Aust. J. Phys., 1985, **38**, 539–45

Scattering at the Positive Energy Bound States

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Abstract

For a rank-n separable potential, some of the conditions for the existence of positive energy bound states are given and discussed. It has been shown that scattering can occur at positive energy bound states and only a particular type of them can be interpreted as zero-width resonances.

1. Introduction

For a class of separable potentials bound states occur at positive energies (Gourdin and Martin 1957; Martin 1958), and these states have been interpreted as zero-width resonances (Bolsterli 1969; Beam 1969). Recently, it has been shown that, in general, a positive energy bound state (PEBS) cannot be interpreted as a zero-width resonance; a rank-two potential can give a PEBS and a scattering phase shift at the same energy (Husain and Suhrabuddin 1980). Here we will derive some general conditions under which a rank-n potential can produce PEBS, and also identify the PEBS which give scattering and the ones which are zero-width resonances. This will be shown by a number of illustrative cases.

2. Theory

We consider the s-wave Schrödinger equation

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} + k^2\right)\psi(r) = \int_0^\infty K(r, r')\,\psi(r')\,\mathrm{d}r', \tag{1}$$

where

$$K(r, r') = \sum_{i=1}^{n} \lambda_i f_i(r) f_i(r') \qquad (\lambda_i \neq 0). \tag{2}$$

The solution of these equations at the energy $k^2 = k_0^2$, such that

$$\psi(k_0, r) \to 0 \qquad \text{as } r \to \infty, \tag{3}$$

$$\psi(k_0, 0) = 0, \tag{4}$$

0004-9506/85/040539$02.00

is known as the PEBS wavefunction. A solution of equations (1) and (2) which satisfies these conditions is

$$\psi(k, r) = \sum_{i=1}^{n} c_i(k)\,\phi_i(k, r) \qquad (c_i \neq 0), \tag{5}$$

where $\phi_i(k, r)$ satisfies

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} + k^2\right)\phi_i(k, r) = f_i(r), \tag{6}$$

with

$$\phi_i(k, r) \to 0 \qquad \text{as } r \to \infty, \tag{7}$$

and where $c_i(k)$ is given by

$$c_i(k) = \lambda_i \sum_{j=1}^{n} d_{ij}(k)\, c_j(k), \tag{8}$$

with

$$d_{ij}(k) = \int_0^\infty f_i(r)\,\phi_j(k, r)\,\mathrm{d}r. \tag{9}$$

Equations (6) and (7) can be solved to give

$$\phi_i(k, r) = -\frac{1}{k}\int_r^\infty \sin\, k(r-r')\, f_i(r')\,\mathrm{d}r', \tag{10}$$

and hence

$$\phi_i(k, 0) = \frac{1}{k}\int_0^\infty \sin\, kr\, f_i(r)\,\mathrm{d}r = g_i(k). \tag{11}$$

From equations (4), (5) and (11) we get

$$\sum_{i=1}^{n} c_i(k_0)\, g_i(k_0) = 0. \tag{12}$$

Therefore $\psi(k, r)$, given by equation (5), gives rise to a PEBS at $k^2 = k_0^2$ provided that equations (8), (9) and (12) are satisfied at that energy.

Moreover, the solution of equations (1) and (2) such that

$$\psi(k, 0) = 0, \tag{13}$$

$$\psi(k, r) \to \sin\, kr + \tan\,\delta \cos\, kr \quad \text{as } r \to \infty \tag{14}$$

is given by

$$\psi_s(k, r) = \frac{1}{k}\sin\, kr + \sum_{i=1}^{n} a_i(k)\{\phi_i(k, r) - g_i(k)\cos\, kr\}, \tag{15}$$

where

$$a_i(k) = \lambda_i g_i(k) + \lambda_i \sum_{j=1}^{n} p_{ij}(k)\, a_j(k), \tag{16}$$

with

$$p_{ij}(k) = d_{ij}(k) - g_j(k) \int_0^\infty f_i(r) \cos kr \, \mathrm{d}r. \tag{17}$$

Now consider the matrix

$$\mathrm{D}(k) = \{(1/\lambda_i)\delta_{ij} - p_{ij}(k)\}, \tag{18}$$

so that from equations (16) and (18) we have

$$a_i(k) = \frac{1}{\det \mathrm{D}(k)} \sum_{j=1}^{n} t_{ij}(k)\, g_j(k), \tag{19}$$

where $t_{ij}(k)$ are the cofactors of the jith element of the matrix $\mathrm{D}(k)$.

