as is the case for the present e^+e^- interaction. It might be argued that it is intuitively obvious that the center-of-mass motion can always be separated out, but for quantitative work, one would like to have a more solid basis for making this simplifying assumption. In general this question seems to have received relatively little attention in the literature, but it has been given more careful consideration elsewhere.[18]

The most straightforward method under the circumstances is to simply work with the original Cartesian coordinates of each particle. The quantum-electrodynamics treatment of the positron uses a similar approach[19,20] in evaluating higher-order effects, including transition probabilities for the decay into photons out of various positronium electronic states, except that it imposes an additional condition of $\mathbf{P} = \Sigma \mathbf{p_i} = 0$. In such a two-particle application this means that $\mathbf{p_1} = -\mathbf{p_2} = \mathbf{p}$. No comparable transformation is employed for the spin coordinates of both particles in this approach, however. Radiation corrections to the Dirac-equation results can also be computed by employing the same condition for the center-of-mass momentum.[19,20]

When more than two particles are involved, complications arise in attempting to generalize this procedure, however, particularly in the relativistic treatment of the kinetic energy. In the transformed coordinate system, one of the particles is effectively singled out as a reference for the internal coordinates, so that $\mathbf{x_i'} = \mathbf{x_i} - \mathbf{x_l}$ is now employed instead of $\mathbf{x_i}$, for example (with $\mathbf{x_l}$ itself being retained in the new basis). As a result the expression for the conjugate momentum of x_l is $\mathbf{p_1} = -\sum_{i \neq 1}{}' p_i'$, i.e. a sum of internal momentum values rather than a single such quantity as in the two-particle case.

In order to develop a computational scheme which can be conveniently applied to systems containing more than two particles, it therefore seemed advisable to avoid making any type of transformation to internal coordinates, and hence to simply employ the original Cartesian coordinates of each constituent particle directly in constructing the corresponding quantum mechanical Hamiltonian operator governing the interactions of a given system. Use of such a coordinate system at all stages of the theoretical treatment carries with it the complicating feature that internal and translational characteristics are mixed together in the resulting wave-functions.

In this connection, it is worth recalling that $\Sigma\mathbf{p_i}$ commutes with each $\mathbf{p_i}$ and $\mathbf{r_{ij}}$ (particle separation) quantity, so that the translational energy operator itself must have a common (complete) set of eigenfunctions[21] with any Hamiltonian containing exclusively these kinds of variables. Hence, any exact solution of a corresponding Schrödinger *equation must always be characterized by a definite value of the translational energy.* This observation underscores another assumption in the usual separation-of-variables argument for internal and center-of-mass coordinates, however. The Breit-Pauli terms mentioned in the last section contain momentum factors as well as internal distances. Consequently, even when the non-relativistic kinetic energy is employed, the desired separation is not complete for a Hamiltonian containing these types of interactions. Again, this presents no real problem for calculations of one-electron atoms, in which the masses of the constituent particles differ greatly, but for a system consisting of only e^+ and e^-, there is need for more careful consideration.

Finally, it should be mentioned that there is a covariant two-electron equation[22] which does employ a separation of internal and translational coordinates just as for the Dirac equation. It is characterized by two separate time coordinates, whereas in what has been described above it is always assumed that there is only one such variable, and that it can be separated from its spatial counterparts in the usual way by virtue of the time-independent nature of the corresponding Hamiltonian operator. Since the stated *modus operandi* in the present study is to depart from the purely quantum-electrodynamics treatment of the e^+e^- system, and especially since no other heavy system is present, it is preferable to work with a relatively simple Schrödinger-equation formulation of this problem which does not make any assumptions regarding the way in which the internal motion is separated from that of the center of mass.

C. SUGGESTED DAMPED FORM FOR THE BREIT-PAULI TERMS

A prerequisite for constructing a Schrödinger equation to investigate high-energy processes is the use of a potential which is suitably bounded. The assumed tight-binding e^+e^- state most likely is the result of a short-range interaction which is strongly attractive over a given region of inter-particle separation but even more strongly repulsive at still smaller distances (see Sect. II. A). The Breit-Pauli approximation employs attractive terms fitting this description but lacks corresponding shorter-range effects which would produce the desired second minimum in the e^+e^- total energy curve sketched in Fig. 1. We have seen how the Breit-Pauli kinetic energy term

(including the mass-velocity correction) can be replaced by the Einstein free-particle square-root expression to avoid variational collapse, without giving up the advantages of having a reliable approximation to the Dirac equation results for hydrogenic atoms. It remains to find a similar means of dealing with the Breit-Pauli potential terms.

If we look upon the spin-orbit and related interactions as terms in a power series,[1] it seems reasonable to look for a closed expression which approaches this result in the low-energy relativistic regime encountered in calculations of atoms with moderately heavy nuclei, something analogous to the Einstein relativistic kinetic energy, in other words. At least one knows from the form of the Lorentz electromagnetic force that the next higher-order terms after those of $\alpha^2\ r^{-3}$ spin-orbit type vary as $\alpha^4\ r^{-4}$.

Simply adding such terms to the Hamiltonian has several disadvantages, however. It falls short of the goal of replacing the Breit-Pauli interactions with closed expressions which themselves correspond to infinite-order power series. In addition, it is difficult to carry out computations with an operator varying as r^{-4} since not all integrals which would be required in a variational treatment possess finite values. For example, those involving only s-type basis functions do not fall in this category.

The form of the desired potential (Fig. 5) is reminiscent of that observed in nuclear scattering, and this suggests the following alternative. The r^{-3} and r^{-4} terms already discussed can be grouped together as $\alpha^2 r^{-3}\ (1 - \alpha^2\ r^{-1} + ...)$. The terms in parentheses are the beginning of a power series expansion of the exponential function $\exp(-\alpha^2\ r^{-1})$, which in turn is quite similar to that appearing in the Yukawa potential[23,24] in nuclear physics, thus making explicit the connection with the nuclear force description. By multiplying the Breit-Pauli α^2 terms with such an exponential function, we have a potential which is capable of producing the second minimum for e^+e^- in Fig. 5 while at the same time retaining the correct behavior needed at relatively large inter-particle separations to properly describe the conventional positronium (hydogenic atom) states.[1]

Since the damping effects produced by the exponential factor are relativistic in nature, it seems somewhat more likely that the corresponding argument is a function of the momentum of the particles rather than the distance between them, i.e. of the form $\exp(1 - \alpha^2 p)$, with $r^{-1} \sim p = |p|$. This choice has computational advantages as well, because it means working with individual

quantum mechanical operators which depend on the coordinates of a single particle rather than two. From the Lorentz classical Hamiltonian we can also anticipate that a given particle's momentum p is multiplied by its charge-to-mass ratio q/m. Finally, to obtain the desired binding energy for a given particle-anti-particle system it is convenient to introduce a free parameter A as an additional factor in the exponential argument.

The negative of the resulting potential is plotted in Fig. 2(atomic units are employed throughout) as a function of the reciprocal inter-particle distance. For this purpose we use the approximate representation $V(r) = -\alpha^2 r^{-3} \exp(-\alpha^2 r^{-1})$. For high particle velocities it can be assumed that the kinetic energy varies as pc in the range of interest, which can therefore be represented in an analogous manner as r^{-1} α^{-1} in atomic units, i.e. as a straight line. This diagram[1] is useful in analyzing how binding can be achieved with such an exponentially damped potential over a very narrow range, consistent with the total energy curve shown in Fig. 1. For small momentum values typical of electrons in atoms, the kinetic energy far outweighs the short-range potential because of the factor of α^2 in the latter expression. Coulomb effects are omitted from consideration for the time being.

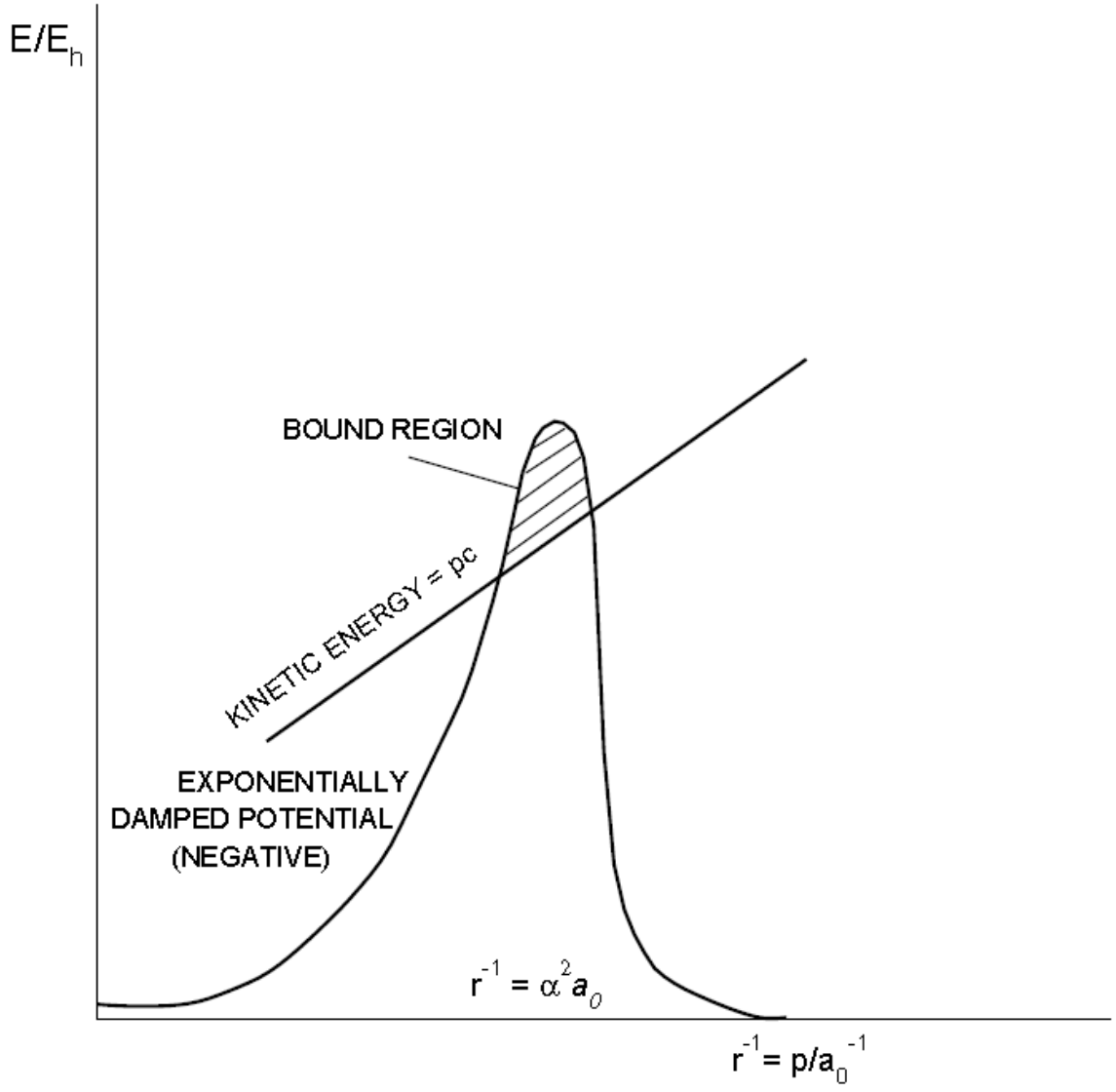

FIG. 2. Schematic diagram exploring the nature of a short-range potential required to produce the type of e^+e^- total energy curve depicted in Fig.1. At relatively small inter-particle distances ($r \approx \alpha^2$) the relativistic kinetic energy varies nearly linearly with momentum $p \approx r^{-1}$. In order to obtain strong binding within a very narrow range of the e^+ - e^- distance, the negative of the attractive potential term must reach a maximum shortly after it crosses the kinetic energy line from the long-distance side of the diagram, and then drop off again very sharply. Such an extreme cancellation effect requires a potential which fulfills at least three conditions: a) a small coupling constant (order α^2), b) a shorter range ($\sim r^{-3}$) than the kinetic energy and c) a momentum-dependent damping which is exponential in nature.

