New Method for Taking into Account Finite Nuclear Mass in the Determination of Absence of Bound States: Application to e^+H

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If the proton is considered to be infinitely massive, no bound state of a system made up of a positron and a hydrogen atom can exist. In this Letter a new method is introduced for taking into account finite nuclear mass. By using this method it is shown that the inclusion of the finite mass of the proton does not result in the appearance of a bound state.

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It has been known since the work of Aronson, Kleinman, and Spruch[1] and Armour[2] that, in the approximation in which the proton is considered to be infinitely massive, a system made up of a hydrogen atom and a positron (e^+) has no bound state below the continuum. Aronson *et al.* showed further that no bound state of the system can exist if the positron mass satisfies $m_p \leq 1.46 m_e$, where m_e is the mass of the electron. This limit has recently been increased to $m_p \leq 1.51 m_e$ by Armour and Schrader.[3]

The approximation of treating the proton as being infinitely massive is a good one as $M/m_e = 1836$, where M is the mass of the proton. However, if the finite mass of the proton is taken into account, small additional terms are introduced into the Hamiltonian for the internal motion of the system. It is the purpose of this Letter to show how these terms can be taken into account by a new method. It is shown in this way that their inclusion does not give rise to a bound state. This is the first time that this result has been established.

If the proton is assumed to be infinitely massive, the Hamiltonian for the internal motion of the system is of the form

$$H_{\mathrm{inf}} = -\frac{1}{2m_p}\nabla_1^2 - \frac{1}{2m_e}\nabla_2^2 + \frac{1}{r_1} - \frac{1}{r_2} - \frac{1}{r_{12}}, \quad (1)$$

where particle 1 is the positron, particle 2 is the electron, r_1 and r_2 are the distances between the proton and the positron and the proton and the electron, respectively, and r_{12} is the distance between the electron and the positron. Units have been chosen for which $\hbar = e = 1$, where e is the charge on the proton.

If the finite mass of the proton is taken into account and the origin of the coordinates is chosen to be at the proton, the Hamiltonian for the internal motion takes the form

$$H_{\mathrm{fin}}(1,2) = -\frac{1}{2\mu_p}\nabla_1^2 - \frac{1}{2\mu_e}\nabla_2^2 - \frac{1}{M}\nabla_1 \cdot \nabla_2 + \frac{1}{r_1} - \frac{1}{r_2} - \frac{1}{r_{12}}, \quad (2)$$

where

$$\mu_p = [M/(M+m_p)]m_p, \quad (3)$$

$$\mu_e = [M/(M+m_e)]m_e \quad (4)$$

are the reduced masses of the positron and the electron, respectively. The inclusion of the finite mass of the proton thus effectively reduces slightly the masses of the positron and the electron and introduces a small coupling term between the momenta of the positron and the electron, the Hughes-Eckart or mass-polarization term (Hughes and Eckart[4]).

Since $m_p = m_e$ and hence $\mu_p = \mu_e$, it can readily be seen that, if the Hughes-Eckart term is omitted in $H_{\mathrm{fin}}(1,2)$, the resulting Hamiltonian and H_{inf} are related by a scaling transformation. Since H_{inf} cannot support a bound state, it follows that H_{fin} certainly could not support a bound state in the absence of the Hughes-Eckart term. Thus the key to the determination of whether or not H_{fin} can support a bound state is the calculation of the effect of this term.

Suppose H_{fin} can support at least one bound state, $\Psi(\vec{r}_1, \vec{r}_2)$, i.e.,

$$H_{\mathrm{fin}}\Psi = E\Psi, \quad (5)$$

where $E <$ lowest continuum threshold $= -\frac{1}{2}\mu_e$. It is convenient to choose Ψ to be normalized so that

$$\langle \Psi | \Psi \rangle = 1. \quad (6)$$

We shall assume that, in the event of there being more than one bound state, Ψ corresponds to the bound state which is lowest in energy.

