Binding in some few-body systems containing antimatter

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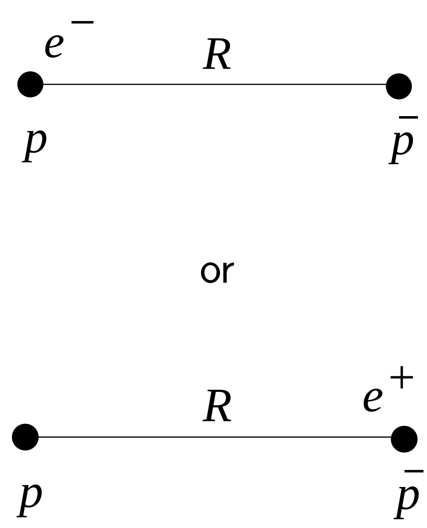
Fixed proton and antiproton + an electron or a positron



Internuclear distance = R

This is a very well-known system – a charge in a dipole field.

Many calculations have been carried out on this system.

First determination of the critical distance, R_c, below which the dipole cannot bind an electron (or a positron).

Fermi and Teller, *Phys. Rev.* **72**, 399 (1947).

They considered binding of an electron by a dipole made up of a negative meson and a proton in connection with the capture of negative mesons in matter.

They stated that $R_c = 0.639a_0$.

No detail given of the calculation.

This system was considered shortly afterwards by

Wightman, *Phys. Rev.* **77**, 521 (1950).

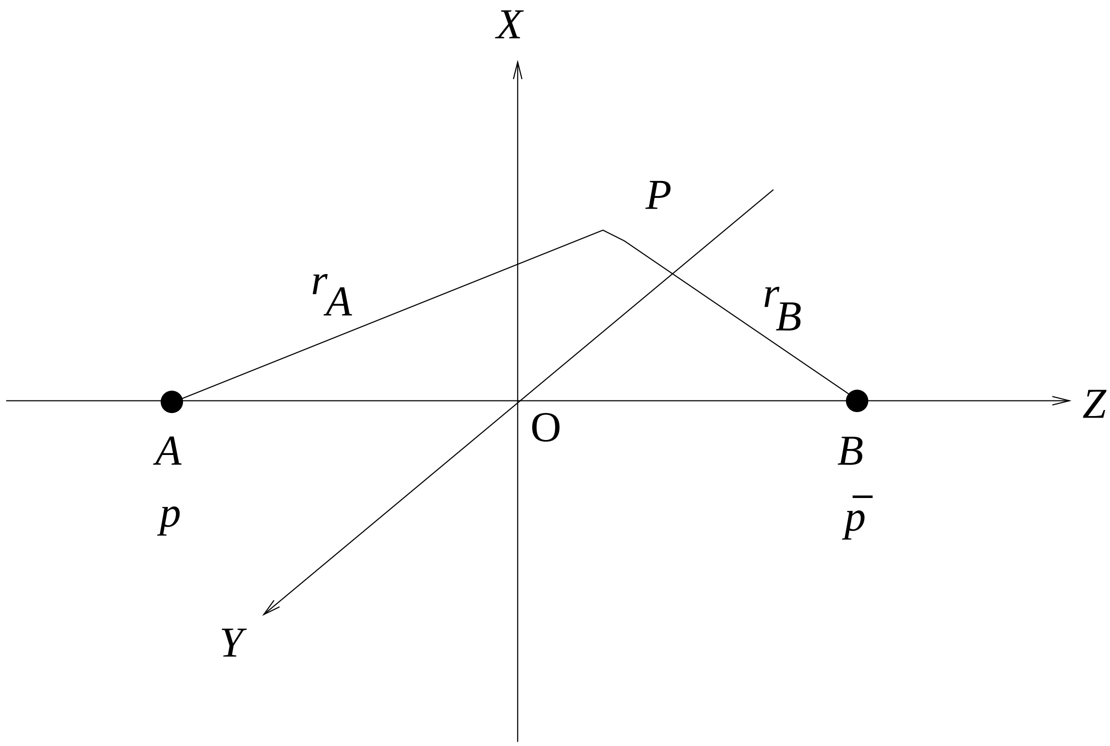
He used the separability of the Schrödinger equation in prolate spheroidal coordinates to deduce that R_c has this value by considering the state of zero energy.

A detailed mathematical treatment of electron binding by a dipole was carried out by

Wallis, Herman and Milnes, *J. Molec. Spectoscopy* **4**, 51 (1960).

Calculation of energies for $R \geq 0.84a_0$ using the separability of the Schrödinger equation in prolate spheroidal coordinates.

Prolate Spheroidal Coordinates (λ, μ, ϕ)



A has coordinates $\left(0, 0, -\frac{R}{2}\right)$

B has coordinates $\left(0, 0, \frac{R}{2}\right)$

$R =$ internuclear distance

$$\lambda = \frac{r_A + r_B}{R}$$
$$\mu = \frac{r_A - r_B}{R}$$

ϕ is the usual azimuthal angle of spherical polar coordinates.

The separability is due to the existence of the complete commuting set of observables:

$\hat{H}$, the Hamiltonian,

$$\hat{\Lambda} = \tfrac{1}{2}(\hat{\boldsymbol{L}}_p \cdot \hat{\boldsymbol{L}}_{\bar{p}} + \hat{\boldsymbol{L}}_{\bar{p}} \cdot \hat{\boldsymbol{L}}_p) + \frac{2R\mu(\lambda^2 - 1)}{\lambda^2 - \mu^2}$$

and $\hat{L}_z$, the component of angular momentum in the z-direction.

$\hat{\boldsymbol{L}}_p$ and $\hat{\boldsymbol{L}}_{\bar{p}}$ are the angular momenta of the electron or the positron about p and $\bar{p}$, respectively. Units are atomic units.

Wallis et al. obtained energies for the electron or the positron for the ground state and several excited states.

The system seems to have been rediscovered around 1965. Several authors obtained the critical value $R_c = 0.639a_0$ obtained by Fermi and Teller in 1947.