The absolute value of the potential increases as the cube of the momentum (or inverse distance) while the kinetic energy changes in a nearly linear manner, so it can be imagined that the two quantities eventually become equal at some point and binding becomes possible. The exponential damping becomes noticeable in the same region, however, and thus the above term does not increase as quickly as before and finally reaches a maximum. At the same time, the kinetic energy continues to increase linearly with p and eventually a second crossing with the negative of the potential occurs in Fig. 2. The area in which the negative of the potential exceeds the kinetic energy corresponds to a very small range of r, but the amount of binding with which it is associated can still be quite large. For example, at $r = \alpha^2$ the un-damped Breit-Pauli potential is of the order α^{-4} hartree, compared to the kinetic energy's order of α^{-3} hartree. Since the assumed binding energy for the e^+e^- system is 1.02 MeV or $2\alpha^{-2}$ hartree, it is clear that an enormous cancellation must occur because of the damping of the potential to obtain physically acceptable results.

This state of affairs is probably the strongest argument for employing an exponential damping to produce such a large degree of binding over a narrow range of interpartic1e separation. The fact that the Coulomb energy is also of order α^{-2} hartree for $r = \alpha^2$ suggests that it is not possible to ignore this effect either, however, despite its relatively long-range character. Nonetheless, the predominant feature in the tight-binding scenario given above is clearly the delicate cancellation at small interpartic1e separations between the exponentially damped Breit-Pauli terms and the relativistic kinetic energy.

D. SCALING PROPERTIES OF THE BREIT-PAULI HAMILTONIAN

One of the key requirements for the Schrödinger equation under discussion is that it leads to maximum binding energies for particle-antiparticle systems of $2Mc^2$, consistent with the Einstein mass-energy equivalence relation. One postulates that a Hamiltonian exists which has the required energy as its *minimal* eigenvalue instead of assuming that annihilation occurs and the total mass of the particles simply appears as the equivalent amount of energy. It is well known that the Schrödinger and Dirac equations for purely electrostatic potentials both have the property that their binding energies are proportional to the reduced mass of the electron in hydrogenic atoms, and this result is easily generalized for systems containing other charged particles such as muons or antiprotons. More interesting in the present context is the fact that the

proportionality between energy and mass also holds when the various Breit-Pauli relativistic corrections are added to the Hamiltonian.

To show this, let us assume that a solution to the Schrödinger equation is known for a particle-antiparticle pair with charge ±q and rest mass m_0.[1] Furthermore, its lowest energy eigenvalue is taken to be $-2m_oc^2=-2m_o\alpha^{-2}$ (in atomic units), corresponding to the eigenfunction $\Psi(r)$. The Hamiltonian itself consists of a series of kinetic and potential energy operators of the type discussed earlier, including exponential damping factors $F(p, q, m_o)$:

$$H(p,r,q,m_o) = (p^2\alpha^{-2} + m_o{}^2\alpha^{-4})^{1/2} - m_o\alpha^{-2} \qquad \text{II.1}$$

$$-q^2r^{-1} - q^2m_o{}^{-2}\alpha^2r^{-3}F(p,q,m_o)$$

If the coordinates are scaled so that

$$p' = M_om_o{}^{-1}p \text{ and } r' = M_o{}^{-1}m_or \qquad \text{II.2}$$

the original Hamiltonian becomes:

$$H(p,r,q,m_o) = M_o{}^{-1}m_o\{(p'^2\alpha^{-2} + M_o{}^2\alpha^{-4})^{1/2} - M_o\alpha^{-2}$$

$$-q^2r'^{-1} - q^2M_o{}^{-2}\alpha^2r'^{-3}F(p',q,M_o)\} \qquad \text{II.3}$$

$$= M_o{}^{-1}m_oH(p',r',q,M_o),$$

provided $F(p,q,m_o)=F(p',q,M_o)$. The corresponding Schrödinger equation in the scaled coordinate system thus becomes:

$$H(p',r',q,M_o)\Psi(r') = -2M_o\alpha^{-2}\Psi(r) \qquad \text{II.4}$$

i.e. by multiplying both sides of the Schrödinger equation for the original Hamiltonian by $M_om_o{}^{-1}$. As a result, it is seen that $\Psi(r)$, or the function $\Psi'(r')$ obtained by making the corresponding coordinate substitution for it, is an eigenfunction of the analogous Hamiltonian for a particle-antiparticle system of the same charge q as before, but with rest mass M_o instead of m_o. Its energy eigenvalue is $-2M_o\alpha^{-2}$, exactly as required by the mass-energy equivalence relation.[1]

Moreover, this result is quite general, since it is easily seen that the above scaling procedure has the effect of producing an entire spectrum of Schrödinger equation eigenvalues which differ by a factor of $M_om_o{}^{-1}$ from those obtained for the original particle-antiparticle

system. Furthermore, by choosing the argument of $F(p, q, m_o)$ to contain the ratio p/m_o, as suggested by the form of the Lorentz electromagnetic force Hamiltonian discussed in Sect. II.A., the requirement that this damping factor be unaffected by such a coordinate scaling is fulfilled.

The Breit-Pauli interactions also contain angular orbital momentum terms not included explicitly in the above Hamiltonian, but these are clearly unaffected by the above scaling procedure because they either involve only products of r and p, or in the case of the spin interactions, are completely independent of spatial coordinates. It is thus shown that the desired proportionality between binding energy and rest mass of the constituents of a particle-antiparticle binary system holds for the Breit-Pauli interaction as long as the charge q of the individual particles remains the same. This is clearly the case in comparing the e^+e^- system to p^+p^-, so the original objective sought at the beginning of this section is guaranteed by the use of such a Hamiltonian.

This result also tells us that the proportionality constant A in the exponential damping factor $F(p,q,m_o) = \exp [-A\alpha^2(q/m_o)p]$ must be the same for proton-antiproton interactions as between electron and positron. Alternatively, one might have assumed a different constant for the electron than for the proton, in which case one would have had to adjust the inverse mass dependence of the present exponential argument in order to obtain the desired scaling property. From the point of view of economy of assumptions and relation to established theoretical models, the former arrangement is clearly superior.

The units for the constant A remain to be discussed. The exponential argument as a whole must be dimensionless. Examination of the damping factor F shows that A must have units of the product of inverse charge and velocity (p/m) in order to ensure that the argument as a whole is dimensionless. The units of A are hidden when one uses atomic units directly in the corresponding calculations, as has been done in the preceding discussion. If mks units are used instead, A must have a unit of $(ec\alpha)^{-1}$ s/Coul m = 2.8530×10^{12} s/Coul m. The actual quantity in the exponential is $A\alpha^2$, however, which has the value of 1.51926×10^8.

E. EXPLICIT REPRESENTATION OF THE EXPONENTIALLY DAMPED HAMILTONIAN

The explicit form of the Hamiltonian discussed above is given in Table I.[1] It will be referred to subsequently as the XBPS Hamiltonian, the abbreviation standing for "Exponentially-

damped Breit-Pauli Schrödinger Equation." As usual, there is a one-particle interaction for each constituent in the system, and a set of two-particle operators for each pair of such species. The Hamiltonian of Table I is given explicitly for only two (representative) particles with respective charges and rest masses q_i (q_j) and m_{oi} (m_{oj}), but in view of the above discussion it is easily generalized for the description of any number and combination of different particle types.

The only one-particle term in the Hamiltonian is the relativistic kinetic energy. Other common one-electron interactions such as the Coulomb nuclear attraction for an electron are to be found among the two-particle interactions. The rest energy $m_{oi}c^2 = m_{oi}\alpha^{-2}$ (atomic units are used throughout) is subtracted from the Einstein square-root operator in the usual way to represent the kinetic energy. This procedure effectively defines the zero of energy as that of the (infinitely) separated particles at rest.

The first two-particle interaction listed in Table I is the Coulomb term and it is the only one which is unchanged relative to the standard Breit-Pauli treatment.[6] The remaining terms are all exponentially damped, but fall into distinct categories, depending on whether they are multiplied with $q_1q_2/m_{o1}m_{o2}$ or q_1^2/m_{o1}^2 (or q_2^2/m_{o2}^2). In the first group are the spin-other-orbit, orbit-orbit and spin-spin terms, the latter including a δ-function component. The spin-same-orbit and Darwin interactions comprise the second category. Since all particles are to be treated equivalently, it is essential that each two-particle interaction be symmetric with respect to interchange of the corresponding indices, as provided for in the original Breit-Pauli Hamiltonian. The Coulomb term obviously satisfies this condition, since r_{12} is a scalar quantity denoting the magnitude of the distance separating the two particles.

The most significant change in the operators of Table I compared to those in the conventional Breit-Pauli Hamiltonian is their multiplication with exponential damping factors. For the terms of orbit-orbit type, it is assumed that two such factors are needed:
$\exp(-A\alpha^2|(q_i/m_{oi})p_i|)$, for i= 1 and 2. To insure that the Hamiltonian be Hermitian, it is necessary that the same pair of factors appear on both sides of the original Breit-Pauli terms, since $\mathbf{p_i}$ and $\mathbf{r_{ij}}$ do not commute with one another. The arguments of all the exponential terms are defined to be negative-definite, hence the absolute value sign in these expressions. The damping factors for the spin-same-orbit and Darwin terms have a somewhat more complicated form, however. Since the q/m_o factors appear squared for these terms in the original Breit-Pauli Hamiltonian,[53] it seems

consistent to also use squares of the corresponding damping factors for the same particle in this instance instead of products of two different kinds as before.

