BOUND STATES OF THE KLEIN–GORDON EQUATION WITH VECTOR AND SCALAR HULTHÉN-TYPE POTENTIALS

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The existence of bound states for the s-wave Klein–Gordon equation for vector and scalar Hulthén-type potentials is shown, provided that the potential "size" is large enough. The solution can be explicitly written down in terms of hypergeometric functions. The effects of strong coupling on the bound states are discussed.

1. Introduction

The nonrelativistic Schrödinger equation with the Hulthén potential can be solved exactly for s-states [1]. This naive potential explains quite well the electronic properties of F′-colour centers in alkali halides [2]. Moreover, the model of the three-dimensional delta-function well could be considered as a Hulthén potential with the radius of the force going down to zero, within a nonrelativistic framework [3]. Nevertheless, relativistic effects for a particle under the action of this potential could become important, especially for strong coupling.

2. Bound state solutions

In order to introduce relativistic corrections in a non-perturbative way, we shall solve the s-wave Klein–Gordon equation ($\hbar = c = 1$)

$$\{d^2/dr^2 + [E - V(r)]^2 - [m + S(r)]^2\}u(r) = 0\,, \quad (1)$$

where the particle wave function is $\psi(r) = u(r)/r$. We consider vector and scalar Hulthén-type potentials which are written as

$$V(r) = -\frac{V_0}{e^{r/a} - 1}\,, \quad S(r) = -\frac{S_0}{e^{r/a} - 1}\,, \quad (2)$$

respectively, where a is the range of the potentials. We should emphasize the Coulomb-like behavior of the potentials near the origin, since it will be used below.

Introducing the parameters $\eta = (m^2 - E^2)^{1/2}$ (real for bound states), $\alpha = \eta a$, $\beta = (2EV_0 + 2mS_0)^{1/2}a$ and $\nu = S_0^2 - V_0^2)^{1/2}a$, and the new variable $x = \exp(-r/a)$, eq. (1) can be rewritten as

$$x^2 \frac{d^2u(x)}{dx^2} + x\frac{du(x)}{dx} - \left(\alpha^2 - \frac{\beta^2 x}{1-x} + \frac{\nu^2 x^2}{(1-x)^2}\right)u(x) = 0\,. \quad (3)$$

Bound state solutions of this equation satisfy the boundary conditions $u(1) = 0$ ($r \to 0$) and $u(0) = 0$ ($r \to \infty$). The trial function

$$u(x) = x^{\alpha}(1-x)^{1+\delta}W(x)\,, \quad (4)$$

with $\delta \equiv \delta_{\pm} = -\frac{1}{2} \pm (\frac{1}{4} + \nu^2)^{1/2}$ leads to the equation

$$x(1-x)\frac{d^2W(x)}{dx^2} + [2\alpha + 1 - (2\alpha + 2\delta + 3)x]\frac{dW(x)}{dx} - [(2\alpha+1)(1+\delta) - \beta^2]W(x) = 0\,. \quad (5)$$

Solutions of eq. (5) can be expressed in terms of hypergeometric functions; taking into account the boundary condition $u(0) = 0$ we find

$$W(x)={}_2F_1(\alpha+\delta+1+\gamma,\ \alpha+\delta+1-\gamma;\ 2\alpha+1;\ x)\ , \tag{6}$$

where

$$\gamma=+(\alpha^2+\beta^2+\gamma^2)^{1/2}$$
$$=a[(m+S_0)^2-(E-V_0)^2]^{1/2}\ .$$

Considering that γ is real for bound states (see below), the condition $E+m>V_0-S_0$ should be fulfilled; thus we avoid discussing the Klein paradox (tunneling of the particle from positive to negative energy states; this effect depends only on the potential strength and is quite independent of the potential shape). We can observe from the last condition that if the scalar potential is stronger than the vector potential, the Klein paradox cannot occur.