Calculations were carried out by:

Mittleman and Myerscough, *Phys. Letts.* **23**, 545 (1966);

Turner and Fox, *Phys. Letts.* **23**, 547 (1966);

Crawford and Dalgarno, *Chem. Phys. Letts.* **1**, 23 (1967);

Coulson and Walmsley, *Proc. Phys. Soc.* (London) **91**, 31 (1967);

Lévy-Leblond, *Phys. Rev.* **153**, 1 (1967);

Byers Brown and Roberts, *J. Chem. Phys.* **46**, 2006 (1967);

Crawford, *Proc. Phys. Soc.* (London) **91**, 279 (1967).

Turner, *J. Am. Phys. Soc.* **45**, 758 (1977), gives a good overall review of the calculations, starting with Fermi and Teller.

Crawford was able to show that if $R > R_c$, a *countable infinity* of bound states exists.

Behaviour of the expectation value of z as $R \to R_c+$

This will be of interest in what follows.

Separable solutions of Schrödinger's equation are of the form:

$$\psi(\lambda, \mu, \phi) = L(\lambda)M(\mu)P(\phi).$$

$R > R_c$

Ground state $P(\phi) = \dfrac{1}{\sqrt{2\pi}}$.

$$L(\lambda) = \mathrm{e}^{-\frac{x}{2}} \sum_{n=0}^{\infty} \frac{c_n}{n!} L_n(x)$$

$$M(\mu) = \mathrm{e}^{-p\mu} \sum_{l=0}^{\infty} f_l P_l(\mu)$$

where

$$x = 2p(\lambda - 1),$$

$$p^2 = -\frac{R^2}{2} E \quad (E < 0)$$

and E is the energy of the electron or the positron. $L_n(x)$ is the Laguerre polynomial of degree n. $P_l(\mu)$ is the Legendre polynomial of degree l. The coefficients $\{c_n\}$ and $\{f_l\}$ are determined by three-coefficient recurrence relations.

$$z = \frac{R}{2}\lambda\mu$$

$\therefore$ The expectation value of z,

$$\langle z \rangle = \frac{R}{2}\frac{\int_1^\infty \int_{-1}^1 |L(\lambda)|^2 |M(\mu)|^2 \lambda\mu(\lambda^2 - \mu^2)\, \mathrm{d}\mu\, \mathrm{d}\lambda}{\int_1^\infty \int_{-1}^1 |L(\lambda)|^2 |M(\mu)|^2 (\lambda^2 - \mu^2)\, \mathrm{d}\mu\, \mathrm{d}\lambda}.$$

By straightforward manipulation it can be shown that

$$\langle z \rangle = \frac{R}{4p}\left[\frac{A_3 B_1 - 4p^2 A_1 B_3}{A_2 B_0 - 4p^2 A_0 B_2}\right],$$

where

$$A_q = \int_0^\infty |L(\lambda)|^2 (x + 2p)^q \, \mathrm{d}x$$

and

$$B_s = \int_{-1}^1 |M(\mu)|^2 \mu^s \, \mathrm{d}\mu.$$

$$\lim_{p \to 0+}\left[\frac{A_3 B_1 - 4p^2 A_1 B_3}{A_2 B_0 - 4p^2 A_0 B_2}\right] = k,$$

where k is a non-zero constant. Thus

$$\lim_{p \to 0+} \langle z \rangle = \pm\infty.$$

As

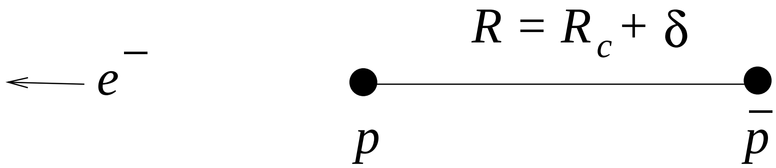
$$p \to 0+,$$

$$E \to 0-$$

and

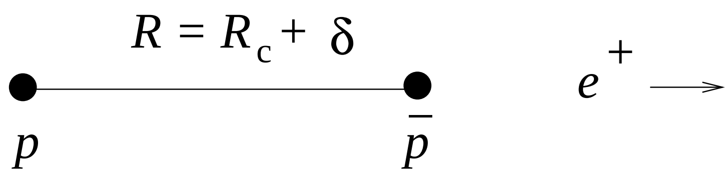
$$R_c \to R_c + .$$

Electron



Thus $\langle z \rangle \to -\infty$ in this case.

Positron



Thus $\langle z \rangle \to \infty$ in this case.

For small $w = R - R_c > 0$, Jonsell (private communication) finds that

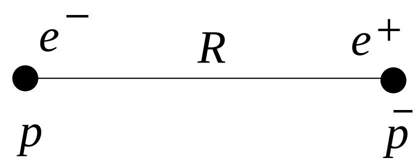
$$p = 9.8178 \exp(-3.6953 w^{-\frac{1}{2}}).$$

Now

$$E = -\frac{2p^2}{R^2}.$$

Thus $E \to 0-$ as $R \to R_c+$, more slowly than any power of $w = R - R_c$.

Hydrogen-Antihydrogen $(\mathrm{H}\bar{\mathrm{H}})$ **with fixed nuclei**



When both the electron and the positron are present, the threshold for binding moves down from zero to $-\frac{1}{4}$ a.u., the ground state energy of positronium (Ps).

Clearly, there is no binding if $R = 0$.

It is reasonable to assume that there exists a critical value of R, R_{cp}, below which the nuclei are unable to bind the electron and the positron.

Upper bounds to R_{cp}

Armour, Zeman and Carr, *J. Phys. B* **31**, L679 (1998).

Variational calculation with trial function with 32 basis functions in terms of prolate spheroidal coordinates, some of them Hylleraas-type functions, and one basis function of the form,

$$\psi_{Ps} = \left(\frac{e^{-\kappa\rho}}{\rho}\right) g(\rho)\Phi_{Ps}(r_{12}),$$

where ρ is the distance of the centre of mass of the Ps from the centre of mass of the nuclei. r_{12} is the distance between the electron (particle 1) and the positron (particle 2)

$$g(\rho) = \left(1 - e^{-\gamma\rho}\right)^3 \quad \text{(Shielding function).}$$

$\Phi_{Ps}(r_{12})$ is the wave function of ground-state Ps.

$$\psi_{Ps} = \left(\frac{e^{-\kappa\rho}}{\rho}\right)\left(1 - e^{-\gamma\rho}\right)^3 \Phi_{Ps}(r_{12})$$

represents weakly bound Ps.

Optimum value of $\kappa \approx 0.06$ a.u.