The sign of the interaction in the latter class of operators requires additional comment as well. Since the pre-multiplying factor is either q_1^2/m_{o1}^2 or q_2^2/m_{o2}^2, it is not possible on this basis alone to specify whether the interaction is attractive or repulsive. This information is contained in the product of the charges of the two particles, which appears explicitly in the orbit-orbit-type terms but not for the Darwin or spin-same-orbit operators. It is thus necessary to define a sign convention based on the product $(q_1/m_{o1})\,(q_2/m_{o2}) \equiv G(1,2)$ according to which a positive result corresponds to a negative sign for both terms, while the opposite choice is made if the result is negative. Similarly as in the other case, the $\exp(-2A\alpha^2|(q_i/m_{oi})\,p_i|)$ factor must appear on both sides of the corresponding Breit-Pauli terms in order to preserve the required Hermitian character. The absolute value sign guarantees that the argument of the exponential is negative, i.e. the factor always reduces the absolute magnitude of the original Breit-Pauli interaction for the same charge distributions.

Designation		Operator
Relativistic Kinetic Energy (one-particle only	KE	$\left(p_i^2\alpha^{-2} + m_{0i}^2\alpha^{-4}\right)^{\frac{1}{2}} - m_{0i}\alpha^{-2}$
Coulomb	C	$q_i q_j r_{ij}^{-1}$
Spin-same-orbit (exponentially damped)	SsO	$-\frac{\alpha^2}{2}G(i,j)$ $\times\left\{\left(\frac{q_i}{m_{0i}}\right)^2 \exp\left(-2A\alpha^2\left\lvert\frac{q_i}{m_{0i}}\mathbf{p}_i\right\rvert\right)\times\left(\mathbf{r}_{ij}\times\mathbf{p}_i\cdot\mathbf{s}_i\right)r_{ij}^{-3}\right.$ $\left.+\left(\frac{q_j}{m_{0j}}\right)^2 \exp\left(-2A\alpha^2\left\lvert\frac{q_j}{m_{0j}}\mathbf{p}_j\right\rvert\right)\times\left(\mathbf{r}_{ji}\times\mathbf{p}_j\cdot\mathbf{s}_j\right)r_{ij}^{-3}\right.,$

$$\text{where } G(i,j)=\begin{cases}1, & \text{if } \dfrac{q_i q_j}{m_{0i}m_{0j}}>1\\ -1, & \text{if } \dfrac{q_i q_j}{m_{0i}m_{0j}}<1\end{cases}$$

Spin-other-orbit (exponentially damped)	SoO	$-\alpha^2\left(\dfrac{q_i}{m_{0i}}\right)\left(\dfrac{q_j}{m_{0j}}\right)$ $\times\exp\left(-A\alpha^2\left\lvert\dfrac{q_i}{m_{0i}}\mathbf{p}_i\right\rvert\right)\exp\left(-A\alpha^2\left\lvert\dfrac{q_j}{m_{0j}}\mathbf{p}_j\right\rvert\right)$ $\times\left(\mathbf{r}_{ji}\times\mathbf{p}_j\cdot\mathbf{s}_i+\mathbf{r}_{ij}\times\mathbf{p}_i\cdot\mathbf{s}_i\right)r_{ij}^{-3}$
Darwin Term (exponentially damped)	D	$-\pi\dfrac{\alpha^2}{2}G(i,j)\delta(r_{ij})$ $\times\left\{\left(\dfrac{q_i}{m_{0i}}\right)^2\exp\left(-2A\alpha^2\left\lvert\dfrac{q_i}{m_{0i}}\mathbf{p}_i\right\rvert\right)\right.$ $\left.+\left(\dfrac{q_j}{m_{0j}}\right)^2\exp\left(-2A\alpha^2\left\lvert\dfrac{q_j}{m_{0j}}\mathbf{p}_j\right\rvert\right)\right\},$
Orbit-orbit (exponentially damped)	OO	$-\dfrac{\alpha^2}{2}\left(\dfrac{q_i}{m_{0i}}\right)\left(\dfrac{q_j}{m_{0j}}\right)$ $\times\exp\left(-A\alpha^2\left\lvert\dfrac{q_i}{m_{0i}}\mathbf{p}_i\right\rvert\right)\exp\left(-A\alpha^2\left\lvert\dfrac{q_j}{m_{0j}}\mathbf{p}_j\right\rvert\right)$ $\times\left[\left(\mathbf{p}_i\cdot\mathbf{p}_j\right)r_{ij}^{-1}+\left(\mathbf{r}_{ij}\cdot\left(\mathbf{r}_{ij}\cdot\mathbf{p}_i\right)\mathbf{p}_j r_{ij}^{-3}\right)\right]$
Spin-spin (exponentially damped)	SS	$-\alpha^2\left(\dfrac{q_i}{m_{0i}}\right)\left(\dfrac{q_j}{m_{0j}}\right)$ $\times\exp\left(-A\alpha^2\left\lvert\dfrac{q_i}{m_{0i}}\mathbf{p}_i\right\rvert\right)\exp\left(-A\alpha^2\left\lvert\dfrac{q_j}{m_{0j}}\mathbf{p}_j\right\rvert\right)$

		$\times\left[\left(\mathbf{s}_i\cdot\mathbf{s}_j\right)r_{ij}^{-3}+3\left(\mathbf{r}_{ij}\cdot\mathbf{s}_i\right)\left(\mathbf{r}_{ij}\cdot\mathbf{s}_j\right)r_{ij}^{-5}\right]$
Spin-spin δ (exponentially damped)	SSδ	$-\frac{8\pi\alpha^2}{3}\left(\frac{q_i}{m_{0i}}\right)\left(\frac{q_j}{m_{0j}}\right)$ $\times\exp\left(-A\alpha^2\left\lvert\frac{q_i}{m_{0i}}\mathbf{p}_i\right\rvert\right)\exp\left(-A\alpha^2\left\lvert\frac{q_j}{m_{0j}}\mathbf{p}_j\right\rvert\right)$ $\times\mathbf{s}_i\cdot\mathbf{s}_j\delta\left(\mathbf{r}_{ij}\right)$

Table I. Definition of quantum mechanical operators present in the exponentially damped Breit-Pauli Hamiltonian employed throughout the present study (α is the fine-structure constant; atomic units employed throughout).[1] The indices i and j are used generically to represent two interacting particles; the quantities q_i (q_j) and m_{oi} (m_{oj}) are the electric charges and rest masses of the i^{th} (j^{th}) particle, A is the exponential damping constant , and $\mathbf{p_i}$ ($\mathbf{p_j}$), $\mathbf{s_i}$ ($\mathbf{s_j}$) and $\mathbf{r_{ij}}$ are the standard vectorial symbols for the linear and spin angular momenta of a single particle and the distance between the i^{th} and j^{th} particles, respectively.

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Note that there is an error in the original version of this table,[1] namely the exponential factors appear more often than above.

It might be argued that the above sign convention for the Darwin and spin-same-orbit terms can be satisfied more simply by replacing q_1^2/m_{o1}^2 by q_1q_2/m_{o1}^2. The result would clearly be the same as before only if $|q_1| = |q_2|$, however. This is the case for interactions between protons and electrons and their antiparticles, but in a more general formulation capable of dealing with other types of particles as well, it seems preferable to employ the former definitions. In this way the charge of a given particle only appears divided by its own rest mass in the damped Breit-Pauli interactions. This prescription at least formally allows for the treatment of charge-less, mass-less neutrinos with such a Hamiltonian, without introducing the types of singularities which otherwise would arise when coupling constants involving ratios of the charge of one particle and the rest mass of another are employed.

Returning to the immediate focus of attention, the e^+e^- system, it can be seen that the XBPS Hamiltonian of Table I exhibits a special symmetry in this case, namely it commutes with the charge conjugation operation C. This means that the corresponding eigenfunctions must be either symmetric or anti-symmetric with respect to interchanging the electron and positron coordinates.

The same result clearly holds for any particle-antiparticle binary system. This is a different situation than one normally encounters in conjunction with the Pauli principle,[25] in which permutation symmetry results because the component particles are indistinguishable. As a result it is not necessary to assume that the only physically meaningful solutions are of one symmetry-type, for example, anti-symmetric in the case of fermions. The symmetry in question arises not because the particles are indistinguishable, but rather because their (different) properties can be exchanged without affecting the form of their mutual interaction. This characteristic applies to all states of positronium, including those of hydrogenic type. In view of its special nature, however, there seems little point in incorporating this symmetry into the basis functions employed in explicit e^+e^- calculations with the XBPS Hamiltonian. In general, it will be assumed that the many-particle basis consists of products of Slater determinants[26] for each particle type, i.e. anti-symmetry is assumed only for indistinguishable fermions. Bosons arise naturally as even products of fermions[27] and therefore require no additional symmetrization procedure.

III. COMPUTATIONS FOR MASSLESSS PARTICLE-ANTIPARTICLE BINARIES

The central hypothesis explored in the previous section is that elemental matter can neither be created nor destroyed. Instead, it is argued that there exist strong attractive forces between elementary particles and their antiparticles which lead to mass-less binary systems whose lack of observability is understandable in terms of the Planck frequency relation
($E = m = 0$ implies $\nu = 0$ and $\lambda = \infty$). The XBPS Hamiltonian given in Table I is deduced in accordance with such expectations, and calculations employing it will be considered below, starting with the electron-positron system.

A. DETAILS OF THE COMPUTATIONAL METHOD

The computational methods employed are modeled after those of electronic structure calculations for atoms and molecules. In essence a matrix representation of the XBPS Hamiltonian is formed with the aid of products of one-particle functions. The first step is to compute integrals for each of the original Breit-Pauli operators[6] (except for the mass velocity terms) over a set of basis functions. Because of the decision to treat all particles in an equivalent manner, with no assumptions about fixed probability distributions for any of them, it can be noted that the Hamiltonian is symmetric with respect to all operations of the full rotation group

plus inversion. Accordingly, it is reasonable to localize all basis functions at a single center, specifically the origin of the coordinate system. As mentioned in the last chapter, the only one-particle operator under the circumstances is that of the (relativistic) kinetic energy. All the other Breit-Pauli terms in the Hamiltonian, including the Coulomb interaction. are treated exclusively as two-particle operators.[6]

To construct the most general possible digital computer program it was decided to employ the same set of basis functions to describe each type of constituent particle. This approach seems reasonable because in a system with no net translation, the momentum of the particles should be similar, which implies basis functions of roughly the same extension for each of them. In the last analysis, it is always possible to employ individually optimized basis functions for each particle type by simply combining all such sets and making them available to describe the probability distributions of all the particles involved.