To obtain a bound on $\langle \Psi | \nabla_1 \cdot \nabla_2 | \Psi \rangle$ let us consider the form taken by the Hamiltonian for the internal motion when transformed to coordinates relative to the electron rather than the proton (Farid and Mattis[5]). In terms of this coordinate system, the Hamiltonian for the internal motion has the form

$$H_{\mathrm{fin}}^{T}(1,3)=-\frac{1}{2\nu_p}\nabla_1^2-\frac{1}{2\mu_e}\nabla_3^2-\frac{1}{m_e}\nabla_1\cdot\nabla_3-\frac{1}{R_1}-\frac{1}{R_3}+\frac{1}{R_{13}},\tag{7}$$

where

$$\nu_p=m_p m_e/(m_p+m_e).$$

Particle 1 is the positron, particle 3 the proton, and R_1 and R_3 are the distances of the positron and proton, respectively, from the electron at the origin. R_{13} is the distance between the proton and the positron. Note that $H_{\mathrm{fin}}^{T}(1,3)$ is readily derived from $H_{\mathrm{fin}}(1,2)$ by interchanging the proton and the electron.

Since $H_{\mathrm{fin}}(1,2)$ and $H_{\mathrm{fin}}^{T}(1,3)$ are related by a canonical transformation, it follows that they must have the same eigenvalue spectrum. In particular, the lowest bound state of $H_{\mathrm{fin}}^{T}(1,3)$ must have energy E.

$H_{\mathrm{fin}}^{T}(1,3)$ involves the coordinates of the positron and the proton with origin at the electron. Let us now consider this Hamiltonian with these coordinates replaced by the coordinates of the positron and the electron with origin at the proton. It takes the form

$$H_{\mathrm{fin}}^{T}(1,2)=-\frac{1}{2\nu_p}\nabla_1^2-\frac{1}{2\mu_e}\nabla_2^2-\frac{1}{m_e}\nabla_1\cdot\nabla_2-\frac{1}{r_1}-\frac{1}{r_2}+\frac{1}{r_{12}}.\tag{8}$$

This operator does not correspond to anything physical. However, it follows from our earlier analysis that $H_{\mathrm{fin}}(1,2)$ and $H_{\mathrm{fin}}^{T}(1,2)$ must have the same eigenvalue spectrum. In particular, the lowest bound-state eigenfunction of $H_{\mathrm{fin}}^{T}(1,2)$ must correspond to the eigenvalue E.

Since Ψ is a ground-state eigenfunction of $H_{\mathrm{fin}}(1,2)$, it follows that

$$\langle\Psi|H_{\mathrm{fin}}^{T}(1,2)-H_{\mathrm{fin}}(1,2)|\Psi\rangle\geq 0,\tag{9}$$

i.e.,

$$\left\langle\Psi\left|-\left(\frac{1}{2\nu_p}-\frac{1}{2\mu_p}\right)\nabla_1^2-\left(\frac{1}{m_e}-\frac{1}{M}\right)\nabla_1\cdot\nabla_2-2\left(\frac{1}{r_1}-\frac{1}{r_{12}}\right)\right|\Psi\right\rangle\geq 0,\tag{10}$$

i.e.,

$$\langle\Psi|\nabla_1\cdot\nabla_2|\Psi\rangle\leq\left(\frac{Mm_e}{M-m_e}\right)\left\langle\Psi\left|-\left(\frac{1}{2\nu_p}-\frac{1}{2\mu_p}\right)\nabla_1^2-2\left(\frac{1}{r_1}-\frac{1}{r_{12}}\right)\right|\Psi\right\rangle.\tag{11}$$