Binding energy of the electron and the positron at $R = 0.8a_0$ is 0.00065 a.u.

Thus the critical value, $R_{cp} \leq 0.8a_0$.

Strasburger, *J. Phys. B* **35**, L435 (2002).

Variational calculation with 64 to 256 explicitly correlated Gaussian basis functions:

$$\psi_\ell = \exp\left[-\sum_{i=1}^{2} \alpha_i^{(\ell)}(\boldsymbol{r}_i - \boldsymbol{R}_i^{(\ell)})^2 - \beta_{12}^{(\ell)}(\boldsymbol{r}_1 - \boldsymbol{r}_2)^2\right],$$

where $\boldsymbol{r}_1$ is the position vector of the electron, $\boldsymbol{r}_2$ is the position vector of the positron and $\alpha_i^{(\ell)}$, $\beta_{12}^{(\ell)}$ and $\boldsymbol{R}_i^{(\ell)}$ are independent, non-linear parameters.

Strasburger showed that $R_{cp} \leq 0.744a_0$.

The existence of the critical radius, R_{cp}, below which the electron and the positron become unbound results in a breakdown of the Born–Oppenheimer approximation for $R < R_{cp}$.

Any calculation of $\mathrm{H}\bar{\mathrm{H}}$ scattering must take account of the inelastic channel

$$\mathrm{H} + \bar{\mathrm{H}} \longrightarrow p\bar{p} + Ps.$$

Kohn method:

Armour and Chamberlain, *J. Phys. B* **35**, L489 (2002).

Optical potential method:

Zygelman, Saenz, Froelich and Jonsell, *Phys. Rev. A* **69**, 042715 (2004).

Towards a lower bound on R_{cp}

$R = 0.744 a_0$ is an upper bound on the value of the critical R value, R_{cp}, for $\mathrm{H\bar{H}}$. Can we obtain a lower bound? For example, can we show that $R_{cp} \geq R_c = 0.639 a_0$, the critical value for $p\bar{p}e^-$ and $p\bar{p}e^+$, when only the electron or the positron present?

One way of proving this would be to show that

$$\text{A bound state of } \mathrm{H\bar{H}} \text{ at } R < R_c \Longrightarrow \text{A bound state of } p\bar{p}e^- \text{ and } p\bar{p}e^+ \text{ at } R < R_c. \tag{1}$$

For we know that no such bound state of $p\bar{p}e^-$ and $p\bar{p}e^+$ exists. Thus taking the *contrapositive* of (1) $\Rightarrow$ no bound state of $\mathrm{H\bar{H}}$ at $R < R_c$.

Alternatively, we can conclude from (1) that the existence of a bound state of $p\bar{p}e^-$ and $p\bar{p}e^+$ at $R < R_c$ is a *necessary condition* for the existence of bound state of $\mathrm{H\bar{H}}$ at $R < R_c$. If this condition is not satisfied, no bound state of $\mathrm{H\bar{H}}$ exists at $R < R_c$.

Can we prove proposition (1)?

The Hamiltonian, $\hat{H}_f$, for the system is of the form

$$\hat{H}_f = -\tfrac{1}{2}\nabla_1^2 - \tfrac{1}{2}\nabla_2^2 + V - \frac{1}{r_{12}}, \tag{2}$$

where V is the dipole potential,

$$V = -\frac{1}{r_{p1}} + \frac{1}{r_{\bar{p}1}} + \frac{1}{r_{p2}} - \frac{1}{r_{\bar{p}2}} \tag{3}$$

and r_{pi} and $r_{\bar{p}i}$ are the distances of particle i from the proton and antiproton, respectively.

$$\hat{H}_f = -\tfrac{1}{2}\nabla_1^2 - \tfrac{1}{2}\nabla_2^2 + V - \frac{1}{r_{12}}, \tag{2}$$

$\hat{H}_f$ can also be expressed in the form

$$\hat{H}_f = -\tfrac{1}{4}\nabla_{\boldsymbol{\rho}}^2 - \nabla_{\boldsymbol{r}_{12}}^2 + V - \frac{1}{r_{12}}, \tag{4}$$

where $\boldsymbol{\rho}$ is the position vector of the centre of mass of the positronium w.r.t. the centre of mass of the nuclei. $\boldsymbol{r}_{12}$ is the position vector of the positron (particle 2) w.r.t. the electron (particle 1).

Suppose that a bound state of the full system does exist for some value of R, i.e. there exists some square-integrable function $\phi(\boldsymbol{r}_1, \boldsymbol{r}_2)$, within the domain of $\hat{H}_f$, for which

$$\hat{H}_f \phi = E\phi \tag{5}$$

where

$$E = -\tfrac{1}{4} - \epsilon \quad (\epsilon > 0). \tag{6}$$

If more than one exists, we shall assume that ϕ is the lowest in energy.

It follows from (5) that

$$(C\hat{H}_f C^{-1})C\phi = EC\phi \tag{7}$$

$$\text{i.e.} \quad \hat{H}_{fc}\phi_c = E\phi_c, \tag{8}$$

where

$$\hat{H}_{fc} = C\hat{H}_f C^{-1} \tag{9}$$

and

$$\phi_c = C\phi. \tag{10}$$

If $C^\dagger = C^{-1}$, this would be a unitary transformation. However, this will not be the case. (9) is a similarity transformation. As C is not unitary, it follows that $\hat{H}_{fc}$ is not Hermitian.

Take

$$C = \exp\left[\frac{ar_{12}}{1+\delta r_{12}}\right], \tag{11}$$

where a and δ are positive constants. Note that C is non-singular as $r_{12} \geq 0$ and $\delta > 0$.

Since

$$\lim_{r_{12}\to\infty} C = \exp\left[\frac{a}{\delta}\right], \tag{12}$$

as ϕ is square-integrable, so is ϕ_c.

Two-particle correlation functions were included in wave functions by Jastrow, *Phys. Rev.* **98**, 1479 (1955) in calculations on many-particle systems interacting through the strong interaction.

Correlation functions of the form of C are used in Monte Carlo calculations of wave functions for atoms and molecules.

See, for example, Umrigar, Wilson and Wilkins, *Phys. Rev. Lett.* **60**, 1719 (1988).