In this approach it is only necessary to compute the various one- and two-particle interaction integrals for electrons in the initial stage of the calculation. These results can then be conveniently adapted for treatment of particles other than electrons at a later stage. It was decided to use real Cartesian Gaussian functions to construct the one-particle basis, although it would also be convenient to use Slater-type exponential functions as more commonly employed in atomic calculations. Since no exact solutions for the Schrödinger equations of primary interest are known, the primary consideration was to choose a basis capable of describing general continuous functions which vanish at infinite distance from the origin.

An option for use of one-center potentials is available in the program which enables conventional atomic calculations to be carried out as well, in which case only two-particle interactions for electrons are assumed, although this restriction could also easily be removed. In such applications the charge of the nuclear center is required as input for the initial integral computations. Otherwise, no input is needed other than the exponents and coefficients of the contracted Cartesian Gaussian basis functions. Formulae for the calculation of Cartesian Gaussian integrals for all the Breit-Pauli operators may be found elsewhere.[28] The computer program for evaluation of these integrals for the present study has been written by Chandra and implemented by Phillips, Liebermann and the author.[29]

Because of the presence of spin variables in the one-particle functions it is desirable to carry out the overall treatment by employing a basis of eigenfunctions of the total angular

momentum operators j^2 and j_z. The corresponding spin-orbitals are formed with the help of the ladder operator technique[31] and conform to the standard Condon-Shortley convention.[31] The transformation of the Breit-Pauli integrals from a basis of spatial functions to the desired spin-orbitals is effected in two steps: the complex spatial eigenfunctions of l^2 and l_z are employed in the first transformation, followed by a second change of basis to the j^2, j_z eigenfunctions. In the process, the number of basis functions is doubled in the usual way because of the duality of the spin representation for fermions. The final two-particle integrals are classified according to quartets of the four quantum numbers, n, l, j and m_j, whereby n simply numbers the different spatial basis functions from unity upwards. Because of the spherical symmetry of the Breit-Pauli terms it is only necessary to specify three m_j values explicitly, since the only non-zero two-particle integrals are characterized by $\sum_i m_j^i = 0$.

Two other indices are required, referred to as Γ and μ. The index μ simply refers to the different operators employed, while Γ is an ordering index with only two values. A standard order of indices is defined, whereby the integral $<\varphi_a(1)\ \varphi_b(2)\ \varphi_\mu(1,2)\ \varphi_c(1)\ \varphi_d(2)>$ is characterized by $\Gamma = 1(2)$ if the standard order can be reached by an even (odd) number of permutations of the orbitals of the same particle. As is common practice,[32] the spin-same-orbit term is treated as two separate operators, one for $\mathbf{1_1.s_1}$ and one for $\mathbf{1_2.s_2}$. All other Breit-Pauli terms are symmetric with respect to particle exchange prior to multiplication by the various q/m_o coupling constants and can therefore be treated as symmetric sums at this stage of the computations, i.e. before the charges and rest masses of the actual constituent particles are introduced. More details concerning these computer programs will be given elsewhere.[33]

B. TRANSFORMATION TO THE MANY-PARTICLE-TYPE BASIS

In Sect. II it was argued that the original Breit-Pauli operators need to be adapted so that a Schrödinger equation employing them can lead to a mass-less state of a particle-antiparticle binary system, i.e. one whose binding energy is exactly equal to the sum of the rest masses of its constituents. The suggested changes have always involved functions of the momentum operator, specifically a square-root and several exponentials. These operators lead to integrals needed for their matrix representation which are relatively complicated to evaluate in a direct manner. This is particularly true for the two-particle exponentially-damped Breit-Pauli terms (Table I). Closed

expressions for the relativistic kinetic energy do exist,[34] but in order to deal with all the required operators in a consistent manner, an approximate integral evaluation technique must be employed.

It was thus decided to apply the matrix procedure referred to above[15] for the treatment of both the square-root and exponential function operators. This involves use of the resolution of the identity formalism[35] and thus results employing it approach their exact values only as the basis set employed to obtain the matrix representation of the Hamiltonian nears completeness. Numerical tests[36,37] comparing the exact and matrix representation values for relativistic kinetic energy integrals indicate that this level of approximation is suitable for the purpose at hand. The situation is more complicated for the damped Breit-Pauli terms of a two-particle nature, because it becomes impractical to saturate the basis to a similar extent as in the square-root operator tests. Nonetheless, it is always possible to judge the numerical stability of the final results of the calculations by comparing with analogous findings obtained with basis sets of different size. Since all the operators which are primarily responsible for these difficulties are functions of the momentum operator, it is possible to proceed in a very similar fashion for all of them.

Briefly, one first needs to form the non-relativistic kinetic energy matrix for electrons in the assumed Gaussian basis and then to diagonalize it. If the basis functions were momentum eigenfunctions, the desired relativistic square-root integrals could be obtained exact1y by simply replacing the $p^2/2$ eigenvalues by the corresponding results for the operator in question. A related diagonal matrix can be formed even if momentum eigenfuctions are not used, but then it is necessary to subsequently carry out a reverse transformation to the original basis. The resulting non-diagonal matrix is then used for all subsequent computations. In the case of the damped Breit-Pauli terms it is necessary to carry out an additional matrix multiplication[36] involving four one-electron exponential matrices and the original two-particle Breit-Pauli counterpart discussed in Sect. V.A. The use of this matrix technique has the disadvantage of rendering the overall treatment non-variational, but again use of a suitably flexible basis set minimizes this effect.

It is at this stage of the computations that the charges and rest masses of the various constituent particle types are first needed. Each of the one-particle matrices for the relativistic kinetic energy and the exponential damping factors requires such input values explicitly. The corresponding matrices are generated for each particle type from the $p^2/2$ non-relativistic counterpart. It should be clearly distinguished between "particle types" and "particles" in this

connection. At this stage it is only necessary to know what kinds of particles are contained in the system at hand, and not how many of each. Once these one-particle matrices are generated it is necessary to carry out a series of four-index transformations for each Breit-Pauli operator μ and pair of particle types ρ. Because of the nature of the total XBPS Hamiltonian, it is necessary to distinguish between Γ = (1, 2) and Γ = (2,1), i.e. the order of particle-types is significant. This becomes obvious at the next step in the procedure, in which each transformed matrix is multiplied with an appropriate set of coupling constants formed from the charges and rest masses of the constituent particles (see Table I).

These results are then added together to form the final one- and two-particle Hamiltonian matrices, which are stored for further use in the many-particle phase of the theoretical treatment. The four-index (two-particle) integrals are ordered by means of quartets of indices for each basis function, as distinguished by their respective values for the quantum numbers n, 1, j and m_j discussed above. In addition there are separate values for each of the two Γ permutations, as well as for each pair of particle-types ρ. The operator index μ has thus effectively been replaced by the particle-pair index ρ at this stage of the treatment as a result of the additions and scalar multiplications of the individual operator matrices to form the Hamiltonian two-particle matrix. The kinetic energy matrix elements are only ordered with respect to n and l because they do not vary with j and m_j. In addition, only diagonal ρ values are needed because of the one-particle nature of this operator.

The method employed to obtain approximation solutions for the Schrödinger equation discussed above is primarily the configuration interaction approach. A self-consistent field calculation is first carried out to generate an orthonormal basis of one-particle functions which allows an optimal description in terms of a single configuration.[38-40] More details of this aspect of the general theoretical treatment are given elsewhere.[41]

C. CALCULATION OF NON-HYDROGENIC STATES OF THE e^+e^- SYSTEM

The basic strategy for obtaining an e^+e^- state with a binding energy of $2m_{0e}c^2$ is to vary the constant A in the XBPS Hamiltonian (Table I) until the lowest energy possible for a given number and type of basis function corresponds to the desired value. Without the exponential damping (A = 0), this goal can never be reached because the Hamiltonian is not bounded from below in this case. The first basis chosen contains two s- and two p-type primitive Gaussians

with initial exponents of $1.0x10^7$ and $1.0x10^8$ a_o^{-2} for both types. The exponents were multiplied by a scale factor η and a full CI calculation was carried out for symmetries spanned by this basis.

The computations show that the lowest energy results *for a state of 0^- symmetry* (J=0 and negative parity). By varying both η and the damping constant A, it is found that a minimum in energy of the desired value ($-2\alpha^{-2}$ =-37557.7 hartree) occurs for the lowest 0^- state for η = 0.11 and A= 1.054 a.u. (this result was first obtained in 1987 at the University of Wuppertal[33]). As expected, the value of the minimal energy increases with the magnitude of A for all η and advantage is taken of this relationship in subsequent optimizations. These calculations thus demonstrate that the XBPS Hamiltonian can be subjected to standard optimization techniques and the energies of the corresponding full CI secular equations can be suitably adjusted with a single free parameter.

The next step was to define a larger basis set consisting of five s- and five p-type primitive Gaussians. The exponents were initially assumed to form a geometrical progression: $ß_N = ß_1 Ξ^{N-l}$. The value of Ξ was taken to be 2.0 after some initial experimentation. As before, the energy optimizations are carried out with respect to a single scaling parameter η which multiplies all the $ß_i$ values. The exponents are taken to be the same for the s and p sets ($ß_1 = 0.25 \times 10^8$ a_o^{-2}). This is already a reasonably large s,p basis, consisting of 80 spin-orbitals or 40 for each particle, considering that a full CI optimization is to be carried out. It is nonetheless considerably smaller than those commonly used to study hydrogenic systems on a definitive basi,[36,37] but it will serve the present purpose adequately, namely to examine the description of the proposed tight-binding states in the XBPS model.

It is again found that the most stable state of the e^+e^- system has 0^- symmetry. The corresponding wave-function consists of products of $s_{1/2}$ and $p_{l/2}$ (± denotes positron or electron function respectively) one-partic1e functions. Four products of spin orbitals are required for any pair of exponents[33]:

$$0^- = p^+_{½}\left(m_j = ½\right)s^-_{½}\left(m_j = -½\right) - p^+_{½}\left(m_j = -½\right)s^-_{½}\left(m_j = ½\right)$$

$$+p^-_{½}\left(m_j = ½\right)s^+_{½}\left(m_j = -½\right) - p^-_{½}\left(m_j = -½\right)s^+_{½}\left(m_j = ½\right). \qquad \text{III.1}$$

This function is seen to not only possess singlet spin but also to be symmetric with respect to the charge conjugation operation (see Sect. II.E for a discussion of the latter symmetry property for

particle-antiparticle pairs). The optimal value for the scale factor η is 0.095 and the correct binding energy of $2\alpha^{-2}$ is obtained for A= 1.078 a.u. One should expect that the value of the damping constant increases with improvement in the one-particle basis and this behavior is observed. The change in A relative to its 2s,2p value is 2.3%, which indicates that we are already relatively close to the limit attainable with s and p basis functions. It is thus of interest to look at the results of the 5s,5p calculations in more detail below.