Note that it follows from our earlier discussion that for a bound state to exist at all,

$$\langle\Psi|\nabla_1\cdot\nabla_2|\Psi\rangle>0.\tag{12}$$

Equations (5) and (11) imply that, if a bound state exists, then

$$\left\langle\Psi\left|-\left[\frac{1}{2\mu_p}-\frac{m_e}{2(M-m_e)}\left(\frac{1}{\nu_p}-\frac{1}{\mu_p}\right)\right]\nabla_1^2-\frac{1}{2\mu_e}\nabla_2^2+\left(1+\frac{2m_e}{M-m_e}\right)\frac{1}{r_1}-\frac{1}{r_2}-\left(1+\frac{2m_e}{M-m_e}\right)\frac{1}{r_{12}}\right|\Psi\right\rangle$$
$$\leq E<-\tfrac{1}{2}\mu_e.\tag{13}$$

It follows that if there exists no normalized square-integrable function, $\Phi(\vec{r}_1,\vec{r}_2)$, for which

$$\langle\Phi|H_{\mathrm{inf}}'|\Phi\rangle<-\tfrac{1}{2}\mu_e,\tag{14}$$

where

$$H_{\mathrm{inf}}'=\frac{1}{2\mu_p'}\nabla_1^2-\frac{1}{2\mu_e}\nabla_2^2+\left(\frac{M+m_e}{M-m_e}\right)\frac{1}{r_1}-\frac{1}{r_2}-\left(\frac{M+m_e}{M-m_e}\right)\frac{1}{r_{12}}\tag{15}$$

and

$$\frac{1}{\mu_p'}=\frac{1}{\mu_p}-\frac{m_e}{(M-m_e)}\left(\frac{1}{\nu_p}-\frac{1}{\mu_p}\right), \tag{16}$$

then no bound state of $H_{\rm fin}$ can exist.

Physically, $H_{\rm inf}'$ represents the internal motion, in the infinite-proton-mass approximation, of a system made up of a proton, a "positron" of charge $(M+m_e)/(M-m_e)$ and mass

$$\mu_p'=(M-m_e)\mu_p\nu_p/(M\nu_p-m_e\mu_p), \tag{17}$$

and an "electron" having mass μ_e and the usual charge. Now $-\frac{1}{2}\mu_e$ is the lowest continuum threshold for such a system. Thus a necessary condition for $H_{\rm fin}$ to be able to support a bound state is that $H_{\rm inf}'$ be able to support a bound state.

The existence, or otherwise, of a bound state of $H_{\rm inf}'$ can be investigated by the method used by Armour,[2] hereinafter referred to as I. The ground state will be an S state. For such states $H_{\rm inf}'$ will reduce to the form

$$H'(R,r,\theta)=t_p(R)+t_e(r)+\left(\frac{1}{2\mu_p'R^2}+\frac{1}{2\mu_e r^2}\right)\mathcal{L}^2+\frac{Z}{R}-\frac{1}{r}-\frac{Z}{r_{12}}, \tag{18}$$

where $R=r_1$, $r=r_2$ and

$$t_p(R)=\frac{1}{2\mu_p'R^2}\frac{\partial}{\partial R}\left(R^2\frac{\partial}{\partial R}\right), \tag{19}$$

$$t_e(r)=-\frac{1}{2\mu_e r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right), \tag{20}$$

$$\mathcal{L}^2=-\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right), \tag{21}$$

$$Z=\frac{M+m_e}{M-m_e}. \tag{22}$$

As was pointed out in I, Spruch[6] has shown that a necessary condition for $H'(R,r,\theta)$ to be able to support a bound state is that the radial Hamiltonian, $H_1(R)$, be able to support a bound state where

$$H_1(R)=t_p(R)+V_1(R), \tag{23}$$

$$V_1(R)=E_0(R)-E_{\rm thr}. \tag{24}$$

$E_0(R)$ is the lowest eigenvalue, for a given R value, of the Hamiltonian

$$H_2'(r,\theta;R)=t_e(r)+\left(\frac{1}{2\mu_p'R^2}+\frac{1}{2\mu_e r^2}\right)^2+\frac{Z}{R}-\frac{1}{r}-\frac{Z}{r_{12}} \tag{25}$$

and

$E_{\rm thr}$ = lowest continuum threshold $=-\frac{1}{2}\mu_e$.

