

POSITIVE-ENERGY BOUND STATES IN QUANTUM MECHANICS

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Conditions are given under which the wave functions of a one-particle Schrödinger equation at points of a positive discrete spectrum superposed on the continuous spectrum have the property of quadratic integrability; this allows us to put this spectrum in correspondence with bound states with positive energy. By means of separable potentials examples are constructed of attractive and repulsive interactions which give rise to positive discrete spectra. The nature of the scattering amplitude and of the wave function at a point of this spectrum is studied. The differential cross section for scattering by a positive discrete level is a characteristic two-hump curve. If a bound state with positive energy plays the role of a virtual state, the cross section is described by the Breit-Wigner formula. This allows us to draw a parallel between different quasiparticle models and positive energy levels. A treatment of these levels as states of unstable equilibrium of a quantum-mechanical system is proposed.

UP to the present time the most fruitful method of approximate solution of many-particle problems has been the use of effective one-particle models. Important examples are the concepts of the selfconsistent field and of quasiparticles in solid-state theory and in atomic and nuclear physics, the quasipotential approach in field theory, and so on. In all of these cases one often has to solve the one-particle Schrödinger equation for the radial wave function:

$$H_l R_l(k, r) = -\frac{\partial^2}{\partial r^2} R_l(k, r) + \frac{l(l+1)}{r^2} R_l(k, r) + V_l R_l(k, r) = k^2 R_l(k, r), \quad (1)$$

where the interaction operator is in general nonlocal and can usually be represented in the following form:

$$V_l R_l = g \int_0^\infty K_l(r, r') R_l(k, r') dr'. \quad (2)$$

We consider a Hermitian Hamiltonian, which means that $K_l^*(r, r') = K_l(r', r)$, and we shall assume that the kernel $K_l(r, r')$ satisfies the relation

$$\int_0^\infty \int_0^\infty \frac{\sqrt{rr'}}{1 + \sqrt{rr'}} K_l(r, r') \mu(r) \nu(r') dr dr' < \infty, \quad (3)$$

where $\mu(r)$ and $\nu(r)$ are arbitrary bounded functions.

For scattering problems one needs continuous solutions of (1) with the required asymptotic behavior for positive k^2 (continuous spectrum), and for the description of bound states one uses continuous quadratically integrable solutions for a discrete set of negative values of k^2 (discrete spectrum). In principle the Hamiltonian H can also have a positive discrete spectrum superposed on the continuous spectrum, but so far as we know there have been no definite statements in the literature as to what the nature of the interaction V must be for this to occur.

It has been shown in^[1,2] that even under broader assumptions about the form of the Hamiltonian than indicated in Eqs. (1)–(3) the scattering amplitude is bounded at points of the positive discrete spectrum (PPDS), and one of the solutions of the Schrödinger equation is a wave function which vanishes at infinity and is peculiarly suited to describe a bound state of positive energy

(BSPE). The question arises as to whether the BSPE is a mathematical abstraction—that is, whether the BSPE has a physical meaning and can be observed experimentally in some other way than through a zero value of the scattering amplitude, since this last also occurs in the Ramsauer-Townsend effect^[3] for sufficiently strong attractive potentials.

We note here the following fact. The theory of the activated complex in quantum chemistry, the concept of the compound nucleus in nuclear physics, and various theories of quasiparticles, often appeal in the last analysis to the idea that a system of a large number of particles can be in an “almost stationary” state with a positive energy. In S-matrix language, as is well known, such states correspond to poles on a nonphysical sheet of complex values of k , near the real axis. It is the fact that $\text{Im } k \neq 0$ that leads to the finiteness of the lifetime of the “almost stationary” states.

In the framework of the one-particle approach of Eqs. (1) and (2), in the present paper we propose a treatment of BSPE as quasi-particles of the type of an activated complex or compound nucleus. The poles of the S matrix then “slide,” as it were, onto the real axis of the k plane (for physical l), thus leading to the formation of stationary BSPE. This picture will be confirmed by the fact that a Hamiltonian which differs by only a small term from the Hamiltonian with PPDS produces near the BSPE a sharp maximum of the scattering cross section, of the type of a Breit-Wigner resonance. Nonlocal separable potentials will be used to construct examples of interaction operators which form BSPE; the special features of these operators and of the wave functions of the BSPE will be studied.