TABLE II. Total full CI energy (in hartree) of the lowest states of various symmetries of the e^+e^- system obtained employing the 5s,5p basis with scale factor η = 0.095 and exponential damping constant A = 1.0775 a.u. for the XBPS Hamiltonian of Table I.

Symmetry	First Root	Second Root
0^+	372025.142	561471.371
0^-	-37656.717	483278.726
1^+	596788.279	646488.246
1^-	592821.494	639727.142
2^+	785793.989	806032.930
2^-	691742.083	763807.974
3^+	853632.944	164188.023

TABLE III. Energy contributions (in hartree) of various operators (see Table I for definitions) for the 0_g^- ground state of the e^+e^- system obtained employing the 5s,5p basis with scale factor η = 0.095 and exponential damping constant A = 1.0775 a.u. for the XBPS Hamiltonian.

Operator	Expectation Value
Kinetic energy	1992262.978
Coulomb	-3233.894
Spin-same-orbit	-378340.098
Spin-other-orbit	-830993.650
Darwin Term	8889.119
Orbit-orbit	-407592.397

Spin-spin	-418648.776
Spin-spin δ	0.000
Total energy	-37656.721

The energies of the most stable e^+e^- states of each symmetry obtained in this treatment are given in Table II, from which it is seen that the lowest-lying 0^- species is favored by a large margin over the other states, being the only one which is bound with respect to the separated particles at this level of treatment. The 0^- total energy is broken down into contributions from each of the terms in the XBPS Hamiltonian in Table III. The total kinetic energy is 1.99×10^6 hartree or 54.2 MeV, so it is clear that the two particles are tightly bound. The main attractive contributions come as expected from the damped Breit-Pauli interactions. The spin-same-orbit, orbit-orbit and spin-spin terms are each in the order of -4×10^5 hartree, while the spin-other-orbit interaction is double this amount. The relative order of these contributions is easily understandable in terms of the constants multiplying each operator in the Breit-Pauli interactions themselves[6] (see Table I). The cancellation between these attractive potential terms and the two repulsive quantities is very delicate, as seen by the fact that the binding energy is only 1.89 % of the total kinetic energy. By way of comparison, it should be recalled that the binding energy is exactly equal to the kinetic energy in non-relativistic treatments of atomic systems (by virtue of the virial theorem).

It is important to note that a state composed of only s orbitals must give zero contribution by symmetry for each of the above Breit-Pauli potential terms, so it is not difficult to understand that substantial $p_{1/2}$ character is present in the optimal 0^- wavefunction. It is well known that the $p_{1/2}$ orbital is stabilized by spin-orbit coupling in atomic calculations, so this observation is also not surprising from that point of view. The binding is considerably enhanced for the e^+e^- system relative to the hydrogen atom because of the much larger magnetic moment of the positron compared to that of the proton, as demonstrated in Table III. In this sense the large binding of the 0^- state can be thought of as resulting from a tremendously large increase in the $p_{1/2}$ - $p_{3/2}$ multiplet splitting in the spectrum of hydrogenic systems. It might be thought that a $p_{1/2}$ $p_{1/2}$ configuration would be even more stable on this basis, but the added kinetic energy of $p_{1/2}$ *vis-a-vis* $s_{1/2}$ is decisive in avoiding this result. If the calculations are carried out under the condition of

vanishing translational energy (**P** = 0; see Sect. III.B), it follows that the corresponding function of the electron-positron separation would be a p orbital (more specifically a $p_{1/2}$ species coupled with the spin of the reference particle to produce a 0^- solution). This point has been verified explicitly in calculations to be discussed subsequently in Sect. III. F.

The 0^- state's composition is noteworthy in another way, namely that it possesses an exactly vanishing expectation value for the Darwin δ-function term appearing in the original Breit-Pauli Hamiltonian, as can be verified using the above sample wave-function. This means that the electron and positron never occupy the same spatial position when their spins are identical. The expectation value of the Darwin term in the XBPS Hamiltonian itself (Table I) is non-zero in value (Table III), but this result stems from the form of the exponential damping factors employed in this case (same as for the spin-same-orbit term). The δ-function term in the spin-spin operator also has a vanishing expectation value for the 0^- wave-function, with and without the XBPS adaptations (Table III). This result shows that the avoidance property for electron and positron is not restricted to species of the same spin component since the $\mathbf{s_1}.\mathbf{s_2}$ scalar product allows α and ß spins to have a non-zero interaction in general. In view of the opposite charges of the electron and positron it might be thought that these particles would prefer to be in the same region of space much more than these results would indicate, but one should not forget that the Darwin term itself is repulsive in this case, and thus its influence should tend to be minimized in a variational treatment. This consideration does not completely explain the observed behavior, however, as it must be assumed that such a relationship between the two charge distributions also maximizes the effects of the attractive terms in the XBPS Hamiltonian, such as the spin-spin, spin-orbit and orbit-orbit interactions. Since the vanishing magnitude for the various δ-function terms is so clearly tied up with the 0^- composition for the e^+e^- wavefunction, there is good reason to expect that similar results will be found regardless of the size of the one-particle basis set employed. In the **P** = 0 limit for this state discussed above, even the expectation value of the exponentially damped Darwin term must vanish exactly since it is forbidden by symmetry from having an admixture of s spatial character, again as demonstrate in the calculations of Sect. III. F. Such a function must also be symmetric with respect to the charge conjugation operation, in agreement with what has been found in the calculations above for the 0^- wave-function with non-vanishing translational energy.

The exceptional nature of the 0^- e^+e^- state also gives added support to the hypothesis formulated in earlier work[42] to the effect that such a mass-less state of positronium is identical with that of the photon at rest. Although this result might be thought to be inconsistent with such an assumption because the photon is normally assigned 1^- symmetry, it should be recalled that the photon state given the latter designation does not correspond to a mass-less system. The experiments which demonstrate that the photon has one unit of angular momentum,[43,44] for example, are based on a radiative emission process. Since the dominant mechanism in such transitions is electric-dipole in character, it follows that a change in angular momentum of one unit must have occurred in the process, for both the atomic system *and the photon itself* (see Fig. 3). In the creation-annihilation hypothesis, attention is centered on the change in the atom's angular momentum, but the premise in the XBPS model is that a mass-less photon is present prior to the transition and thus that its angular momentum is also altered upon emission. On this basis one can conclude from the rule for the vector addition of angular momentum that the original mass-less photon must have possessed one of three possible J values: 0, 1 or 2. Since it is difficult to imagine how a system with zero momentum, as must be assumed for a photon with E = 0, can have other than zero angular momentum, the finding that J = 0 is greatly preferred in the present calculations for the proposed e^+e^- tight-binding state is completely in line with the results of the photon angular momentum measurements.

Since the electric dipole moment has negative parity, one is also led to conclude that *the photon state after emission has a different parity than the initial mass-less state.* This deduction would appear to contradict the presently calculated finding that the symmetry of the latter is 0^-, but closer consideration shows that *the assignment of negative parity to the state of the emitted photon is perfectly arbitrary.* Parity designations of particles are always based on assigning one of two possible values to some standard system, and as such it is not possible to speak of absolute parity determinations[45] on the basis of experimental evidence alone. If one believes that the photon is created from nothing, it is perhaps natural to assign even parity to the initial photon state, and consequently odd parity to a photon generated as a result of an electric-dipole transition. The present calculations suggest a definite structure for the mass-less photon state, with 0^- symmetry, so that in this view one is led to conclude that the state of a photon observed after an electric-dipole transition is actually 1^+, i.e. the opposite parity as conventionally assumed.

At the same time, one can point to more general discussions[46] of the dynamics of relatively light particles such as electrons or neutrinos when confined to small (nuclear-like) volumes which clearly suggest that it is highly unlikely that they exist in other than the lowest possible angular momentum state under these circumstances, which again in the case of a photon would be J = 0. Higher values of J are easily conceivable in conjunction with the translation of a tightly-bound system, however, which corresponds to the natural condition of a photon with non-zero energy. With regard to the positronium decay process, it is interesting to note that the present assignment for the photon's mass-less state implies that the most common process involving a singlet initial state corresponds to a $0^+ \rightarrow 0^-$ transition. Such a process is well known to be forbidden by any radiative mechanism involving only a single photon, consistent with what is observed. A possible two-photon transition would proceed with the aid of a $1^{\pm}$ virtual photon state, in which case the two decay photons would possess respectively 1^+ and 1^- symmetry, i.e. of opposite parity to one another but of the same total J value. Since there is no net change of total angular momentum in the overall process, it follows that the two photons must have complementary polarizations, again as observed. On the other hand, there appears to be no definitive means of establishing their relative parity experimentally. All in all, it can be concluded that the calculations appear to be perfectly consistent with both experimental observations and fundamental theoretical considerations with regard to the symmetry properties expected for particles of light.

The variation of the energy of the 0^- state with the scaling parameter η and the exponential damping constant A is shown in Fig. 3. The minimal energy always becomes higher as A is increased, as already noted. The E vs. η curve is closely related to the schematic total energy diagram given in Fig. 1, whereby η plays much the same role as the reciprocal of the square root of the inter-particle distance r by virtue of the scaling properties of Gaussian functions. For example, the expectation value <r> approaches zero to the right in Fig. 3 as η increases. The damping of the Breit-Pauli terms (Table I) produces a sharp minimum consistent with this interpretation, and the depth of the minimum is seen to be very sensitive to the value of the constant A. Qualitatively, it is easy to imagine from this diagram that a system trapped in such a deep potential well would be extremely stable. At distances to the left of the minimum's location the energy increases sharply, passing well beyond the zero value for the separated particles.

Eventually as the Gaussian exponents are decreased to their hydrogenic values ($\eta \cong 10^{-8} - 10^{-9}$), the total energy peaks and then the positronium ls minimum is reached on the basis of the same Hamiltonian. A change of state occurs along the way, however, so that the $s^{1/2}$ $s^{1/2}$ configuration becomes most stable. At this point the mean values of the exponential damping factors are very nearly unity, but they have the advantage of allowing a variational treatment of the hydrogenic states while still retaining a form of the Breit-Pauli interactions in the Hamiltonian. At distances smaller than that of the location of the deep potential minimum in Fig. 1, the energy is seen to increase very sharply as a result of the steep decrease in the magnitudes of' the exponential damping factors in this region combined with the corresponding increase in the magnitude of the kinetic energy (see Fig. 2). Altogether, a consistent picture emerges of a tightly bound e^+e^- state with a binding energy of exactly $2m_{0e}c^2$, resulting primarily from an exponentially damped attractive potential of relatively short range.