Correlation functions of this form are also used in the transcorrelated method of Boys and Handy, *Proc. Roy. Soc.* (London) A **310**, 43 (1969) – an ingenious attempt to take a very accurate account of electron correlation. See also, Armour, *Molec. Phys.* **24**, 181 (1972).

However, the use to which C be will be put here is quite different. As $\delta \to 0+$, ϕ_c becomes more and more diffuse, and the effect of the Coulombic interaction becomes less and less. The aim is to use this to uncover the role in binding of the dipole potential V in $\hat{H}_f$.

It follows from equation (6) and (8) that

$$\frac{\langle \phi_c \mid \hat{H}_{fc} \mid \phi_c \rangle}{\langle \phi_c \mid \phi_c \rangle} = E = -\tfrac{1}{4} - \epsilon \quad (\epsilon > 0). \tag{13}$$

Now

$$\begin{aligned} \hat{H}_{fc}\phi_c &= C\hat{H}_f C^{-1}\phi_c \\ &= C\left\{ -\left[\phi_c \frac{\partial^2 C^{-1}}{\partial r_{12}^2} + 2\frac{\partial C^{-1}}{\partial r_{12}}\frac{\partial \phi_c}{\partial r_{12}} + C^{-1}\frac{\partial^2 \phi_c}{\partial r_{12}^2} \right.\right. \\ &\qquad \left.\left. + \frac{2}{r_{12}}\left(\phi_c \frac{\partial C^{-1}}{\partial r_{12}} + C^{-1}\frac{\partial \phi_c}{\partial r_{12}} \right) - C^{-1}\frac{\hat{L}^2(\theta_{12},\phi_{12})}{r_{12}^2}\phi_c \right] \right\} \\ &\qquad - \tfrac{1}{4}\nabla_{\boldsymbol{\rho}}^2 \phi_c + V\phi_c - \frac{\phi_c}{r_{12}}, \end{aligned} \tag{14}$$

where $\hat{L}^2(\theta_{12}, \phi_{12})$ is the operator for the square of the angular momentum.

Using expression (11) for C, it can be shown that

$$\begin{aligned} \hat{H}_{fc}\phi_c \;=\; & -\frac{\{a^2 + 2a\delta(1+\delta r_{12})\}}{(1+\delta r_{12})^4}\phi_c + \frac{2a}{(1+\delta r_{12})^2}\left(\frac{\partial}{\partial r_{12}} + \frac{1}{r_{12}} \right)\phi_c \\ & + \left(-\nabla_{\boldsymbol{r}_{12}}^2 - \tfrac{1}{4}\nabla_{\boldsymbol{\rho}}^2 + V - \frac{1}{r_{12}} \right)\phi_c. \end{aligned} \tag{15}$$

Thus from (2), (4), (13) and (15),

$$\begin{aligned}
\frac{\langle \phi_c \mid \hat{H}_{fc} \mid \phi_c \rangle}{\langle \phi_c \mid \phi_c \rangle} &= \Bigg[-\frac{\langle \phi_c \mid \{a^2 + 2a\delta(1+\delta r_{12})\} \mid \phi_c \rangle}{(1+\delta r_{12})^4} \\
&\qquad + 2a \langle \phi_c \mid \frac{1}{(1+\delta r_{12})^2} \left(\frac{\partial}{\partial r_{12}} + \frac{1}{r_{12}} \right) \mid \phi_c \rangle \\
&\qquad - \langle \phi_c \mid \frac{1}{r_{12}} \mid \phi_c \rangle + \langle \phi_c \mid \hat{H}_{\rm dip} \mid \phi_c \rangle \Bigg] \left[\langle \phi_c \mid \phi_c \rangle \right]^{-1} \\
&= -\tfrac{1}{4} - \epsilon \quad (\epsilon > 0),
\end{aligned} \tag{16}$$

where

$$\hat{H}_{\rm dip} = -\tfrac{1}{2}\nabla_1^2 - \tfrac{1}{2}\nabla_2^2 + V \tag{17}$$

is the Hamiltonian for the non-interacting particles in the field of the nuclei.

From which it follows that

$$\frac{\langle\phi_c \mid \hat{H}_{\rm dip} \mid \phi_c\rangle}{\langle\phi_c \mid \phi_c\rangle} = -\tfrac{1}{4} + a^2 \frac{\langle\phi_c \mid \frac{1}{(1+\delta r_{12})^4} \mid \phi_c\rangle}{\langle\phi_c \mid \phi_c\rangle} + 2a\delta \frac{\langle\phi_c \mid \frac{1}{(1+\delta r_{12})^3} \mid \phi_c\rangle}{\langle\phi_c \mid \phi_c\rangle}$$
$$- \frac{\langle\phi_c \mid \frac{2a}{(1+\delta r_{12})^2} \left(\frac{\partial}{\partial r_{12}} + \frac{1}{r_{12}}\right) \mid \phi_c\rangle}{\langle\phi_c \mid \phi_c\rangle} + \frac{\langle\phi_c \mid \frac{1}{r_{12}} \mid \phi_c\rangle}{\langle\phi_c \mid \phi_c\rangle} - \epsilon \quad (\epsilon > 0). \qquad (18)$$

As

$$\frac{\langle\phi_c \mid \frac{1}{(1+\delta r_{12})^n} \mid \phi_c\rangle}{\langle\phi_c \mid \phi_c\rangle} < 1 \quad \forall \quad \delta > 0 \quad (n > 0) \qquad (19)$$

it follows that

$$\frac{\langle\phi_c \mid \hat{H}_{\rm dip} \mid \phi_c\rangle}{\langle\phi_c \mid \phi_c\rangle} \leq -\tfrac{1}{4} + a^2 + 2a\delta \frac{\langle\phi_c \mid \frac{1}{(1+\delta r_{12})^3} \mid \phi_c\rangle}{\langle\phi_c \mid \phi_c\rangle}$$
$$-2a \frac{\langle\phi_c \mid \frac{1}{(1+\delta r_{12})^2} \left(\frac{\partial}{\partial r_{12}} + \frac{1}{r_{12}}\right) \mid \phi_c\rangle}{\langle\phi_c \mid \phi_c\rangle}$$
$$+ \frac{\langle\phi_c \mid \frac{1}{r_{12}} \mid \phi_c\rangle}{\langle\phi_c \mid \phi_c\rangle} - \epsilon. \qquad (20)$$

Now

$$\hat{A} = \frac{\partial}{\partial r_{12}} + \frac{1}{r_{12}} \tag{21}$$

is an anti-Hermitian operator. This can be seen by integrating a given integral involving $\hat{A}$, using integration by parts, or by noting that

$$-i\hat{A} = -i\left(\frac{\partial}{\partial r_{12}} + \frac{1}{r_{12}}\right) \tag{22}$$

is the Hermitian operator for radial momentum. See, for example, Messiah, *Quantum Mechanics*, Vol I, p 346. It is not an observable, but this is not relevant to the present analysis.