INTERACTIONS WHICH LEAD TO THE APPEARANCE OF BOUND STATES IN THE SPECTRUM OF POSITIVE ENERGIES

We can write Eqs. (1) and (2), together with the boundary conditions

$$R_l(k, r) \rightarrow r j_l(kr) + i^{-l} A_l(k) e^{ihr}, \quad r \rightarrow \infty$$

in the equivalent form of the integral equation

$$R_l(k, r) = r j_l(kr) - g \int_0^\infty R_l(k, x) dx \int_0^\infty ikrx' j_l(kr_{<}) h_l^{(1)}(kx_{>}) K_l(x', x) dx', \tag{4}$$

where $j_l(z)$ and $h_l^{(1)}(z)$ are the usual notations for spherical Bessel functions. At PPDS there are nontrivial solutions of the homogeneous integral equation

$$\rho_l^n(k, r) = -g \int_0^\infty \rho_l^n(k, x) dx \int_0^\infty ikrx' j_l(kr_{<}) h_l^{(1)}(kx_{>}) K_l(x', x) dx', \tag{5}$$

but by using a method of proof due to Fadeev^[4] it is not hard to show that the original equation (4) is soluble and that the solution consists of a term $r j_l(kr)$ and a quite definite linear combination of solutions of Eq. (5). The functions $\rho_l^n(k, r)$ vanish at infinity and satisfy the relation

$$\int_0^\infty kr j_l(kr) dr \int_0^\infty K_l(r, x) \rho_l^n(k, x) dx = 0. \tag{6}$$

If an inequality stronger than (3), namely

$$\int_0^\infty \int_0^\infty \sqrt{rr'} (1 + \sqrt{rr'}) \mu(r) \nu(r') K_l(r, r') dr dr' < \infty, \tag{7}$$

is satisfied, then the eigenfunctions $\rho_l^n(k, r)$ of the BSPE belong to $L_2(0, \infty)$ and consequently satisfy all of the requirements for wave functions of bound states in quantum mechanics. Since $\rho_l^n(k, \infty) = 0$, the asymptotic behavior of $R_l(k, r)$ is determined only by the free term $r j_l(kr)$, and there is no scattering at a PPDS.

We can write Eq. (5) together with the condition (6) in the form

$$\rho_l^n(k, r) = g i k \int_r^\infty r x [j_l(kx) h_l^{(1)}(kr) - j_l(kr) h_l^{(1)}(kx)] \int_0^\infty K_l(x, y) \rho_l^n(k, y) dy. \tag{8}$$

In the special case of a local potential $K_l(x, y) = V(x)\delta(x - y)$ the integral equation (8) contains a Volterra kernel, and consequently has no solution which is not identically zero. This is the well known result (cf., e.g.,^[5]) that there is no positive discrete spectrum for a central local potential under the conditions

$$V(x) = o(x^{-1-\epsilon}), \quad V(x) = o(x^{-2+\delta}); \quad \epsilon, \delta > 0.$$

It is shown in^[6] that there is also no discrete spectrum of positive energies in the case of a noncentral potential $\mathcal{V}(x)$ which satisfies the estimate

$$\int_{R_0}^\infty \sup_{|x|=r} |\mathcal{V}(x)| dr < \infty, \quad R_0 > 0.$$

Let us take as the interaction the nonlocal separable potential

$$K_l(x, y) = \frac{4\pi}{2l+1} \sum_{m=1}^{N_l} \beta_m^l g_m^l f_m^l(x) [f_m^l(y)]^*, \tag{9}$$

with $\beta_m^l = \pm 1$, $g_m^l > 0$,

$$f_m^l(r) = o(r^{-3/2+\delta}), \quad f_m^l(r) = o(r^{-1-\epsilon}); \quad \epsilon, \delta > 0. \tag{10}$$

In this case we can write an explicit expression for the scattering amplitude^[7]

$$A_l(k) = 2i \operatorname{Im} [D_l(k)] / D_l(k), \tag{11}$$

where

$$D_l(k) = \det_{N_l} \left[\delta_{ij} - \frac{4g_j^l \beta_j^l}{2l+1} P \int_{-\infty}^\infty \frac{B_i^l(q) \bar{B}_j^l(q)}{q^2 - k^2} dq + \frac{4\pi i}{2l+1} g_j^l \beta_j^l \frac{B_i^l(k) \bar{B}_j^l(k)}{k} \right], \tag{12}$$

$$B_j^l(k) = i^{-l} \int_0^\infty kr j_l(kr) f_j^l(r) dr$$

(P indicates the principal value of the integral).