Recalling eq. (1) and using the transformation formulas for hypergeometric functions [4] we write the wave function as

$$u(x)=x^\alpha(1-x)^{1+\delta}\frac{\Gamma(2\alpha+1)\Gamma(-1-2\delta)}{\Gamma(\alpha-\delta+\gamma)\Gamma(\alpha-\delta-\gamma)}$$
$$\times{}_2F_1(\alpha+\delta+1+\gamma,\ \alpha+\delta+1-\gamma;\ 2+2\delta;\ 1-x)$$
$$+x^\alpha(1-x)^{-\delta}\frac{\Gamma(2\alpha+1)\Gamma(1+2\delta)}{\Gamma(\alpha+\delta+1+\gamma)\Gamma(\alpha+\delta+1-\gamma)}$$
$$\times{}_2F_1(\alpha-\delta+\gamma,\ \alpha-\delta-\gamma;\ -2\delta;\ 1-x)\ . \tag{7}$$

Note that the first term is obtained from the second term replacing $\delta+1$ by $-\delta$; since $1+\delta_\pm=-\delta_\mp$ we can choose a unique value of δ. Hence, we take $\delta=\delta_+=-\frac{1}{2}+(1+4\nu^2)$ hereafter. Near the origin $(x\to 1)$ the wave function behaves as

$$u(r)\sim r^{1+\delta}\frac{\Gamma(-1-2\delta)}{\Gamma(\alpha-\delta+\gamma)\Gamma(\alpha-\delta-\gamma)}$$
$$+r^{-\delta}\frac{\Gamma(1+2\delta)}{\Gamma(\alpha+\delta+1+\gamma)\Gamma(\alpha+\delta+1-\gamma)}\ . \tag{8}$$

The square of the potential energy, which appears in the Klein–Gordon equation, takes the form const$\times r^{-2}$ as $r\to 0$. Therefore, $V^2(r)$ and $S^2(r)$ have finite expectation values only if $u(r)\sim r^{1-p}$ with $p<\frac{1}{2}$. The second term of eq. (8) does not satisfy this condition and it should vanish, leading to $\Gamma(\alpha+1+\delta-\gamma)\to\infty$. Thus we obtain the quantum condition $\alpha+\delta-\gamma=-1,\ -2,\ ...$ so allowed energy values are given through the equation

$$\alpha=[\beta^2-n^2-(2n-1)\delta]/2(n+\delta),$$
$$n=1,2,\dots\ . \tag{9}$$

Combining everything, the (unnormalized) s-wave function can be written as

$$\psi_n(r)=\frac{e^{-\eta r}}{r}(1-e^{-r/a})^{1+\delta}$$
$$\times{}_2F_1(1-n,\ 2\alpha+2\delta+n+1;\ 2\alpha+1;\ e^{-r/a})\ , \tag{10}$$

where the hypergeometric function degenerates into a polynomial of degree $n-1$ in the variable $\exp(-r/a)$. In particular, the ground state wave function is found to be

$$\psi_g(r)=\frac{e^{-\eta r}}{r}(1-e^{-r/a})^{1+\delta}\ , \tag{11}$$

which behaves like the wave function of the delta-well potential $\psi(r)\sim\exp(-\eta r)/r$ for large r values. The ground state energy E_g is given by

$$2a(m^2-E_g^2)^{1/2}$$
$$=\frac{E_gV_0+mS_0}{S_0^2-V_0^2}\{[1+4(S_0^2-V_0^2)a^2]^{1/2}-1\}-1\ . \tag{12}$$

3. Discussion

After solving the Klein–Gordon equation (1) for scalar plus vector Hulthén-type potentials, we should make some remarks.

(a) For pure vector potentials ($V_0\neq 0$, $S_0=0$), a bound state can exist irrespective of the sign of V_0 (attractive or repulsive), as seen by inspection of eq. (12). When $V(r)$ is weakly attractive (repulsive), a bound state may exist with energy somewhat below m (above $-m$).

