

Quantum-mechanical Wave Equation for Two Particles of Spin 0

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Abstract

A quantum-mechanical wave equation for two particles of spin 0 is presented in Hamiltonian formalism and is then simplified and discussed. Solutions are found for square-well and Coulomb interactions, and energy levels are determined. It is shown that, for the Coulomb interaction, the energy levels to the lowest order agree with those given by the hydrogen atom formula.

Introduction

A quantum-mechanical wave equation for two particles of any spin with an arbitrary instantaneous interaction was recently derived by the author (Tam 1973). This equation contains the sum of the Hamiltonians of the two particles, and it can be explicitly written for any specific particles once the Hamiltonians and the interaction of the particles are known. In this paper, solutions to the equation for spin-0 particles with some common interactions such as square-well and Coulomb are presented and discussed. The two-particle wave equation originally in matrix form is first reduced to four simultaneous equations with four unknown components of the wavefunction, and the four equations are then combined to yield a single equation for one component. This equation holds for any arbitrary instantaneous interaction. For square-well and Coulomb interactions, solutions are found and energy levels are determined.

Throughout this paper, quantities are expressed in natural units with $\hbar = c = 1$, that is, with \hbar , Planck's constant divided by 2π , and c , the speed of light, taken as unity. The imaginary fourth component convention is also used, in which the space-time four-vectors are $x_\mu = (x, y, z, it)$ and the invariant is

$$x_\mu x_\mu = x^2 + y^2 + z^2 - t^2.$$

Two Spin-0 Particles

For a spin-0 particle, the Hamiltonian is (see Tam 1973)

$$H = \nabla^2 \sigma / 2m - m\rho, \tag{1}$$

where

$$\sigma = \begin{bmatrix} 0 & 0 \\ 2 & 0 \end{bmatrix} \quad \text{and} \quad \rho = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

Squaring the operator (1) gives

$$H^2 = (-\nabla^2 + m^2)I,$$

where I is a 2×2 unit matrix, so that the spin-0 Hamiltonian equation $H\psi = i\partial\psi/\partial t$ reduces to the Klein-Gordon equation

$$(-\nabla^2 + m^2)\psi = -\partial^2\psi/\partial t^2.$$

The time-independent wave equation for two particles of any spin is (see Tam 1973)

$$(H_1 + H_2 + V)\psi = E\psi,$$

which, for two spin-0 particles, becomes symbolically

$$\left(\frac{\nabla_1^2 \sigma_1}{2m_1} + \frac{\nabla_2^2 \sigma_2}{2m_2} - (m_1 \rho_1 + m_2 \rho_2) + V \right) \psi(x_1, x_2) = E\psi(x_1, x_2), \quad (2)$$

where the two-particle wavefunction is

$$\psi(x_1, x_2) = \begin{bmatrix} \psi_{11} & \psi_{12} \\ \psi_{21} & \psi_{22} \end{bmatrix}.$$

The first index in the components of the wavefunction is associated with the first particle and the second index with the second particle. Equation (2) has the following matrix form

$$\begin{aligned} & \frac{\nabla_1^2}{2m_1} \begin{bmatrix} 0 & 0 \\ 2 & 0 \end{bmatrix} \begin{bmatrix} \psi_{11} & \psi_{12} \\ \psi_{21} & \psi_{22} \end{bmatrix} + \frac{\nabla_2^2}{2m_2} \begin{bmatrix} \psi_{11} & \psi_{12} \\ \psi_{21} & \psi_{22} \end{bmatrix} \begin{bmatrix} 0 & 2 \\ 0 & 0 \end{bmatrix} \\ & - \left[m_1 \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \psi_{11} & \psi_{12} \\ \psi_{21} & \psi_{22} \end{bmatrix} + m_2 \begin{bmatrix} \psi_{11} & \psi_{12} \\ \psi_{21} & \psi_{22} \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \right] + V \begin{bmatrix} \psi_{11} & \psi_{12} \\ \psi_{21} & \psi_{22} \end{bmatrix} = E \begin{bmatrix} \psi_{11} & \psi_{12} \\ \psi_{21} & \psi_{22} \end{bmatrix}. \end{aligned} \quad (3)$$

After equating each component of the matrix equation (3), we obtain

$$\begin{bmatrix} E-V & m_2 & m_1 & 0 \\ -\nabla_2^2/m_2 + m_2 & E-V & 0 & m_1 \\ -\nabla_1^2/m_1 + m_1 & 0 & E-V & m_2 \\ 0 & -\nabla_1^2/m_1 + m_1 & -\nabla_2^2/m_2 + m_2 & E-V \end{bmatrix} \begin{bmatrix} \psi_{11} \\ \psi_{12} \\ \psi_{21} \\ \psi_{22} \end{bmatrix} = 0. \quad (4)$$