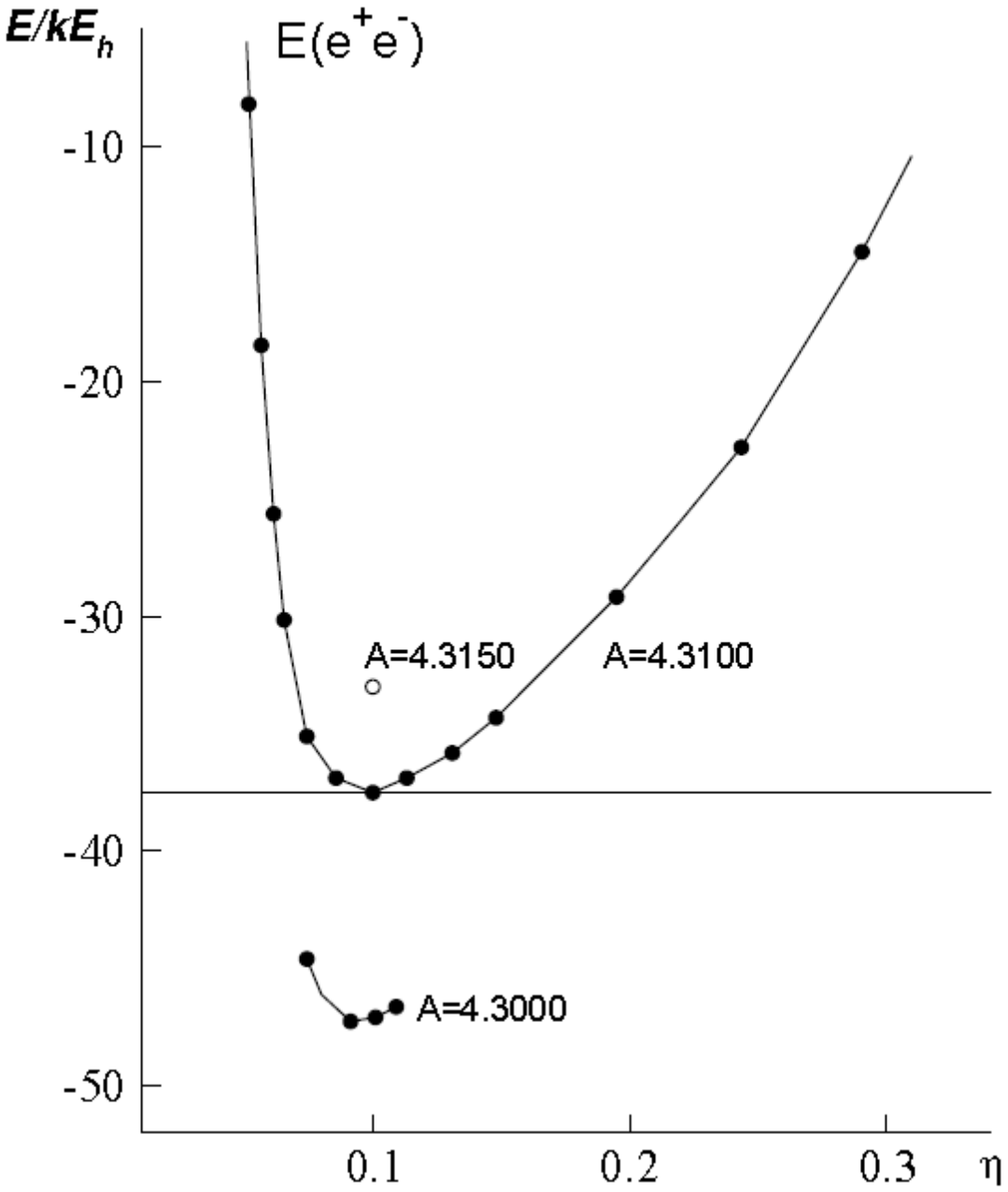

FIG. 7. Variation of the computed total energy (in khartree) of the e^+e^- system as a function of the 5s,5p basis set scaling factor η in the XBPS treatment for various values of the damping constant A. The horizontal line at the center of the diagram corresponds to the negative of the rest energy ($2m_{0e}c^2$) of the system. A value of A is sought which leads to this energy result for the optimum choice of η. Results for several other A values are also shown for comparison. Note that the values of A given in the diagram are 4.0 times larger than those given in the text due to a difference in definition.

D. CONSIDERATION OF TRANSLATIONAL EFFECTS IN THE XBPS CALCULATIONS

The calculations discussed thus far have yet to consider the magnitude of the translational component of the total energy. This can be done in several ways, the simplest of which in the present context involves the computation of the expectation value of $(\Sigma \mathbf{p_i})^2$ for the wave-function already obtained. On this basis it is found that the translational energy is 1.3483×10^6 hartree, a very considerable amount. This result needs to be kept in perspective, however, when comparing with conventional calculations in which the center-of-mass motion is factored out. We have therefore carried out the analogous treatment for the hydrogen atom (employing a slightly larger 10s,5p basis), i.e. by also treating the translational and internal motion together explicitly. A total energy of -0.4660 hartree results, which is 0.0340 hartree higher than the non-relativistic Schrödinger equation value. The expectation value of the translational energy <T> obtained with this wavefunction is 0.015 hartree, which corresponds to a mean center-of-mass momentum of 7.42 a.u. Assuming that momentum increases proportionally with r^{-1} and comparing the value of the $0^- e^+e^-$ expectation value Table III (Coulomb term, -3233.89 hartree) to the unit value known for the H atom ground state leads to an estimate of the translational momentum of 2.400×10^4 a.u., which upon multiplication with $c = \alpha^{-1}$ corresponds to a translational energy for a mass-less system of 3.29×10^6 hartree, roughly two-and-one-half times larger than the above computed value.

The $p_{1/2}s_{1/2}$ form for this state helps to minimize the expectation value of T because it leads to a $\langle \mathbf{p}_1 \cdot \mathbf{p}_2 \rangle$ cross term which is necessarily negative (it is proportional to $-|\langle p_{1/2}\ \mathbf{p}\ s_{1/2}\rangle|^2$). In other words, it is also possible to look upon the relatively high stability of the 0^- state as resulting from its ability to minimize the translational energy with this type of wave-function. More details regarding further calculations to study the effects of translation on the present XPBS results are given elsewhere.[47]

E. CALCULATIONS WITH ELIMINATION OF TRANSLATIONAL ENERGY EFFECTS

It is possible to carry out the calculations in a different way using the Hamiltonian of Table I in order to eliminate the effects of translation on the wavefunctions. As discussed in Sect. II.B, this can be done by simply applying the condition that the momentum difference of the two

particles always be equal to zero, that is by requiring that $\mathbf{p_1}$=-$\mathbf{p_2}$. There remains only one spatial co-ordinate as a result, the $\mathbf{r_{12}}$ inter-particle vector. In effect the calculations correspond to those carried out for atoms with a single center. It is merely necessary to replace the two kinetic energy terms in the original calculations with a single square-root operator in which the reduced mass ($\mu = 0.5$) of the electron-positron pair is used.

As a result, it is possible to employ a much larger Gaussian basis set in this series of calculations than in those already discussed in Sect. III. B. It contains 70 functions for each l value (s,p,d…) whose exponents range in a geometric series from 0.00158 to 1.00000×10^{10}. In contrast to the first set of calculations, this basis set is large enough to describe the lowest-lying Rydberg states of positronium in the same treatment as for those with much smaller average radial distances. The energy results obtained for the lowest states of 0^+ and 0^- symmetry are given in Table IV. The corresponding results for J=1 and 2 have also been obtained and they produce no low-energy states other than the Rydberg species shown for the 0+ and 0- symmetries. It would be possible to obtain accurate energies for many more Rydberg states by simply adding more small-exponent Gaussian basis functions to the theoretical treatment, e.g. by expanding the above progression by several orders of magnitude downward to 1.0×10^{-7}.

The point which needs to be emphasized, however, is that the present calculations demonstrate explicitly that it is possible to construct a Hamiltonian operator whose eigenvalues not only include those of all the positronium Rydberg states, but in addition a single value with energy equal to $2m_{0e}c^2$, i.e. the 0^- value that corresponds to complete elimination of rest mass from the e^+e^- system. This result comes out most clearly in the above calculations in which the energy of the center-of-mass of the system has been completely removed, i.e. no translation. To do this quantitatively, it is necessary to increase the value of A in the XBPS Hamiltonian from 1.0775 a.u. in Table II to 1.54666 a.u. to obtain the results of Table IV. This change demonstrates that the amount of exponential damping must be significantly increased in order to make up for removing the effects of translational motion in the lowest 0^- state.

Root No.	0^+	0^-
1	-0.250041 (n=1)	-37561.376228 ($2m_ec^2$)
2	-0.062507 (n=2)	-0.062502 (n=2)
3	-0.027779 (n=3)	-0.027778 (n=3)

4	-0.015626 (n=4)	-0.015625 (n=4)
5	-0.010000 (n=5)	-0.010000 (n=5)
6	-0.006943 (n=6)	-0.006944 (n=6)
7	-0.004686 (n=7)	-0.004903 (n=7)

TABLE IV. Total full CI energy (in hartree) of the lowest states of 0^+ and 0^- symmetry of the e^+e^- system obtained in the calculations with the condition of $\mathbf{p_1}$=-$\mathbf{p_2}$ using the XBPS Hamiltonian of Table I.. In the 0^+ case 70 s-type functions are employed, while the same number of p-type functions are employed in the corresponding 0^- treatment. The value of the exponential damping constant A in the XBPS Hamiltonian has been varied so as to obtain a minimal energy for the 0^- states of $2m_{0e}c^2$= 1.02 Mev. The value of A = 1.54666 a.u. is found to fulfill this condition to a satisfactory degree. The principal quantum number n of each Rydberg state is indicated in parentheses next to the corresponding energy value.