As all quantities being considered are real,

$$\begin{aligned}
&\langle\phi_c \mid \frac{1}{(1+\delta r_{12})^2}\left(\frac{\partial}{\partial r_{12}} + \frac{1}{r_{12}}\right) \mid \phi_c\rangle \\
&\quad = -\langle\phi_c \mid \left(\frac{\partial}{\partial r_{12}} + \frac{1}{r_{12}}\right)\frac{1}{(1+\delta r_{12})^2} \mid \phi_c\rangle \\
&\quad = -\langle\phi_c \mid \left(\frac{1}{1+\delta r_{12}}\right)^2\left(\frac{\partial}{\partial r_{12}} + \frac{1}{r_{12}}\right) \mid \phi_c\rangle \\
&\qquad\quad + 2\delta\langle\phi_c \mid \frac{1}{(1+\delta r_{12})^3} \mid \phi_c\rangle \qquad (23) \\
&\therefore \quad \langle\phi_c \mid \frac{1}{(1+\delta r_{12})^2}\left(\frac{\partial}{\partial r_{12}} + \frac{1}{r_{12}}\right) \mid \phi_c\rangle \\
&\quad = \delta\langle\phi_c \mid \frac{1}{(1+\delta r_{12})^3} \mid \phi_c\rangle.
\end{aligned}$$

It follows from (18) that

$$\frac{\langle\phi_c \mid \hat{H}_{\rm dip} \mid \phi_c\rangle}{\langle\phi_c \mid \phi_c\rangle} \le -\tfrac{1}{4} + a^2 + \frac{\langle\phi_c \mid \frac{1}{r_{12}} \mid \phi_c\rangle}{\langle\phi_c \mid \phi_c\rangle} - \epsilon \quad (\epsilon > 0). \tag{24}$$

I have obtained this result by evaluating

$$\frac{\langle\phi_c|\hat{H}_{fc}|\phi_c\rangle}{\langle\phi_c|\phi_c\rangle},$$

where $\hat{H}_{fc}$ is the non-Hermitian operator

$$\hat{H}_{fc} = C\hat{H}_f C^{-1} \tag{9}$$

where

$$C = \exp\left[\frac{ar_{12}}{1+\delta r_{12}}\right]. \tag{11}$$

This is not necessary. It can also be obtained by evaluating

$$\frac{\langle\phi_c|\hat{H}_f|\phi_c\rangle}{\langle\phi_c|\phi_c\rangle}.$$

A more precise bound on $\dfrac{\langle\phi_c|\hat{H}_{\mathrm{dip}}|\phi_c\rangle}{\langle\phi_c|\phi_c\rangle}$

As

$$\frac{\langle\phi_c \mid \hat{H}_{\mathrm{dip}} \mid \phi_c\rangle}{\langle\phi_c \mid \phi_c\rangle} \le -\tfrac{1}{4} + a^2 + \frac{\langle\phi_c \mid \frac{1}{r_{12}} \mid \phi_c\rangle}{\langle\phi_c \mid \phi_c\rangle} - \epsilon \quad (\epsilon > 0), \tag{24}$$

to obtain a more precise bound, we need to consider the behaviour of

$$I(\delta) = \frac{\langle\phi_c|\frac{1}{r_{12}}|\phi_c\rangle}{\langle\phi_c|\phi_c\rangle} \tag{25}$$

as a function of δ.

Now

$$\phi_c = \exp\left[\frac{ar_{12}}{1+\delta r_{12}}\right]\phi, \tag{11}$$

where

$$\hat{H}_f\phi = E\phi_f. \tag{5}$$

Thus we need to consider

$$M(r) = \langle\phi|\delta(r_{12} - r)|\phi\rangle.$$

As $r \to \infty$, $M(r)$ will show a behaviour intermediate between ground-state positronium and the behaviour of $M(r)$ if the Coulomb attraction between the electron and the positron is set to zero.

$M(r)$ will tend to zero no faster than in the case of the ground-state positronium wave function, i.e. no faster than $r^2 e^{-r}$.

Earlier inclusion of basis function

$$\psi_{Ps} = \left(\frac{e^{-\kappa\rho}}{\rho}\right)(1 - e^{-\gamma\rho})^3 \Phi_{Ps}(r_{12})$$

where $\Phi_{Ps}(r_{12}) = \dfrac{1}{\sqrt{8\pi}} e^{-\frac{1}{2}r_{12}} =$ (normalized) Ps ground-state wave function in a variational calculation of the energy, E, of the electron and the positron.

Very beneficial effect.

It is to be expected that for small ϵ, ψ_{Ps} will be a large component of ϕ.

However, $\phi \neq \psi_{Ps}$.

As the dipole potential V is antisymmetric w.r.t. interchange of the electron and the positron, no binding can occur if ϕ is symmetric, as in the case of ψ_{Ps}, or antisymmetric w.r.t. this interchange.