Free Particles

Consider first the case of two free particles, in which we put $V = 0$. Going to momentum space, we replace ∇_1^2 by $-p_1^2$ and ∇_2^2 by $-p_2^2$. In order that the solution be nontrivial, the determinant of the matrix must be zero, that is, we must have

$$\det \begin{bmatrix} E & m_2 & m_1 & 0 \\ p_2^2/m_2 + m_2 & E & 0 & m_1 \\ p_1^2/m_1 + m_1 & 0 & E & m_2 \\ 0 & p_1^2/m_1 + m_1 & p_2^2/m_2 + m_2 & E \end{bmatrix} = 0.$$

Expanding the determinant and solving for E gives

$$E = \pm \{(p_1^2 + m_1^2)^{\frac{1}{2}} \pm (p_2^2 + m_2^2)^{\frac{1}{2}}\}.$$

Arbitrary Interaction

Next consider equation (4) in the c.m. frame in which $\nabla_1^2 = \nabla_2^2 = \nabla_x^2$, where $\mathbf{x} = \mathbf{x}_1 - \mathbf{x}_2$ is the relative coordinate; we suppress the subscript x in ∇_x^2 in the following discussion. Then, in the c.m. frame with ∇_1^2 and ∇_2^2 replaced by ∇^2 in equation (4), the resulting expression can be simplified to obtain an equation involving only ψ_{11} , namely

$$\left(\nabla^2 - (m_1^2 + m_2^2) + \frac{1}{2}(E - V)^2 + \frac{(m_1 + m_2)^2(m_1 - m_2)^2}{2(E - V)^2} + \frac{\nabla^2(E - V)}{E - V} \right) \psi_{11} = 0, \quad (5)$$

where ψ_{11} corresponds to the usual Klein-Gordon wavefunction for two particles.

Square-well Interaction

For a square-well potential

$$\begin{aligned} V(r) &= -V_0 & \text{for } r \leq a, \\ &= 0 & r > a, \end{aligned}$$

equation (5) becomes, for $r \leq a$,

$$\left(\nabla^2 + \frac{(m_1 + m_2)^2(m_1 - m_2)^2}{4(E + V_0)^2} - \frac{1}{2}(m_1^2 + m_2^2) + \frac{1}{4}(E + V_0)^2 \right) \psi_{11} = 0. \quad (6)$$

With the substitution $\psi_{11} = f_{11}(r) Y_{lm}(\theta, \phi)$ in equation (6), the radial equation becomes

$$\left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} + K^2 - \frac{l(l+1)}{r^2} \right) f_{11}(r) = 0, \quad (7)$$

where

$$K^2 = \frac{1}{4}(m_1 + m_2)^2(m_1 - m_2)^2 / (E + V_0)^2 - \frac{1}{2}(m_1^2 + m_2^2) + \frac{1}{4}(E + V_0)^2.$$

The solution of equation (7) is

$$f_{11}(r) = A j_l(Kr).$$

The other components of the wavefunction can be obtained from equation (4), with $\nabla_1^2 = \nabla_2^2 = \nabla^2$. They are:

$$\psi_{22} = \frac{A}{m_1 m_2} \left(\frac{1}{4}(E + V_0)^2 - \frac{(m_1 + m_2)^2(m_1 - m_2)^2}{4(E + V_0)^2} \right) j_l(Kr) Y_{lm}(\theta, \phi),$$

$$\psi_{12} = -\frac{A}{m_2} \left(\frac{1}{2}(E + V_0) - \frac{(m_1^2 - m_2^2)}{2(E + V_0)} \right) j_l(Kr) Y_{lm}(\theta, \phi),$$

$$\psi_{21} = -\frac{A}{m_1} \left(\frac{1}{2}(E + V_0) - \frac{(m_2^2 - m_1^2)}{2(E + V_0)} \right) j_l(Kr) Y_{lm}(\theta, \phi).$$

For $r > a$, equation (5) reduces to

$$\left(\nabla^2 + \frac{(m_1 + m_2)^2(m_1 - m_2)^2}{4E^2} - \frac{1}{2}(m_1^2 + m_2^2) + \frac{1}{4}E^2 \right) \psi_{11} = 0.$$

With the substitution $\psi_{11} = g_{11}(r) Y_{lm}(\theta, \phi)$, the radial equation becomes

$$\left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} + \alpha^2 - \frac{l(l+1)}{r^2} \right) g_{11}(r) = 0, \tag{8}$$

where

$$\alpha^2 = \frac{1}{4}(m_1 + m_2)^2(m_1 - m_2)^2/E^2 - \frac{1}{2}(m_1^2 + m_2^2) + \frac{1}{4}E^2.$$