An analysis of the energy contributions to the lowest-energy state is given in Table V. These results can be compared with the corresponding values given in Table III for the calculations in which translational effects are not excluded. For example, the Coulomb energy is

Operator	Expectation Value
Kinetic energy	1262707.2926853
Coulomb	-2662.0961756246
Spin-same-orbit	-230447.7644808
Spin-other-orbit	-460895.52896168
Darwin Term	0.000000
Orbit-orbit	-375815.5148147
Spin-spin	-230447.7644808
Spin-spin δ	0.000000
Total energy	-37561.396228

TABLE V. Energy contributions (in hartree) of various operators (see Table I for definitions) for the 0_g^- ground state of the e^+e^- system obtained with exponential damping constant A = 1.54666 a.u. for the XBPS Hamiltonian under the $\mathbf{p_1}$=-$\mathbf{p_2}$ (zero translational energy) condition.

increased by 571.798 hartree, showing that the distance between the electron and positron is greater in the present treatment excluding translational effects. Because of the definition of the Coulomb operator in Table I, it is possible to obtain an average value for this separation simply by taking the reciprocal of the corresponding energy value. The inter-particle distance is therefore estimated to be 3.756×10^{-4} bohr in the present treatment, as opposed to the corresponding value of 3.09228×10^{-4} bohr when translational effects are included. The corresponding value for the positronium 0+ ground state is 2.00 bohr, which is 5324.8 times larger. This value in turn is equal to 7.05 α^2 bohr. It is still more than an order of magnitude larger than a typical separation between nuclear particles ($\alpha^2/2$ bohr). The smaller distances in the latter case are reasonable in view of the much smaller kinetic energies expected for proton and neutron constituents of nuclei as opposed to that of the electron and positron in the present XBPS treatment.

The average value of the momentum p in the lowest root can be estimated by dividing the kinetic energy by in Table V by α^{-1}, the speed of light in a.u. The result is 9214.42 a.u., which is 18428.8 times the corresponding value in the 0^+ positronium ground state. The product of this value and the above distance is 3.46, which may be compared to the corresponding product in the positronium ground state of 1.0, which is the same ratio as found in the hydrogen atom calculations. Thus, it is found that the momentum of the lowest-energy state in Table V increases notably faster than the corresponding inter-particle distance decreases. This relationship is expected on the basis of Fig. 2, which shows that the kinetic energy, which is proportional to the momentum in this region, is increasing linearly toward shorter distances while the mean distance is increasing at a slower rate because of the effects of exponential damping.

The Breit-Pauli terms have an interesting relationship to one another, namely exactly the same value is obtained for the spin-same-orbit and spin-spin operators, which in turn is exactly one-half of that found for the spin-other-orbit term. The value of the orbit-orbit term lies between these two values. The values shown in Table III for the calculations which do exclude translational effects on the energy eigenvalues are much more irregular. Finally, the value of the Darwin term's energy is exactly zero in Table V, which is the expected result given the l=1 value of the (p) basis functions in this case. The non-zero value in Table III shows that translational effects tend to allow the wavefunctions to avoid having a node at the origin, although they do not

change the fact that the spin-spin delta term must be of vanishing magnitude for L=1 symmetry, also as found in Table V, i.e. with or without consideration of the effects of translation.

F. THE PROTON-ANTIPROTON BINARY

As pointed out in Sect. II.D, there is a scaling property for the XBPS Hamiltonian (Table I) which requires that for every e^+e^- wavefunction, there exists a corresponding p^+p^- solution with an energy eigenvalue which is exactly m_{op}=1836 times greater in magnitude. The desired p^+p^- eigenvector can always be obtained from the relation: $\Psi_{e+e-}(r) = \Psi_{p+p-}(m_{oe}r/m_{op})$. In other words for the p^+p^- system everything is played out in a coordinate system which is contracted by a factor of 1836 relative to that of e^+e^-. The Gaussian exponents in the e^+e^- basis must each be multiplied with 1836^2 in order to obtain the desired scaling relationships for each energy quantity. The same scaling property exists for the translational energy operator T, so all energy results obtained above for the electron-positron system can be converted over to those of p^+p^- simply by multiplying the corresponding e^+e^- value with 1836. In particular, this scaling relationship allows one to employ the same value for the exponential damping constant as before, thereby giving this quantity more of a general character than might otherwise be assumed.

It might come as a surprise to see that the required binding energy of $2m_{0p}c^2 = 1.876$ GeV comes from short-range effects which are generally associated with magnetic interactions, i.e. Breit-Pauli terms, because the magnetic moment of the proton is so small compared to that of the electron. Closer examination of the effects involved, however, underscores the fact that the relatively large mass of the proton is actually quite beneficial in forming a tight-binding state which takes extensive advantage of such short-range interactions. To begin with, there is the obvious fact that the kinetic energy associated with a given momentum value is substantially smaller for a proton than for an electron. The occurrence of the mass in the denominator of the exponential arguments of the XBPS Hamiltonian (Table I) is an even more significant factor, however, since it leads to a drastic reduction in the exponent of the damping function for a given momentum *vis-a-vis* that for a lighter particle (Sect. II.D). This means the short-range potential terms are still going down in energy for inter-particle distances much shorter than the $r \cong 7\alpha^2$ value favored by the e^+e^- system (Fig. 1). As usual, the exponential damping ultimately prevents the situation from getting out of hand, but the corresponding p^+p^- energy minimum occurs for r =

7.05 α^2/m_{op} (see the discussion after Table V) or 2.044 x 10^{-7} a_0 (1.08 x 10^{-17} m), making this probably one of the shortest-range interactions which occurs in nature.

The small magnetic moment of the proton only means that magnetic-type interactions occurring at typical atomic separations (Bohr radius a_0) are nearly negligible compared to those of electrons. By contrast, at the much smaller inter-particle distances preferred by the p^+p^- system, even the Coulomb attraction is far from negligible. For $r = 7.05\alpha^2/m_{op}$ the expectation value for this relatively long-range interaction would be -133 MeV, for example, which would be 0.071 times the total binding energy of the p^+p^- system (1876 MeV). From this point of view, the corresponding Breit-Pauli energy contributions, though considerably larger at such distances, do little more than counter the system's enormous kinetic energy, which at $r = 7.05\alpha^2/m_{op}$ can be estimated to be 63.1 GeV based on the result of Table V for the e^+e^- kinetic energy value of 34.3 MeV.

By either of the above measures the cancellation of the kinetic energy due to the Breit-Pauli terms is seen to be almost total, with a net binding energy which is only 2.97 % of the total kinetic energy in either system. As is evident from Fig. 2, it is difficult to imagine that anything other than an exponentially damped potential could achieve such a delicate balance on a general basis.

On the other hand, the main argument against assuming that electrons are actually present in nuclei has been that no such potential can supposedly be found. The present experience strongly suggests that this position should be reevaluated. The Hamiltonian employed in the above investigation allows for a quantitatively equivalent variational treatment of systems with binding energies varying between 1.0 MeV and nearly 2.0 GeV, respectively, as well as a reliable description of conventional atomic systems by virtue of its close association with the Dirac and Breit-Pauli formulations of quantum electrodynamics interactions.

G. THE INTERACTION OF A PROTON AND AN ELECTRON

It remains to be considered whether a strongly bound state also results from an analogous treatment of the electron-proton system. This is done by simply inserting a very large mass for the proton so that the reduced mass of the electron is 1.0. The answer is clearly that *no such second minimum is found which corresponds to an inter-partic1e distance smaller than 1.0*

bohr (Table VI). The corresponding 0^+ results for the treatment in which translational effects are eliminated are shown in Table VII.

Moreover, the reason for this distinction between the e^+e^- and p^+e^- systems is easily understandable from the previous calculations with the XBPS Hamiltonian. The results of Table III for the e^+e^- system are changed dramatically by the substitution of a proton for the positron because of the disparity in the masses of these two particles. The magnitudes of the various Breit-Pauli terms are substantially reduced upon making this substitution because of the importance of the q/m_o factors in the corresponding operators (Table I). Only the spin-same-orbit and Darwin terms with the electron's $(e/m_{oe})^2$ pre-factor survive for all practical purposes. By contrast the kinetic energy is doubled to a value of 0.5 a.u. because of the change in particle mass, thereby destroying the delicate balance mentioned in the last section between the attractive and repulsive components of the total energy for both the e^+e^- and p^+p^- binary systems.

η	E
0.30	710408.14
0.20	560400.24
0.10	374890.12
0.08	329689.40
0.07	305334.70
0.06	279471.535
0.02	148434.705
0.005	64715.8077
5.0×10^{-4}	12839.8600
5.0×10^{-5}	1623.358959
5.0×10^{-6}	159.118214
5.0×10^{-8}	0.173309
3.0×10^{-8}	-0.195469
2.0×10^{-8}	-0.339412
1.0×10^{-8}	-0.425769
9.0×10^{-9}	-0.428911

8.0×10^{-9} (*)	-0.430521
7.0×10^{-9}	-0.430349
6.0×10^{-9}	-0.428057
5.0×10^{-9}	-0.423152
4.0×10^{-9}	-0.414828
3.0×10^{-9}	-0.401501
1.0×10^{-9}	-0.333257
5.0×10^{-10}	-0.281758
1.0×10^{-10}	-0.168834

TABLE VI. Total full CI energy E (in hartree) for the lowest state of the p^+e^- hydrogen atom system obtained employing the 3s,2p,2d basis for various scale factors η and a fixed value of the exponential damping constant A = 1.2648 a.u. for the XBPS Hamiltonian of Table I (* indicates minimum).

Root No.	0^+
1	-0.4999727 (n=1)
2	-0.1249970 (n=2)
3	-0.0555547 (n=3)
4	-0.0312496 (n=4)
5	-0.0199998 (n=5)
6	-0.0138887 (n=6)
7	-0.0102039 (n=7)

TABLE VII. Total full CI energy (in hartree) of the lowest states of 0^+ symmetry of the p^+e^- (H atom) system obtained in the calculations with the condition of $\mathbf{p_1}=-\mathbf{p_2}$ using the XBPS Hamiltonian of Table I.. As in the e^+e^- calculations in Table III, 70 s-type functions are employed. The value of the exponential damping constant A in the XBPS Hamiltonian is the same as for the e^+e^- treatment, although this choice is not critical for the H- atom. The principal quantum number n of each Rydberg state is indicated in parentheses next to the corresponding energy value.

The results of Table III correspond to an e^+e^- inter-particle distance on the order of $r = 7\ \alpha^2$, but as we have seen, the maximum binding for the p^+p^- system occurs when the corresponding separation is m_{0p}/m_{0e} times smaller. At this distance all energy values in Table III can be multiplied by a factor of 1836 to obtain the corresponding p^+p^- results because of the

scaling property discussed in Sect. II.D. If the mass of the electron is substituted for that of the antiproton at such a small distance, the kinetic energy is halved according to the classical Einstein free-particle expression. On the other hand, the corresponding damping factors for the electron are very close to zero for such high momentum, and so only the two Breit-Pauli terms with the $(e/m_{0p})^2$ pre-factor are left (relatively) unaffected.