Let us begin by considering the case when $M(r)$ behaves like $r^2 e^{-r}$ as $r \to \infty$. Let

$$\int \ldots \int |\phi_c|^2 \sin\theta_{12}\; d\theta_{12}\, d\phi_{12}\, d\boldsymbol{\rho} = f(r_{12}) e^{\frac{2ar_{12}}{1+\delta r_{12}}} e^{-r_{12}} r_{12}^2. \quad (26)$$

It follows that

$$\langle \phi_c \mid \phi_c \rangle = \lim_{A\to\infty} \int_0^A f(r_{12}) e^{\frac{2ar_{12}}{1+\delta r_{12}}} e^{-r_{12}} r_{12}^2 \; dr_{12},$$

$$\langle \phi_c \mid \frac{1}{r_{12}} \mid \phi_c \rangle = \lim_{A\to\infty} \int_0^A f(r_{12}) e^{\frac{2ar_{12}}{1+\delta r_{12}}} e^{-r_{12}} r_{12} \; dr_{12}$$

and

$$f(r_{12}) r_{12}^2 \underset{r_{12}\to\infty}{\sim} N r_{12}^2,$$

where N is a positive constant.

$$\therefore \quad \frac{\langle \phi_c \mid \frac{1}{r_{12}} \mid \phi_c \rangle}{\langle \phi_c \mid \phi_c \rangle} = \frac{\lim_{A\to\infty} \int_0^A f(r_{12}) e^{\frac{2ar_{12}}{1+\delta r_{12}}} e^{-r_{12}} r_{12} \; dr_{12}}{\lim_{A\to\infty} \int_0^A f(r_{12}) e^{\frac{2ar_{12}}{1+\delta r_{12}}} e^{-r_{12}} r_{12}^2 \; dr_{12}}. \quad (27)$$

Let us consider the factor

$$e^{\frac{2ar_{12}}{1+\delta r_{12}}} e^{-r_{12}} = \exp\left[\frac{2ar_{12} - r_{12} - \delta r_{12}^2}{1 + \delta r_{12}}\right]. \tag{28}$$

Recall that

$$\frac{\langle \phi_c \mid \hat{H}_{\rm dip} \mid \phi_c \rangle}{\langle \phi_c \mid \phi_c \rangle} \leq -\tfrac{1}{4} + a^2 + \frac{\langle \phi_c \mid \frac{1}{r_{12}} \mid \phi_c \rangle}{\langle \phi_c \mid \phi_c \rangle} - \epsilon \quad (\epsilon > 0), \tag{24}$$

If $a > \frac{1}{2}$, the RHS of (24) > 0 for sufficiently small $\epsilon > 0$. Thus not a suitable choice of a.

If $a < \frac{1}{2}$,

$$\frac{2ar_{12} - r_{12} - \delta r_{12}^2}{1 + \delta r_{12}} = \frac{-br_{12} - \delta r_{12}^2}{1 + \delta r_{12}}$$

where $b = 1 - 2a > 0$. Thus the RHS of (28) declines exponentially. Thus not a suitable choice.

Therefore, choose $a = \frac{1}{2}$.

If $a = \frac{1}{2}$,

$$\frac{2ar_{12} - r_{12} - \delta r_{12}^2}{1 + \delta r_{12}} = \frac{-\delta r_{12}^2}{1 + \delta r_{12}}.$$

Also

$$0 < \frac{\delta r_{12}^2}{1 + \delta r_{12}} < \delta r_{12}^2.$$

In view of this, it is instructive to evaluate $\dfrac{\langle \phi_c \mid \frac{1}{r_{12}} \mid \phi_c \rangle}{\langle \phi_c \mid \phi_c \rangle}$ with $\phi_c = r_{12}^n e^{-\delta r_{12}^2}$ ($n \in \mathbb{N}$),

$$\frac{\langle \phi_c \mid \frac{1}{r_{12}} \mid \phi_c \rangle}{\langle \phi_c \mid \phi_c \rangle} = \frac{\int_0^\infty r_{12}^{n-1} e^{-\delta r_{12}^2} r_{12}^2 \, dr_{12}}{\int_0^\infty r_{12}^{n} e^{-\delta r_{12}^2} r_{12}^2 \, dr_{12}}.$$

If n is even, so that $m = \frac{n}{2} \in \mathbb{N}$,

$$= \frac{2^{m+1} m!}{1.3 \ldots (2m+1)\sqrt{\pi}} \delta^{\frac{1}{2}}.$$

If n is odd, so that $p = \frac{n+1}{2} \in \mathbb{N}$

$$= \frac{1.3 \ldots (2p-1)\sqrt{\pi}}{2^p p!} \delta^{\frac{1}{2}}.$$

Thus, in this case,

$$\frac{\langle \phi_c \mid \frac{1}{r_{12}} \mid \phi_c \rangle}{\langle \phi_c \mid \phi_c \rangle} \longrightarrow 0+$$

like $\delta^{\frac{1}{2}}$ as $\delta \to 0+$.

Conjecture: In the more general case when $M(r)$ behaves like $r^2 e^{-r}$ as $r \to \infty$

$$\frac{\langle \phi_c \mid \frac{1}{r_{12}} \mid \phi_c \rangle}{\langle \phi_c \mid \phi_c \rangle} \longrightarrow 0+ \text{ like } \delta^{\frac{1}{2}} \text{ as } \delta \to 0+.$$

Tentative proof. It follows from (27) that

$$I(\delta) = \frac{\langle \phi_c \mid \frac{1}{r_{12}} \mid \phi_c \rangle}{\langle \phi_c \mid \phi_c \rangle}$$

$$= \frac{\int_0^\alpha f(r_{12}) e^{-\frac{\delta r_{12}^2}{1+\delta r_{12}}} r_{12}\, dr_{12} \;+\; \lim_{A\to\infty} \int_\alpha^A f(r_{12}) e^{-\frac{\delta r_{12}^2}{1+\delta r_{12}}} r_{12}\, dr_{12}}{\int_0^\alpha f(r_{12}) e^{-\frac{\delta r_{12}^2}{1+\delta r_{12}}} r_{12}^2\, dr_{12} \;+\; \lim_{A\to\infty} \int_\alpha^A f(r_{12}) e^{-\frac{\delta r_{12}^2}{1+\delta r_{12}}} r_{12}^2\, dr_{12}},$$

where α is any positive number. As $f(r_{12}) \geq 0$, we can apply the mean value theorem of the integral calculus to the first term in the numerator and both terms in the denominator on the right-hand side of this equation to obtain the inequality.

$$I(\delta) \leq \frac{\int_0^\alpha f(r_{12}) r_{12}\, dr_{12} \;+\; \lim_{A\to\infty} \int_\alpha^A f(r_{12}) e^{-\frac{\delta r_{12}^2}{1+\delta r_{12}}} r_{12}\, dr_{12}}{e^{-\delta\alpha^2} \int_0^\alpha f(r_{12}) r_{12}^2\, dr_{12} \;+\; \alpha \lim_{A\to\infty} \int_\alpha^A f(r_{12}) e^{-\frac{\delta r_{12}^2}{1+\delta r_{12}}} r_{12}\, dr_{12}}. \tag{29}$$