The solution of equation (8) is

$$g_{11}(r) = B h_l^{(1)}(\alpha r).$$

Again, the other components of the wavefunction can be obtained from equation (4):

$$\psi_{22} = \frac{B}{m_1 m_2} \left(\frac{1}{4}E^2 - \frac{(m_1 + m_2)^2(m_1 - m_2)^2}{4E^2} \right) h_l^{(1)}(\alpha r) Y_{lm}(\theta, \phi),$$

$$\psi_{12} = -\frac{B}{m_2} \left(\frac{1}{2}E - \frac{(m_1^2 - m_2^2)}{2E} \right) h_l^{(1)}(\alpha r) Y_{lm}(\theta, \phi),$$

$$\psi_{21} = -\frac{B}{m_1} \left(\frac{1}{2}E - \frac{(m_2^2 - m_1^2)}{2E} \right) h_l^{(1)}(\alpha r) Y_{lm}(\theta, \phi).$$

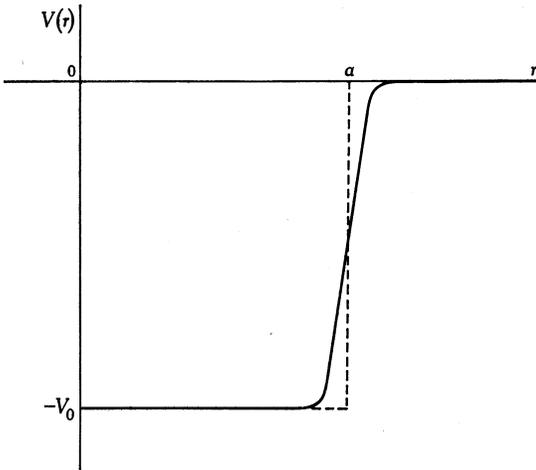


Fig. 1. A more realistic modified square-well potential.

To determine the energy levels, the solutions inside and outside the well are matched at $r = a$. If ψ_{11} and the first derivative of ψ_{11} correspond at $r = a$, we have

$$A j_l(Ka) = B h_l^{(1)}(\alpha a) \quad \text{and} \quad KA j_l'(Ka) = \alpha B h_l^{(1)'(\alpha a)},$$

and thus their ratio

$$j_l(Ka)/Kj_l'(Ka) = h_l^{(1)}(\alpha a)/\alpha h_l^{(1)'(\alpha a)}$$

will give the energy levels. If other components of the wavefunction are matched at

$r = a$ then, for $r < a$, the wavefunction will contain in the coefficient of the spherical Bessel function a term involving $E + V_0$, whereas, for $r > a$, a term involving only E . This is due to the discontinuous change of the potential at $r = a$. For a more realistic potential of the form shown in Fig. 1, the function is continuous at $r = a$ and, since the value of the limit of the potential from both sides is the same, a matching of any component of the wavefunction will give the same result.

Coulomb Interaction

The wave equation for two spin-0 particles is now used to describe a pionic atom which consists of a negatively charged pion circulating around a positively charged pion. For this system, $m_1 = m_2 = m$ and the potential between the two pions is Coulombic and is given by $V(r) = -e^2/r$.

Equation (5) becomes in this case

$$\left(\nabla^2 - 2m^2 + \frac{1}{2}(E + e^2/r)^2 + \frac{E \nabla^2}{E + e^2/r} \right) \psi_{11} + \frac{\nabla^2(e^2 \psi_{11}/r)}{E + e^2/r} = 0. \tag{9}$$

The last term in this equation can be simplified. We consider the region $r \neq 0$ because the potential is singular at the origin. For this region,

$$\nabla^2(r^{-1} \psi_{11}) = r^{-1} \nabla^2 \psi_{11} - 2r^{-2} \partial \psi_{11} / \partial r$$

and therefore equation (9) becomes

$$\left(\nabla^2 - m^2 + \frac{1}{4}(E + e^2/r)^2 - \frac{e^2/r^2}{E + e^2/r} \frac{\partial}{\partial r} \right) \psi_{11} = 0.$$

Putting $\psi_{11} = f_{11}(r) Y_{lm}(\theta, \phi)$, we have for the radial equation

$$\left\{ \frac{d^2}{dr^2} + \frac{1}{r} \left(2 - \frac{e^2/r}{E + e^2/r} \right) \frac{d}{dr} + \frac{(E + e^2/r)^2}{4} - \frac{l(l+1)}{r^2} - m^2 \right\} f_{11}(r) = 0. \tag{10}$$