For simplicity let us consider the s wave. Then Eq. (8) can be written in the form

$$\rho_0(r) = - \int_r^\infty \frac{\sin k(r-x)}{k} dx \int_0^\infty K_0(x, y) \rho_0(y) dy, \tag{13}$$

and the condition (6) has the quite intuitive meaning

$$\rho_0(0) = 0. \tag{14}$$

In the special case $l = 0$, $N_0 = 1$ we have (dropping the indices)

$$A(k) = \frac{8\pi i \beta g}{k} |B(k)|^2 \left[1 - 4\beta g P \int_{-\infty}^\infty |B(q)|^2 \frac{dq}{q^2 - k^2} + \frac{4\pi i \beta g}{k} |B(k)|^2 \right]^{-1}, \tag{15}$$

$$B(k) = \int_0^\infty f(r) \sin kr dr.$$

The condition for solubility of Eq. (5), or, what is the same thing, (8), is the vanishing of the Fredholm determinant, i.e., in the present case

$$D_l(k) = 0, \tag{16}$$

or in more concrete form, in view of (15),

$$1 - 4\beta g P \int_{-\infty}^\infty \frac{|B(q)|^2}{q^2 - k_0^2} dq + 4\pi i \beta g \frac{|B(k_0)|^2}{k_0} = 0. \tag{17}$$

From this we get a necessary condition for the formation of a BSPE:

$$B(k_0) = 0, \tag{18}$$

which imposes a definite restriction on the form of the functions $f(r)$ which describe the interaction operator. If (18) is satisfied, then by the choice of the sign β and the size of the coupling constant g one can always satisfy the relation (17). The only exceptions are the extremely rare cases in which (18) necessarily brings with it the equation

$$\int_{-\infty}^\infty |B(q)|^2 \frac{dq}{q^2 - k_0^2} = 0. \tag{19}$$

The spectrum of eigenvalues corresponding to (17) is actually discrete and consists of a finite number of points, as is directly verified without difficulty if the function $|B(q)|^2 = o(q)$ for $q \rightarrow \infty$ and has no nonintegrable singularities. In fact, let us consider a point of the spectrum

$$B(k_0) = 0, \tag{20}$$

$$u(k_0) = 1 - 8\beta g \int_0^\infty |B(q)|^2 (q^2 - k_0^2)^{-1} dq = 0.$$

Let us assume that for $\gamma(k_0) > 0$ we have $B(k_1) = B(k_0 + \gamma) = 0$ (the necessary condition is satisfied); then

$$u(k_1) = u(k_1) - u(k_0) = -8\beta g \int_0^{\infty} \frac{|B(q)|^2}{(q^2 - k_0^2)(q^2 - k_1^2)} dq.$$

The integrand is negative only in the interval $q \in (k_0, k_0 + \gamma)$, and for sufficiently small but finite γ it is obvious that everywhere in the interval $k \in (k_0, k_0 + \gamma)$ we have $u(k) \neq 0$. Noting that for sufficiently large finite $K \in (k_0, \infty)$ the integral in (20) becomes less than unity and that a uniform estimate for $\gamma(k)$ can be chosen in the interval $k \in (0, K)$, we conclude that the set of points at which (17) can be solved is finite. A general theorem stating that the set of PPDS is finite under other conditions is proved in^[4].