From equations (14), (15) and (19) we get the scattering phase shift as

$$\tan \delta(k) = -\frac{k}{\det \mathrm{D}(k)} \sum_{i,j} t_{ij}(k)\, g_i(k)\, g_j(k), \tag{20}$$

and to satisfy the condition (12) we may take

$$g_i(k_0) = 0, \qquad \text{for } i = 1, 2, \ldots, n \tag{21}$$

or

$$\begin{aligned} g_i(k_0) &\neq 0, \qquad \text{for } i = 1, 2, \ldots, m \\ &= 0, \qquad\quad\;\; i = m+1, \ldots, n. \end{aligned} \tag{22}$$

The coefficients $c_i(k_0)$ for $i = 1, 2, \ldots, m$ are related by the equation

$$\sum_{i=1}^{m} c_i(k_0)\, g_i(k_0) = 0. \tag{23}$$

When condition (21) is satisfied and keeping in mind equation (18), it may be possible that $g_i(k)$ and $\mathrm{D}(k)$ have $k^2 - k_0^2$ as a factor, and hence we may write $\tan \delta(k)$ in the form

$$\tan \delta(k) = v(k)(k^2 - k_0^2)^2/(k^2 - k_0^2), \tag{24}$$

where $v(k)$ is free from the factor $k^2 - k_0^2$. We note that $\tan \delta$, having this form, can be interpreted as a zero-width resonance. In general, equation (24) is difficult, if not formidable, to derive explicitly; however, in the following section we will study a few different cases and describe the correct interpretations.

3. A Few Cases for the PEBS

Case 1

We consider the form factor

$$f_i(r) = \left(\beta_i r - \frac{2\beta_i^2}{k_0^2+\beta_i^2}\right)\exp(-\beta_i r), \tag{25}$$

which has been shown to be equivalent to a Coulomb potential (Husain and Awin 1985). In this case we have $g_i(k_0) = 0$ for all i. Moreover, when $n = 1$ the form factor (25) contains both repulsion and attraction so that the phase shift changes sign at $k^2 = k_0^2$. This can be compared with the one given by Tabakin (1968) which has similar properties. We now consider two situations:

Rank-one potential. In this case $n = 1$ and from equations (5) and (10) the PEBS wavefunction is given by

$$\psi_b(k_0, r) = Nr\exp(-\beta_1 r), \tag{26}$$

provided that

$$\lambda_1 = 4\beta_1(k_0^2+\beta_1^2)^2/(k_0^2-\beta_1^2). \tag{27}$$

The phase shift at the energy k^2 is given by

$$\tan\delta(k) = \frac{-(k^2-k_0^2)^2 16k\beta_1^5/(k^2-k_0^2)}{(k_0^2-\beta_1^2)(k^2+\beta_1^2)^3+2\beta_1^2(k^2+\beta_1^2)^2(k_0^2+\beta_1^2)-8\beta_1^4(k^2-k_0^2)(k^2-\beta_1^2)}. \tag{28}$$

Rank-two potential. We take $n = 2$ and the PEBS wavefunction in this case is given by

$$\psi_b(k_0, r) = \sum_{i=1}^{2} \frac{c_i\beta_i}{k_0^2+\beta_i^2} r\exp(-\beta_i r), \tag{29}$$

where one of the c_i is arbitrary and the λ_i are determined from equation (8). In a similar manner, one can get $\tan\delta(k)$ in the form given by equation (24).

Case 2

Here we use condition (22) to determine both the PEBS wavefunction and the scattering phase shift at the same energy. We consider the form factor (Yamaguchi 1954)

$$f_i(r) = \exp(-\beta_i r), \tag{30}$$

where $i = 1, 2$, and $g_i(k_0) \neq 0$ for $i = 1, 2$. The PEBS wavefunction at $k^2 = k_0^2$ is (Husain and Suhrabuddin 1980)

$$\psi_b(k_0, r) = N\{\exp(-\beta_1 r) - \exp(-\beta_2 r)\}, \tag{31}$$

with

$$\lambda_1 = 2\beta_1(\beta_1+\beta_2)(k_0^2+\beta_1^2)/(\beta_2-\beta_1), \tag{32}$$

$$\lambda_2 = 2\beta_2(\beta_1+\beta_2)(k_0^2+\beta_2^2)/(\beta_1-\beta_2). \tag{33}$$

The phase shift at the PEBS $k^2 = k_0^2$ is given by

$$k_0 \cot \delta(k_0) = (k_0^2 - \beta_1\beta_2)/(\beta_1+\beta_2). \tag{34}$$

Case 3

Here we consider a rank-three potential with the form factor

$$\begin{aligned} f_i(r) &= \exp(-\beta_i r), \qquad i = 1,2 \\ &= \left(\beta_i r - \frac{2\beta_i^2}{k_0^2+\beta_i^2}\right)\exp(-\beta_i r), \qquad i = 3, \end{aligned} \tag{35}$$

so that $g_i(k_0) \neq 0$ for $i = 1,2$ and $g_3(k_0) = 0$. From equations (5) and (10) the PEBS wavefunction is given by

$$\psi_b(k_0, r) = \sum_{i=1}^{2} \frac{c_i}{k_0^2+\beta_i^2}\exp(-\beta_i r) + \frac{c_3\beta_3 r}{k_0^2+\beta_3^2}\exp(-\beta_3 r), \tag{36}$$