But, since

$$-\frac{e^2}{r(Er + e^2)} = -\frac{1}{r} + \frac{1}{r + e^2/E},$$

equation (10) becomes

$$\left\{ \frac{d^2}{dr^2} + \left(\frac{1}{r} + \frac{1}{r + e^2/E} \right) \frac{d}{dr} + (\frac{1}{4}E^2 - m^2) + \frac{Ee^2}{2r} + \frac{\frac{1}{4}e^4 - l(l+1)}{r^2} \right\} f_{11}(r) = 0. \tag{11}$$

Now consider the ratio e^2/E . In SI units, e^2 is of the order of 10^{-38} C^2 while E is of the order of the mass of a pion and is 10^2 MeV or 10^{-11} J . Therefore, the ratio e^2/E is of the order of 10^{-17} m , where a constant $9 \times 10^9 \text{ N m C}^{-2}$ has been inserted for the SI system. Thus we have

$$e^2/E \sim 10^{-17} \text{ m} \ll 10^{-15} \text{ m} = r_e,$$

r_e being the radius of an electron. Equation (11) has no exact solution because of

the presence of the term $(r + e^2/E)^{-1}$. However, since e^2/E is very much less than the radius of an electron, it can be neglected and we can approximate the former term by r^{-1} . With this approximation, equation (11) takes the form

$$\left\{ \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} + \left(-\kappa^2 + \frac{Ee^2}{2r} + \frac{\beta^2}{r^2} \right) \right\} f_{11}(r) = 0, \quad (12)$$

where

$$\kappa^2 = m^2 - \frac{1}{4}E^2, \quad \beta^2 = \frac{1}{4}e^4 - l(l+1).$$

Equation (12) can be solved by the usual method (see e.g. Schiff 1968). The energy eigenvalue is given as

$$E = 2m \left\{ 1 - \frac{e^4}{8n^2} + \frac{e^8}{16n^3} \left(\frac{3}{8n} - \frac{1}{2l+1} \right) + \dots \right\} \quad (13)$$

to terms of order e^8 , where the principal quantum number n can take positive integral values. In terms of the reduced mass of the system $\mu = \frac{1}{2}m$, equation (13) becomes

$$E = 2m - \frac{\mu e^4}{2n^2} + \frac{\mu e^8}{4n^3} \left(\frac{3}{8n} - \frac{1}{2l+1} \right) + \dots$$

The first term on the right-hand side is the rest mass of the system and the second term is identical with the one for nonrelativistic particles. The third term is the fine-structure energy which differs from usual Klein-Gordon and Dirac one-particle levels.

The radial wavefunction is

$$f_{11} = \exp(-\kappa r) r^s L_q^p(2\kappa r),$$

where

$$s = -\frac{1}{2} + \frac{1}{2} \{ (2l+1)^2 - e^4 \}^{\frac{1}{2}}, \quad p = 2s+1, \quad q = Ee^2/4\kappa + s.$$

The other components of the wavefunction can be found from equation (4). The complete wavefunction is

$$\psi = C \begin{bmatrix} f_{11} Y_{lm}(\theta, \phi) & -\frac{1}{2}m^{-1}(E+e^2/r) f_{11} Y_{lm}(\theta, \phi) \\ -\frac{1}{2}m^{-1}(E+e^2/r) f_{11} Y_{lm}(\theta, \phi) & \frac{1}{4}m^{-2}(E+e^2/r)^2 f_{11} Y_{lm}(\theta, \phi) \end{bmatrix},$$

f_{11} being defined as above.

Conclusions

We have seen that the wavefunction for two spin-0 particles in the Hamiltonian formalism has four components and that the corresponding wave equation can be simplified to give four equations for these four components which can then be combined to yield a single equation for one component. The resulting equation holds for two particles of unequal mass and an arbitrary potential which is a function of the magnitude of the relative position of the two particles. The solutions found for a square-well interaction are the product of spherical harmonics and spherical Bessel functions. An approximate solution has also been found for a Coloumb interaction and the corresponding energy levels have been determined. In the

expression for these energy levels, the first two terms are identical with the corresponding terms for nonrelativistic particles, while the third term gives a fine-structure energy which is of the order of e^8 . This result thus shows why the energy level formula for the nonrelativistic hydrogen atom can be used for a system of two pions to obtain a result which agrees with experiment. In fact, when dealing with any two-body system, a two-body equation should be used rather than a single-body one like the Klein-Gordon or Dirac equation as has often been used.

In subsequent papers, the present two-body equation will be applied to two-body systems with spins of $\frac{1}{2}$ and 1.

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