(b) For pure attractive scalar potentials ($V_0=0$, $S_0>0$), all bound states appear in pairs, with energies $\pm E_n$. Since the Klein–Gordon equation is independent of the sign of E for scalar potentials, the wave functions become the same for both energy values. For pure repulsive scalar potentials ($V_0=0$, $S_0<0$) no bound states can occur at all.

(c) There exists a minimum potential "size" to obtain a bound state, as we can see from eq. (12).

The left- and the right-hand sides may be regarded as a positive semicircle and a straight line versus the bound state energy, respectively. A bound state does exist if both curves cross one another. This leads to a condition on the potential parameters for binding a particle. For pure vector, pure scalar and equally mixed potentials the condition can be easily found to be $1<m/|V_0|<\frac{1}{2}+2m^2a^2$, $(S_0/m)(a^2m^2-\frac{1}{4})>\frac{1}{2}$ and $2m|V_0|a^2>\frac{1}{2}$, respectively.

(d) In the case of equally mixed potentials $V(r)=S(r)$, eq. (1) reduces to a Schrödinger-like equation for the potential $-2V_0/[\exp(r/a)-1]$. Energy levels are easily computed from eq. (9) with $\delta=0$ and $V_0=S_0$. In particular, we obtain $(m^2-E_g^2)^{1/2}=aV_0(E_g+m)-1/2a$ for the ground state energy (if any).

(e) If the vector potential is stronger than the scalar potential, i.e. $V_0>S_0$, the parameter δ becomes a complex number when $(V_0^2-S_0^2)a^2>\frac{1}{4}$. Thus the wave function $\psi(r)=u(r)/r$ oscillates rapidly near the origin (see eq. (8)), without reaching any limit. This behavior should be regarded as a particle falling to the center [5]. Also, the expectation value of the square of the potential energy becomes infinite. Note that a particle falls even for finite values of the potential parameters V_0, S_0 and a. The difficulties arising in quantum mechanics when the potential is highly singular were considered earlier by Case [6].

(f) Unlike the previous case, if $S_0>V_0$ the parameter δ is always a real number, and therefore the particle does not collapse to the center for finite values of the potential parameters. For very strong scalar potentials ($S_0\to+\infty$), the bound state energy is given by $E_g=(m/2a-1/4a^2)^{1/2}$, whenever $m>1/2a$. Therefore, the particle cannot fall to the center, no matter how large S_0. We think this is a nontrivial feature of relativistic quantum mechanics.

(g) For equally mixed potential ($V_0=S_0$), the particle energy tends to $-m$ as the potential depth becomes infinite. The particle is pushed down to the negative energy continuum. The corresponding wave function (11) cannot be normalised in the usual form and hence there is no particle binding.

(h) Finally, we should remark that nonrelativistic results [1] are found for weak coupling as the particle mass becomes very large. For strong coupling we need a relativistic wave equation.

4. Conclusions

We may conclude that the Klein–Gordon equation for vector and scalar Hulthén-type potentials can be solved exactly for s-states, so we can include relativistic mass–energy corrections in a non-perturbative way. The obtained wave functions may be used as a starting point to evaluate the spin–orbit interaction or the Darwin energy by perturbative or variational methods. Bound state can occur provided that the potential parameters (depth and range) verify adequate conditions. The effects of strong potentials have been discussed, within the limitations of a single-particle relativistic wave equation.

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References

[1] S. Flügge, Practical quantum mechanics, Vol. I (Springer, Berlin, 1974) p. 175.

[2] A.A. Berezin, Phys. Stat. Sol. (b) 50 (1972) 71; J. Phys. C 12 (1979) L363.

[3] A.A. Berezin, Phys. Rev. B 33 (1986) 2122.

[4] M. Abramowitz and I.A. Stegun, Handbook of mathematical functions (US Government Printing Office, Washington DC, 1964).

[5] V.B. Berestetskii, E.M. Lifshitz and L.P. Pitaevskii, Relativistic quantum theory, Part I (Pergamon, Oxford, 1971).

[6] K.M. Case, Phys. Rev. 80 (1950) 797.