with

$$\sum_{i=1}^{2} \frac{c_i}{k_0^2+\beta_i^2} = 0. \tag{37}$$

Moreover, the phase shift at $k^2 = k_0^2$ can be shown to be

$$\begin{aligned} k_0 \cot \delta(k_0) = {} & \frac{k_0^2 - \beta_1\beta_2}{\beta_1+\beta_2} \\ & + \frac{c_3}{c_1}\frac{\beta_3(k_0^2+\beta_1^2)(k_0^2+\beta_2^2)}{(k_0^2+\beta_3^2)\{(k_0^2+\beta_1^2)(\beta_2+\beta_3)^2 - (k_0^2+\beta_2^2)(\beta_1+\beta_3)^2\}}. \end{aligned} \tag{38}$$

Case 4

We consider the form factor

$$f_i(r) = \exp(-\beta_i r), \qquad i = 1,2,3, \tag{39}$$

so that $g_i(k_0) \neq 0$ for all i, and the PEBS wavefunction is

$$\psi_b(k_0, r) = \sum_{i=1}^{3} \frac{c_i}{k_0^2+\beta_i^2} \exp(-\beta_i r), \tag{40}$$

with

$$\sum_{i=1}^{3} \frac{c_i}{k_0^2+\beta_i^2} = 0. \tag{41}$$

The phase shift, in this case, is given by

$$k_0 \cot \delta(k_0) =$$

$$\frac{(k_0^2-\beta_1\beta_2)(k_0^2+\beta_3^2)^2(\beta_1-\beta_2)+(c_3/c_1)(k_0^2-\beta_2\beta_3)(k_0^2+\beta_1^2)^2(\beta_3-\beta_1)}{(k_0^2+\beta_3^2)^2(\beta_1^2-\beta_2^2)+(c_3/c_1)(k_0^2+\beta_1^2)^2(\beta_3^2-\beta_2^2)}. \tag{42}$$

Hence, we see that cases 2, 3 and 4 have given rise to both a PEBS as well as a scattering phase shift.

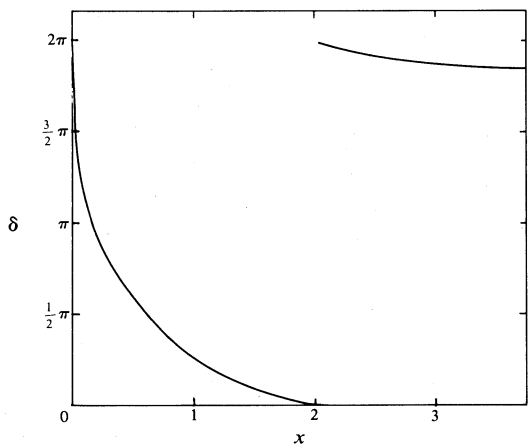

Fig. 1. Phase shift δ as a function of the energy x for case 1, with $n = 1$.

4. Sample Calculations

To get a clearer idea about the behaviour of the phase shift we perform some sample calculations for the two cases 1 and 2.

Case 1 ($n = 1$). If we put $x = k^2/\beta_1^2$ (with $x_0 = k_0^2/\beta_1^2$) then we can write

$$\tan \delta = -\frac{(x-x_0)^2 16x^{\frac{1}{2}}/(x-x_0)}{(x_0-1)(x+1)^3+2(x+1)^2(x_0+1)-8(x-x_0)(x-1)}.$$

To determine x_0 we solve equation (27) to get

$$x_0 = \tfrac{1}{2}[(\mu-2)\pm\{\mu(\mu-6)\}^{\frac{1}{2}}],$$

where $\mu = \frac{1}{4}\lambda_1 \beta_1^3$. If we choose $\mu = 6$ we get $x_0 = 2$; the corresponding phase shift is shown in Fig. 1.

Case 2. If we take $\beta_2 = 2\beta_1$, then

$$\tan \delta(k_0) = 3x_0^{\frac{1}{2}}/(x_0-2).$$

Moreover, if $\lambda_2 = 4\lambda_1$, we get $x_0 = 2$ and the resulting phase shift is equal to $\frac{1}{2}\pi$.

5. Conclusions

For a certain class of separable potentials [with $g_i(k_0) = 0$] the PEBS can be interpreted as a zero-width resonance, while for potentials satisfying the condition that not all $g_i(k_0)$ are zero and linearly dependent, PEBS and scattering can occur at the same energy. In addition, we note that for a rank-n potential, we have $n+1$ equations relating the $2n-1$ parameters λ_i $(i = 1, 2, \ldots, n)$ and c_i $(i = 1, 2, \ldots, n-1)$ and both the PEBS and the scattering phase shift have $n-2$ parameters. This result is quite clear from the cases studied. From these arguments, it is obvious that the interpretation of PEBS as a zero-width resonance does not hold in general and a different interpretation is necessary.

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Manuscript received 21 August 1984, accepted 18 March 1985