The method employed in I for showing that $H_1(R)$ could not support a bound state in the case of e^+H with the proton assumed to be infinitely massive was to calculate a lower bound, $V_L(R)$, to $V_1(R)$ and then show that $V_L(R)$ could not support a bound state. As $m_p=m_e$ and thus $\mu_p'=m_e$, $\mu_e=0.9995m_e$ and $Z=1.0011$, it seems almost certain that $H_1(R)$ in this case will also be unable to support a bound state. We can readily show that this is so as follows. For $R>20$ bohr, $V_L(R)$ is certainly given accurately by treating the system as a hydrogen atom perturbed by a charge Z (see, for example, Wind[7]).

We can obtain $V_L(R)$ for the region $R\leq 20$ bohr as follows.

$$H_2'(r,\theta;R)\geq ZH_3(r,\theta;R), \tag{26}$$

where

$$H_3(r,\theta;R)=-\frac{1}{2\mu r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\left(\frac{1}{2\mu R^2}+\frac{1}{2\mu r^2}\right)\mathcal{L}^2+\frac{1}{R}-\frac{1}{r}-\frac{1}{r_{12}} \tag{27}$$

and

$$\mu = Z\mu_p' = 1.0011 m_e.$$

$H_3(r,\theta;R)$ is essentially the same as the Hamiltonian $H_2(r,\theta;R)$ of I; it differs from it only in that m_e is replaced by μ. This makes it possible to use a lower bound potential already calculated.

It can be shown by solving the appropriate radial Schrödinger equation that $V_L(R)$ cannot support a bound state and consequently no bound state of $H_1(R)$ exists. It follows that no bound state of H_{inf}' exists. Hence H_{fin}, the Hamiltonian for the internal motion of e^+H in the case of finite proton mass, can have no bound state. This proves, for the first time, that no bound state of e^+H exists in the case when the finite mass of the proton is taken into account.

It is intended as a next stage to apply the method to try to prove the absence of a bound state for a system made up of muonium and a positron. The mass of the muon is $207m_e$ and, consequently, the effect of the Hughes-Eckart term can be expected to be more important in this case.

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Quantum Mechanical Models of Turing Machines That Dissipate No Energy

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Quantum mechanical Hamiltonian models of Turing machines are constructed here on a finite lattice of spin-$\frac{1}{2}$ systems. The models do not dissipate any energy and they operate at the quantum limit in that the system (energy uncertainty)/(computation speed) is close to the limit given by the time-energy uncertainty principle.

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There has been much discussion in the literature recently about the physical limitations of the computation process and information transfer.[1-12] Early work[1,2] assumed that the computation process was irreversible because of the necessity to discard information. However, this was shown to be false by Bennett.[3] More recently Landauer[7] has stressed the importance of the energy dissipation problem for the computation process. Recent work[8,9] has assumed that energy dissipation must occur, and on the basis of this, Bekenstein[8] derived an upper limit of 10^{15} steps/sec for computation speeds. However, this work has been criticized by Deutsch[10] and Landauer.[11] Fredkin and Toffoli[12] have constructed a classical mechanical model of the computation process which dissipates no energy.

The purpose of this note is to briefly present and discuss quantum mechanical Hamiltonian models of the computation process as represented by standard Turing machines.[3] These models also dissipate no energy and operate at essentially the quantum limit in that the total system (energy uncertainty)/(computation speed) $\lesssim 2\pi\hbar$. Unlike the models constructed in other work,[13] the models constructed here do not use successive scattering to drive the process.

A Turing machine consists of three parts, an internal machine part L which is capable of assuming any one of a finite number of states, a computation tape T infinite in both directions, and a computation head h. T is divided into an infinite number of cells at positions $\ldots -1, 0, 1, \ldots$. Each cell contains any symbol s of an