We shall consider several examples.

$$1. f(r) = e^{-\gamma r}, \quad \gamma > 0. \quad (21)$$

By means of (15) we find $B(k) = k/(\gamma^2 + k^2)$. For $k > 0$ the condition (18) cannot be satisfied; there can be no PPDS in this case.

$$2. f(r) = \begin{cases} 1, & 0 \leq r \leq a; \\ 0, & r > a \end{cases}; \quad (22)$$

$B(k) = (1 - \cos ka)/k$. Obviously $B(k_n) = 0$ for

$$k_n = 2\pi n/a, \quad n = 0, 1, 2, \dots \quad (23)$$

Equation (17) takes the form

$$1 - 4\pi a \beta g k^{-2} = 0, \quad (24)$$

and can be satisfied only in the case $\beta = 1$, i.e., only in the case of a repulsive interaction.

$$3. f(r) = (\gamma^2 + k_0^2)e^{-\gamma r} - (\delta^2 + k_0^2)e^{-\delta r}. \quad (25)$$

Here $B(k) = 0$ at a single point $k = k_0$, and (17) leads to the equation

$$1 - 4\pi g \beta \frac{(\gamma - \delta)^2(k_0^2 - \gamma\delta)}{\gamma\delta(\gamma + \delta)(k_0^2 + \gamma^2)(k_0^2 + \delta^2)} = 0,$$

which for a sufficiently large coupling constant has solutions for both repulsive and attractive potentials.

It is not hard to show that in the last example there can be values of the parameters for which the condition for the formation of bound states is satisfied simultaneously for both positive and negative energies. The examples considered give a single PPDS, but it is easy to assume functions $f(r)$ such that there will be as many BSPE as one wishes. In this connection it is important to point out that the potentials we have given can form only one ordinary level each with negative energy^[8,9] (the case of attractive interaction is of course that with $\beta = -1$).

It is interesting to find out the shape of the eigenfunctions of the positive discrete spectrum. For the Yamaguchi nonlocal potential^[10] with functions of the form (22) we find $\rho(r)$ by means of Eq. (13). Writing

$$\int_0^{\infty} f(y)\rho(y)dy = C, \quad (26)$$

we get

$$\rho(r) = -4\pi C g \beta k^{-2} \begin{cases} \cos k(r-a) - 1, & 0 \leq r \leq a \\ 0, & r \geq a \end{cases}.$$

From (14) we find the condition (23) and

$$\rho(r) = 8\pi g \beta C k_n^{-2} \begin{cases} \sin^2(k_n r/2), & 0 \leq r \leq a \\ 0, & r \geq a \end{cases}$$

Comparing this expression with (26), we easily arrive at the previously obtained relation (24). The eigenfunction $\rho(r)$ can obviously be normalized. In the given special case it is finite.

In concluding this section let us study the BSPE for a somewhat more complicated kernel $K(x, y)$, namely for the sum of a local potential $V(x) = \delta(x-a)$ and a Yamaguchi potential:

$$K(x, y) = \frac{g_1}{a} \delta(x-a)\delta(x-y) + \frac{2g_2}{b^3} e^{-(x+y)/b}. \quad (27)$$

In order not to introduce β_1 and β_2 , we shall suppose that the coupling constants g_1 and g_2 can have either sign. The normalization of the potentials is chosen in the following way: for $g_1 = 0$ and $g_2 \leq -1$ there is an ordinary level; the same is true for $g_2 = 0$, $g_1 \leq -1$. The local potential $V(x)$ considered here has the unique property that it can be put in the form of a nonlocal separable potential

$$K'(x, y) = \delta(x-a)\delta(x-y) = \delta(x-a)\delta(y-a),$$

and we could use the general expression (12), but it is more convenient to go back again to (13). We note that the potentials which compose the expression (27) cannot separately form BSPE: for the second this has been shown earlier, and the first is a local potential [if we regard it as a nonlocal separable potential, then at points where $B(k) = 0$ we arrive at Eq. (19)].