Now

$$\int_0^{\alpha} f(r_{12}) r_{12}^p \, dr_{12} = [g_p(r_{12})]_0^{\alpha},$$

where $g_p(r_{12})$ is an indefinite integral of $f(r_{12})r_{12}^p$. For sufficiently large but finite values of α, we can take $g_p(\alpha)$ to be of the form

$$g_p(\alpha) = \frac{N\alpha^{p+1}}{p+1} + s_p(\alpha),$$

where $s_p(\alpha)$ is of $O(\alpha^p)$. Thus for such α values,

$$\int_0^{\alpha} f(r_{12}) r_{12}^p \, dr_{12} = \frac{N\alpha^{p+1}}{p+1} + s_p(\alpha) - g_p(0).$$

Let $\alpha = \dfrac{1}{\delta^{\frac{1}{2}}}$. Thus for sufficiently small positive values of δ,

$$\int_0^{\frac{1}{\delta^{\frac{1}{2}}}} f(r_{12}) r_{12}^p \, dr_{12} = \left(\frac{N}{p+1}\right) \frac{1}{\delta^{\frac{p+1}{2}}} + s_p\left(\frac{1}{\delta^{\frac{1}{2}}}\right) - g_p(0),$$

where $s_p\left(\dfrac{1}{\delta^{\frac{1}{2}}}\right)$ is of order $\dfrac{1}{\delta^{\frac{p}{2}}}$.

It follows that for such values of $\dfrac{1}{\delta^{\frac{1}{2}}}$,

$$I(\delta) \leq \frac{\frac{N}{2\delta} + s_1\left(\frac{1}{\delta^{\frac{1}{2}}}\right) - g_1(0) + W(\delta)}{e^{-1}\left(\frac{N}{3\delta^{\frac{3}{2}}} + s_2\left(\frac{1}{\delta^{\frac{1}{2}}}\right) - g_2(0)\right) + \frac{1}{\delta^{\frac{1}{2}}}W(\delta)},$$

where

$$W(\delta) = \lim_{A\to\infty}\int_{\frac{1}{\delta^{\frac{1}{2}}}}^{A} f(r_{12})e^{-\frac{\delta r_{12}^2}{1+\delta r_{12}}}r_{12}\ dr_{12} > 0.$$

Thus

$$\begin{aligned}
I(\delta) &\leq \tfrac{3}{2}e\delta^{\frac{1}{2}}\left[\frac{N + 2\delta s_1\left(\frac{1}{\delta^{\frac{1}{2}}}\right) - 2\delta g_1(0) + 2\delta W(\delta)}{N + 3\delta^{\frac{3}{2}}s_2\left(\frac{1}{\delta^{\frac{1}{2}}}\right) - 3\delta^{\frac{3}{2}}g_2(0) + 3e\delta W(\delta)}\right] \\
&= \tfrac{3}{2}e\delta^{\frac{1}{2}}\left[\frac{N + 3\delta^{\frac{3}{2}}s_2\left(\frac{1}{\delta^{\frac{1}{2}}}\right) - 3\delta^{\frac{3}{2}}g_2(0) + 2\delta W(\delta)}{N + 3\delta^{\frac{3}{2}}s_2\left(\frac{1}{\delta^{\frac{1}{2}}}\right) - 3\delta^{\frac{3}{2}}g_2(0) + 3e\delta W(\delta)}\right. \\
&\qquad \left. + \frac{2\delta s_1\left(\frac{1}{\delta^{\frac{1}{2}}}\right) - 2\delta g_1(0) - 3\delta^{\frac{3}{2}}s_2\left(\frac{1}{\delta^{\frac{1}{2}}}\right) + 3\delta^{\frac{3}{2}}g_2(0)}{N + 3\delta^{\frac{3}{2}}s_2\left(\frac{1}{\delta^{\frac{1}{2}}}\right) - 3\delta^{\frac{3}{2}}g_2(0) + 3e\delta W(\delta)}\right] \\
&= \tfrac{3}{2}e\delta^{\frac{1}{2}}[B + O(\delta^{\frac{1}{2}})] \quad (0 < B < 1).
\end{aligned}$$

It follows that

$$I(\delta) \leq \omega\delta^{\frac{1}{2}} + O(\delta), \tag{30}$$

where $0 < \omega < \frac{3}{2}e$.

Thus in the case where

$$M(r) = \langle \phi \mid \delta(r_{12} - r) \mid \phi \rangle$$

tends to zero like $r^2 e^{-r}$ asymptotically, it follows from the relation

$$\frac{\langle \phi_c \mid \hat{H}_{\text{dip}} \mid \phi_c \rangle}{\langle \phi_c \mid \phi_c \rangle} \leq -\tfrac{1}{4} + a^2 + \frac{\langle \phi_c \mid \frac{1}{r_{12}} \mid \phi_c \rangle}{\langle \phi_c \mid \phi_c \rangle} - \epsilon \quad (\epsilon > 0) \qquad (24)$$

with $a = \frac{1}{2}$, that

$$\frac{\langle \phi_c \mid \hat{H}_{\text{dip}} \mid \phi_c \rangle}{\langle \phi_c \mid \phi_c \rangle} \leq \omega \delta^{\frac{1}{2}} + O(\delta) - \epsilon \quad (\epsilon > 0) \qquad (31)$$

where $0 < \omega < \frac{3}{2}e$.

$M(r)$ will tend to zero more slowly asymptotically than $r^2 e^{-r}$.

Proof can be extended to this case, though some features still need clarification.

$$\frac{\langle \phi_c \mid \hat{H}_{\rm dip} \mid \phi_c \rangle}{\langle \phi_c \mid \phi_c \rangle} \leq \omega \delta^{\frac{1}{2}} + 0(\delta) - \epsilon \quad (\epsilon > 0) \tag{31}$$

implies that, for sufficiently small δ, there exists a square-integrable function, ϕ_c, such that

$$\frac{\langle \phi_c \mid \hat{H}_{\rm dip} \mid \phi_c \rangle}{\langle \phi_c \mid \phi_c \rangle} < 0. \tag{32}$$

It follows from the variational theorem that a bound state of the system exists when the interaction between the electron and the positron is set to zero.