As a result the required cancellation of the attractive and repulsive terms no longer takes place and an extremely large positive total energy results for the p^+e^- system in this range of inter-particle separation. No choice of basis set succeeds in binding the electron and proton more strongly together than is the case for the hydrogenic 1s state. For example, the use of electronic functions which are optimal for the strongly bound e^+e^- system along with proton functions which are 1836 times more compact (corresponding to their optimal p^+p^- counterparts) also produces only negative binding energies.

These results can again be understood on a qualitative basis by considering the p^+e^- system in its own center-of-mass coordinate system. The condition of equal and opposite momentum (see Sect. III.E) now requires that the electron move at a speed which is 1836 times greater than that of the proton. This requirement forces the particles to avoid each other by wide margins if high speeds are to be maintained, making the type of short-range momentum-dependent interaction represented by the Breit-Pauli interactions very ineffective in producing binding under these circumstances. Such distinctions in the relative particle masses for binary systems are of only minor importance when the Coulomb interaction dominates, however, *which explains why we normally regard* positronium as just another *hydrogenic system.* By simply decreasing the values of the exponents employed for the Gaussian basis functions, one eventually finds that the variational treatment of the XBPS Hamiltonian leads to binding energies in the 0.5 hartree range (Table VI) expected for the ground state of the hydrogen atom. No amount of exponent optimization produces a second minimum at shorter inter-particle separations for this system, in marked contrast to what is observed when employing the analogous Hamiltonian for the e^+e^- and p^+p^- systems.

IV. CONCLUSION

In order to give quantitative substance to the above theoretical model, it is imperative that one clearly identify the nature of the interactions responsible for high-energy processes, especially the prototype example in which an electron and a positron combine to form a tightly bound binary complex with exactly zero rest mass. Emphasis is placed thereby on the fact that no corresponding state of a proton and an electron is known, i.e. the $1s_{1/2}$ state of the hydrogen atom is perfectly stable when left in an isolated condition, whereas that of positronium has only a short lifetime. Similarly, a massless p^+p^- binary must also be assumed to exist based on the analogous experimental results for the interaction of a proton and an antiproton.

The high energies associated with the formation of these two systems suggest that similar short-range interactions are involved as in the binding of nuclei, in which case an exponential form for the corresponding potential has been deduced from scattering experiments. Because of the participation of electrons, positrons and photons in the electromagnetic interaction, it is suggested that a good starting point in the search for such a potential is the relativistic Dirac equation or some approximation to it. It is noted that the Breit-Pauli reduction of this equation contains short-range terms varying inversely as the cube of the inter-particle distance which are of the order of α^2 (10^{-4} hartree) for typical electron-proton separations in an atomic system. The unbounded character of these terms in the limit of vanishingly small separations, particularly in relation to the corresponding relativistic kinetic energy, makes it clear, however, that the desired short-range bonding of elementary particles can only be satisfactorily described by interactions of this type *if they are somehow modified to become considerably less attractive at extremely small interparticle distances.*

An exponential damping of the Breit-Pauli interactions is thus suggested (Sect. II.C). This is in analogy to that proposed by Yukawa fifty years earlier for the description of nuclear binding, except that in that case it was applied to an r^{-1} potential. Similar quantities of r^{-3} type present in the $\mathbf{p} \cdot \mathbf{A}$ cross terms of the Maxwell-Lorentz Hamiltonian are kept in check by the $\mathbf{A} \cdot \mathbf{A}$ component of a perfect square, which in turn varies as r^{-4}. This suggests that the exponent of the damping function for the Breit-Pauli interactions should vary as r^{-1} or p, and that it should contain a factor of the charge-to-mass ratio of a given particle multiplied by a constant of order α^2.

Since the motion of charged particles is involved in such interactions, it seems reasonable to choose a momentum-dependent exponential damping whose argument is always negative. Ultimately these arguments lead to the following explicit form for the damping function: $\exp(-A\,\alpha^2\,|\,\mathbf{p}\,q/m_0|)$. At the same time, the unbounded correction to the Breit-Pauli kinetic energy, which varies as p^4, is introduced via the Einstein relativistic operator $(p^2 + m_0^2\,c^4)^{1/2} - m_o\,c^2$ (with $c = \alpha^{-1}$ in atomic units). The resulting set of interactions is subsequently referred to as the exponentially damped Breit-Pauli Hamiltonian and is employed in a Schrödinger equation (XBPS) of the standard $H\,\Psi = E\,\Psi$ form. The potentially crucial advantage of this Hamiltonian is that it is bounded from below and thus can be treated using standard variational techniques, unlike the un-damped Breit-Pauli terms themselves. The explicit form of the XBPS Hamiltonian is given in Table I.

The above Schrödinger equation has an interesting scaling property of relevance to the positronium decay process. The total energy of any state of a particle-antiparticle system with a given charge and rest mass is exactly M times larger than that obtained by a coordinate scaling for an analogous binary system with the same charge but a rest mass which is M times smaller. This means that the same Hamiltonian which produces the $2m_{oe}c^2$ binding energy assumed for the e^+e^- system leads to the corresponding value of exactly $2m_{op}c^2$ for the p^+p^- counterpart. The latter system's average inter-particle separation is smaller by a factor of the proton-electron rest-mass ratio m_{op}/m_{oe} than that for the e^+e^- system. The form of the XBPS Hamiltonian is thus seen to guarantee the condition required by the Einstein mass-energy equivalence relation, namely that the maximum energy lost in a particle-antiparticle interaction is directly proportional to the rest masses of the isolated systems (Sect. IV.D). This condition places a restriction on the form of the exponential damping factor in the XBPS Hamiltonian, specifically that the momentum p be divided by the particle's rest mass in the corresponding argument.

The use of the relativistic kinetic energy operator in the XBPS model raises a fundamental question of a different nature, however, namely how to deal with the translational motion of the combined system being treated (Sect. II.B). Analysis indicates that, contrary to the non-relativistic case, a transformation to center-of-mass coordinates for such a Hamiltonian does not lead to a total separation of the internal and translation motion. This fact is related to the requirement of the theory of special relativity that distances measured in an inertial system moving with constant velocity relative to the observer are found by him to be different. Such

findings clearly cannot result if it is simply assumed that the center-of-mass motion is completely separable, since properties involving only internal variables are thereby forced to be independent of the state of translation of the combined system. It was therefore decided to carry out calculations with the XBPS Hamiltonian in terms of the Cartesian coordinates of the constituent particles without introducing a center-of-mass transformation, so as not to prejudice the results of the treatment in this respect, despite the fact that this procedure brings with it certain computational difficulties otherwise avoided by such a change in coordinates.

Allowing the internal and center-of-mass motion to remain coupled in the theoretical treatment gives insight as to how the $e^+ e^-$ system can have a tightly bound ground state below the familiar 1s state of positronium, unlike the case for the hydrogen atom of proton-electron composition. The essence of this argument is contained in the observation that the Σp_i condition for a binary system whose center of mass is at rest in the origin of the coordinate system implies that $\mathbf{p_1} = -\mathbf{p_2}$ or $\mathbf{v_1} = -(m_2/ m_1)\, \mathbf{v_2}$**.** Since the mass of the proton is so much greater than that of the electron, this condition requires that their respective velocities be quite different from one another in the hydrogen atom. This circumstance is incompatible with the need to keep the particles close to one another while each is moving at high speed in order to take maximum advantage of the short-range momentum-dependent attractive terms in the XBPS Hamiltonian such as the damped spin-orbit coupling (Sect. III.G).

By contrast, the analogous condition for the electron-positron and proton-antiproton systems leads to a perfectly correlated relative motion of the two particles. This relationship lends considerable support to the proposition that such systems possess non-hydrogenic states of exceptionally large binding energies. As the translational energy increases beyond zero the correlated motion is gradually disturbed, however. At first glance the smaller q/m_o value of the proton relative to the electron appears to be inconsistent with the requirement that p^+p^- have a much larger binding energy than the corresponding $e^+ e^-$ system, especially when one only considers the magnitude of their respective coupling constants in the short-range XBPS interactions. The same quantity also causes the argument of the exponential damping factors to be correspondingly smaller for the proton-antiproton system, however, which in turn allows its two particles to approach each other far more closely than is preferable for the lighter electron-positron pair.

A full CI treatment of the Schrödinger equation discussed above for the e^+e^- system employing various primitive Cartesian Gaussian one-particle basis sets has indicated that the lowest-energy state for this system possesses 0^- symmetry and is symmetric with respect to the charge conjugation operation, which commutes with the corresponding Hamiltonian (Tables II-III). The constant A in the exponential damping factors has been chosen so as to obtain the desired e^+e^- binding energy of $2\ m_{oe}c^2$ for an optimal choice of orbital exponents in the full CI treatment (Sect. III.C).

Additional calculations have also been carried out using the $\mathbf{p_1} = -\mathbf{p}_2$ condition that eliminates translational energy from the theoretical treatment (Tables IV-V). In this case, the 0_g^- symmetry of the lowest-energy e^+e^- (ground) state is found to possess a vanishing expectation value for the conventional (undamped) Darwin term, as well as for the corresponding δ-function term in the spin-spin interaction. This result shows in a particularly striking manner that the two constituent particles must effectively avoid one another completely in order to achieve maximum stability.

The value of the damping constant A is found to be 1.54666 a,u, using the above criterion. As a result, the range of the damping interaction conforms to the expectations discussed previously, becoming significant for inter-particle distances smaller than or equal to $r = 10\ \alpha^2$. In accordance with the XBPS scaling property, the optimum proton-antiproton wave function is characterized by Gaussian exponents which are larger by a factor of $(m_{op}/m_{oe})^2$ relative to those for e^+e^-, giving the desired $2m_{op}c^2$ binding energy relative to the separated proton and antiproton for the same choice of A as for the electron-positron system, as discussed in Sect. II. D.

The well-known Rydberg states of positronium are obtained with high accuracy using the same XBPS treatment. This experience shows that it is quite feasible that the suggested e^+e^- state does indeed exist as the true ground state of the e^+e^- system. The value of the Coulomb energy in the latter state indicates that the average separation between the electron and positron is $3.756\text{x}10^{-4}$ bohr or $7.05\ \alpha^2$, whereas the corresponding value for the 1s Rydberg ground state is 2.0 bohr.

Finally, analogous calculations have been carried out using the XBPS Hamiltonian for the electron-proton system. The results are shown in Tables VI and VII. As expected, no low-energy state comparable to that for the electron-positron system is found in this case. Instead, only an accurate calculation of the H-atom Rydberg spectrum is obtained, especially when the

effects of translation are eliminated (Table VII). There is no question that the lowest-energy state obtained is the completely stable ground state of the hydrogen atom.

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