Substituting (27) in (13) and using notations of the form (26), we get expressions for the eigenfunction of a BSPE:

$$\rho(r) = -\frac{2g_2 C}{b(1+k^2 b^2)} e^{-r/b} - \frac{g_1}{ka} \rho(a) \begin{cases} \sin k(r-a), & 0 \leq r \leq a \\ 0, & r \geq a \end{cases}. \quad (28)$$

From this we have

$$\rho(a) = -\frac{2g_2 C}{b(1+k^2 b^2)} e^{-a/b}.$$

By means of (14) we arrive at the equation

$$g_1 \frac{\sin ka}{ka} e^{-a/b} + 1 = 0, \quad (29)$$

and after substituting $\rho(r)$ in (26) we find a second relation:

$$\frac{g_2}{1+k^2 b^2} \left\{ 1 + \frac{2}{(1+k^2 b^2) \sin ka} [kb(\cos ka - e^{-a/b}) - \sin ka] \right\} + 1 = 0. \quad (30)$$

The eigenfunction (28) falls off exponentially at infinity and can be normalized, and the system of equations (29) and (30) can almost always be solved for g_1 and g_2 . If, however, we regard (29) and (30) as equations for k for given g_1, g_2, a, b , it can be seen that the set of such solutions has zero measure.

It follows from (29) that the inequality $|g_1| \geq 1$ is necessary, i.e., that the local potential must be above a certain strength. For $b \gg a$ and $kb \ll 1$ it is not hard to show that $g_1 \approx -e^{-a/b} \approx -1$, $g_2 \approx -a/2b$: the nonlocal interaction term can be arbitrarily small, but then the energy of the bound state is close to zero and the interaction reduces to a pure attraction. For example, in the

case $ka = 3\pi/2$, $b = 2a$ the local potential is repulsive and the nonlocal potential is attractive: $g_1 \approx 8$, $g_2 \approx -100$. It is very easy to get the opposite situation $g_1 < 0$, $g_2 > 0$. Finally, taking as an example $\cos ka = e^{-a/b}$, $0 < kb < 1$, we find that both potentials are repulsive.

POSITIVE-ENERGY BOUND STATES AND RESONANCE SCATTERING

We have so far been mainly considering only the question of the legitimacy of the concept of BSPE in the one-particle problem from the mathematical side. It can already be said, however, that at a PPDS there is no scattering of the corresponding partial wave; the asymptotic form of the wave function is $rj_l(k_0r)$, and the amplitude $A_l(k_0) = 0$. Since in general this last equation does not hold for $k \neq k_0$, in the neighborhood of a PPDS $k = k_0$ the differential scattering cross section $\sigma_l(k) = \pi k^{-2} |A_l(k)|^2$ must follow a two-hump curve with a zero at the PPDS. It is shown in^[1,2] that $\sigma(k) = o(k - k_0)$ for $k \rightarrow k_0$, and in our case the cross section has a zero of at least the second degree at $k = k_0$. In the case of the nonlocal separable potential (9), (10) this result clearly follows when we use (11), (12). Using the Yamaguchi potential with the functions (22) under the condition (23) and with $n \geq 1$, we get from 15

$$A(k) \approx \frac{2i(1 - \cos ka)^2}{k^3 a (k_n^{-2} - k^2) + i(1 - \cos ka)^2}. \quad (31)$$

The relation (31) allows us to answer the question as to what the minimum degree of nonmonochromaticity of the beam of incident particles must be for it to be impossible to resolve the dip in the cross section at $k = k_0$. If we set

$$\sigma_{av}(k) = \frac{1}{2\Delta k} \int_{k-\Delta k}^{k+\Delta k} \sigma(k) dk,$$

the indicated condition is obviously satisfied by a value of Δk such that $d^2\sigma_{av}/dk^2|_{k=k_0} \leq 0$. From this we get the equation

$$\sigma'(k_0 + \Delta k_{min}) - \sigma'(k_0 - \Delta k_{min}) = 0,$$

and after substituting (31) and performing some manipulations we get $a\Delta k_{min} \approx \text{tg}(a\Delta k_{min}/2)$, and consequently

$$\Delta k_{min} \sim a^{-1}. \quad (32)$$

We can also arrive at the same relation when we study Yamaguchi potentials of different form. In spite of the dip at the point $k = k_0$ the unaveraged cross section in the neighborhood of the PPDS is characterized by a spike. The width of this spike is obviously roughly indicated by (32) also for the case of a general form of the interaction-operator kernel $K_l(x, y)$, a being given by the size of the region where the interaction is intense, that is, where $K_l(x, y)$ is large.