This implies that a bound state of the dipole system made up of the proton and the antiproton and the electron or the positron exists.

This is close to the desired result.

Qualifications

$I(\delta) = \dfrac{\langle \phi_c \mid \frac{1}{r_{12}} \mid \phi_c \rangle}{\langle \phi_c \mid \phi_c \rangle}$ involves infinite integrals containing $\lim_{A \to \infty} \int_0^A \ldots dr_{12}$. Thus if we take the limit, $\lim_{\delta \to 0+}$ a double limit is involved. Further analysis is necessary to clarify this.

This would be a problem if we wished to consider binding energies, ϵ, as small as we please.

However, we know from Strasburger's variational calculation that for $R = 0.8a_0$,

$$\epsilon \geq 0.0013148 \; a.u. \tag{33}$$

Also we know from Wallis *et al.*'s exact solution for the system made up of a proton, an antiproton and an electron or a positron, that in the case of the binding energy, ϵ_{ni}, for the two non-interacting particles, if $R = 0.8a_0$,

$$\epsilon_{ni} < 0.0000464 \; a.u. \tag{34}$$

Consider the relation obtained earlier

$$\frac{\langle \phi_c \mid \hat{H}_{\rm dip} \mid \phi_c \rangle}{\langle \phi_c \mid \phi_c \rangle} \leq \omega \delta^{\frac{1}{2}} + O(\delta) - \epsilon \quad (\epsilon > 0) \tag{31}$$

where $0 < \omega < \frac{3}{2}e$.

Take

$$\epsilon > 0.0013148. \tag{33}$$

The inequality (31) implies that it should be possible to find a δ such that

$$\frac{\langle \phi_c \mid \hat{H}_{\rm dip} \mid \phi_c \rangle}{\langle \phi_c \mid \phi_c \rangle} < -\epsilon_{ni} = -0.0000464,$$

without taking the limit $\delta \to 0+$.

This is a contradiction.

Further investigation is necessary.

What does the existence of a bound state of the non-interacting system imply about the existence of a bound state of the interacting system?

Suppose that the electron and the positron interact through a potential, $-\dfrac{\gamma}{r_{12}}$, where $\gamma > 0$.

Suppose $\hat{H}_{\rm dip}$ has a bound state, ϕ_d, of energy $-\eta$, where $\eta > 0$.

Then

$$\frac{\langle \phi_d \mid \hat{H}_f(\gamma) \mid \phi_d \rangle}{\langle \phi_d \mid \phi_d \rangle} = \frac{\langle \phi_d \mid \hat{H}_{\rm dip} \mid \phi_d \rangle - \gamma \langle \phi_d \mid \frac{1}{r_{12}} \mid \phi_d \rangle}{\langle \phi_d \mid \phi_d \rangle}$$

$$= -\eta - \gamma \frac{\langle \phi_d \mid \frac{1}{r_{12}} \mid \phi_d \rangle}{\langle \phi_d \mid \phi_d \rangle} \quad (\eta > 0).$$

The threshold below which states are bound is $-\frac{1}{4}\gamma^2$. Thus there must exist a region $0 < \gamma < \gamma_c$, in which

$$\frac{\langle \phi_d \mid \hat{H}_f(\gamma) \mid \phi_d \rangle}{\langle \phi_d \mid \phi_d \rangle} = -\eta - \gamma \frac{\langle \phi_d \mid \frac{1}{r_{12}} \mid \phi_d \rangle}{\langle \phi_d \mid \phi_d \rangle} < -\frac{1}{4}\gamma^2 \quad (\gamma > 0)$$

i.e. $\quad -\eta - \gamma A < -\frac{1}{4}\gamma^2 \quad (\gamma > 0)$

where $A = \dfrac{\langle \phi_d \mid \frac{1}{r_{12}} \mid \phi_d \rangle}{\langle \phi_c \mid \phi_c \rangle}$.

It is easy to show that

$$\gamma_c = 2A + 2\sqrt{A^2 + \eta}.$$

Recall that there are a countable infinity of bound states of the non-interacting system if $R > R_c$. Thus, for sufficiently small γ,

$$\frac{\langle \phi_d \mid \hat{H}_f(\gamma) \mid \phi_d \rangle}{\langle \phi_d \mid \phi_d \rangle} < -\tfrac{1}{4}\gamma^2$$

for as many of these states as we please.

Take $\{\phi_{di}\}_{i=1}^{N}$ to be an orthonormal set of such eigenfunctions.

If we diagonalise the matrix representation, $\boldsymbol{H}_f(\gamma)$, of $\hat{H}_f(\gamma)$ over these eigenfunctions, the trace of the matrix will be invariant.

$$\therefore \quad \sum_{i=1}^{N} \langle \psi_{di} \mid \hat{H}_f(\gamma) \mid \psi_{di} \rangle = \sum_{i=1}^{N} \langle \phi_{di} \mid \hat{H}_f(\gamma) \mid \phi_{di} \rangle < -\tfrac{N}{4}\gamma^2$$

where $\{\psi_{di}\}_{i=1}^{N}$ are orthonormal wave functions in terms of which $\boldsymbol{H}_f(\gamma)$ is diagonal.

Thus for M of these wave functions, $1 \leq M \leq N$,

$$\langle \psi_{di} \mid \hat{H}_f(\gamma) \mid \psi_{di} \rangle < -\tfrac{1}{4}\gamma^2$$

$$\langle \psi_{di} \mid \hat{H}_f(\gamma) \mid \psi_{di} \rangle < -\tfrac{1}{4}\gamma^2$$

for M of the wave functions, $\{\psi_{di}\}_{i=1}^{N}$, where $1 \leq M \leq N$.

It follows from the Hylleraas–Undheim theorem that M bound states exist of the system with interaction $-\dfrac{\gamma}{r_{12}}$.

M can be expected to increase as N increases.

Strasburger has shown that a bound state of $\hat{H}_f(\gamma)$ exists for $\gamma = 1$ if $R \geq 0.744a_0$.

It would thus seem likely that $\gamma_c > 1$ if $R \geq 0.744a_0$.

Critical mass at which a ‘positron’ would form a bound state with a hydrogen molecule

Connection with the very large positron annihilation rates that have been observed in low-energy positron scattering by some larger molecules.

I am willing to discuss this with anyone who is interested.