It is necessary to point out that it is in general rather rarely that all of the conditions for the appearance of a BSPE are realized. Negative levels necessarily appear when the coupling constant is sufficiently large, if the interaction is not purely repulsive. Here, however, we need, first, some special form of the functions that describe the interaction, for example (18) for the Yamaguchi potential, and in the general case the solubility in principle of Eq. (8), which does not depend

on the coupling constant. Secondly, the conditions for occurrence of a BSPE [cf. (11), (12)],

$$\text{Re } [D_l(k)] = 0, \quad \text{Im } [D_l(k)] = 0$$

are two equations for a single quantity k , even in cases in which the form of the functions $f_l^j(r)$ allows us to satisfy these equations separately.^j The same can be said also in the general case of $K_l(r, r')$.

Let us suppose that for a given form of the kernel $K_l(x, y)$ or for a given value of the coupling constant it is impossible for both the real and the imaginary parts of the function $D_l(k)$ to vanish simultaneously, so that no BSPE is formed. Suppose, however, that at the point where $\text{Re } [D_l(k_0)] = 0$ the quantity $\text{Im } [D_l(k_0)]$ is small. For simplicity we shall conduct the treatment with nonlocal separable potentials, although similar results can be regarded as characteristic for the nonlocal operator of the general form (2). In the case of a Yamaguchi potential which is of the form (22) near k_0 and satisfies (24), when we assume that (23) does not hold we get from (31) as the approximate result for the differential cross section the usual Breit-Wigner formula

$$\sigma(k) = \frac{\pi}{k^2} \frac{\Gamma^2}{(k^2 - k_0^2)^2 + \Gamma^2/4}, \quad \Gamma = \frac{2k_0}{a}(1 - \cos ka)^2. \quad (33)$$

The form of the interaction is here such as to allow the formation of a BSPE, and none has appeared only because of the unsuitable value of the coupling constant. In such situations when there is a certain change of the energy of the incident particles $\text{Im } [D_l(k)]$ and the cross section $\sigma_l(k)$ become zero, and because of this the Breit-Wigner maximum is asymmetrical; the sharper the maximum, the more marked is the asymmetry.

If we take a Yamaguchi potential of the form (21), we again get Eq. (33), where $\Gamma \approx 4\gamma k_0(k_0^2 + \gamma^2)/(3\gamma^2 - k_0^2)$. In the case in which $g \approx \gamma k_0/\pi$ and $\beta = -1$ (attraction), the inequality $k_0 \gg \gamma$ holds here. Then $\Gamma = -4\gamma k_0$ and (33) describes a rather sharp resonance, although, as was shown earlier, the nonlocal potential (21) in principle does not form any BSPE. In any given case the width of the resonance peak is determined by a relation of the form (32), but it is easy to assume more complicated functions $f(r)$ which produce much more sharply marked maxima in the cross section.

We note that $\text{Re } [D_l(k)]$ cannot always become zero, but if this quantity is small there will be resonance scattering described by relations somewhat different from (33). It is important to emphasize that resonance formulas of the form (33) must rather be the rule, and the form (31) the exception. In fact, however small the quantity $\text{Im } [D_l(k)]$ may be at the point k_0 where $\text{Re } [D_l(k_0)] = 0$, the scattering is described by the Breit-Wigner formula, and only at energies corresponding to PPDS will a relatively flat two-hump curve appear. This finds its expression in the fact that the dependence of $\sigma_l(k_0)$ on the coupling constant is almost everywhere given by the factor $4\pi/k^2$; only the PPDS are exceptional, and there $\sigma_l(k_0) = 0$.

It is not hard to see that the resonance formula (33) can be connected with a pole of the amplitude (31) in the lower half of the complex k plane; besides this, we can here propose a different intuitive interpretation of the resonances—the near approach to a virtual level with positive energy. Since PPDS are not associated with minimum values of the energy functional and are unsta-

ble with respect to small variations of the Hamiltonian, we can regard BSPE as states of unstable equilibrium of the quantum-mechanical system. The presence of a virtual level with positive energy leads to a great increase in the speed of a reaction, since it is well known that quantum-mechanical transitions occur more easily between states which are close together in energy.

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