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# Resonance states as solutions of the Schrödinger equation with a nonlocal boundary condition*

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Resonance states of a system consisting of a particle interacting with a finite-range potential are introduced in a novel way, independent of the notion of scattering. It is shown that a resonance wave function satisfies a certain nonlocal boundary condition on the surface that delimits the range of the potential. With a central potential our general boundary condition reduces to a set of local ones that are identical with those obtained previously by Humblet and Rosenfeld by different methods.

There exist several definitions of resonance parameters and resonance states of a system consisting of a particle interacting with a potential. Some of them are related to singularities of the scattering cross section, of a Green's function, or of the scattering matrix.[1] When the potential is spherically symmetric and of finite range, some of the definitions have been shown to be equivalent to a boundary-value formulation that involves the boundary values of the radial wave function of a resonance state and of its normal derivative on a spherical surface delimiting the domain throughout which the potential is effective.[2-4] This boundary-value formulation is a refinement of a procedure introduced by Kapur and Peierls in a well-known paper[5] dealing with the dispersion formula for nuclear reactions. All these definitions have one feature in common, namely that they introduce the resonance state as a kind of extrapolation or as a limit of scattering states. Mittleman[6] has stressed the desirability of defining resonance states without using a "preconceived notion" of its structure.

In a recent paper[7] we have reformulated in a novel way the problem of determining the scattering states and the bound states of a nonrelativistic particle interacting with a finite-range potential. We showed that such states are represented by solutions of the Schrödinger equation that satisfy a certain boundary condition, which is nonlocal in general, on the surface that delimits the effective range of the potential. In the present paper we use the same approach to introduce resonance states in a new way. Our definition of a resonance state will be seen to be entirely independent of the notion of scattering and applies to a particle interacting with any finite-range potential, central as well as noncentral ones. With a central potential our definition will be shown to reduce to the boundary-value formulation of Siegert,[2] Humblet,[3] and Humblet and Rosenfeld.[4]

Consider a particle of mass $m$ interacting with a finite-range potential $\mathcal{V}(\vec{r})$, which vanishes outside a volume $V$ bounded by a closed surface $S$. The time-independent part $\psi_E(\vec{r})$ of the wave function $\psi_E(\vec{r},t)=\psi_E(\vec{r})\exp(-iEt/\hbar)$ then satisfies, throughout the whole space, the time-independent Schrödinger equation

$$(\nabla^2+k^2)\psi_E(\vec{r})=U(\vec{r})\psi_E(\vec{r}), \tag{1}$$

where

$$k^2=\frac{2m}{\hbar^2}E \tag{2}$$

and

$$U(\vec{r})=\frac{2m}{\hbar^2}\,\mathcal{V}(\vec{r}). \tag{3}$$

We have shown in Ref. 7 by an elementary argument involving nothing more than the use of Green's theorem that the following four equations (not all independent of each other) are a necessary consequence of the fact that $\psi_E(\vec{r})$ satisfies the Schrödinger equation:

$$\psi_E(\vec{r}_<)=-\frac{1}{4\pi}\int_V\psi_E(\vec{r}\,')U(\vec{r}\,')G_E(\vec{r}_<,\vec{r}\,')d^3r'-\frac{1}{4\pi}\Sigma(\vec{r}_<), \tag{4}$$

$$0=\frac{1}{4\pi}\Sigma(\vec{r}_<)-\frac{1}{4\pi}\Sigma^{(\infty)}(\vec{r}_<), \tag{5}$$

$$\psi_E(\vec{r}_>)=\frac{1}{4\pi}\Sigma(\vec{r}_>)-\frac{1}{4\pi}\Sigma^{(\infty)}(\vec{r}_>), \tag{6}$$

$$0=-\frac{1}{4\pi}\int_V\psi_E(\vec{r}\,')U(\vec{r}\,')G(\vec{r}_>,\vec{r}\,')d^3r'-\frac{1}{4\pi}\Sigma(\vec{r}_>). \tag{7}$$

In these formulas $\vec{r}_<$ represents any point inside $V$, $\vec{r}_>$ represents any point outside $V$, and

$$G_E(\vec{r},\vec{r}\,')=\frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|}\,, \tag{8}$$

$$\Sigma(\vec{r})=\int_S\left[\psi_E(\vec{r}\,')\,\frac{\partial G_E(\vec{r},\vec{r}\,')}{\partial n}-G_E(\vec{r},\vec{r}\,')\,\frac{\partial\psi(\vec{r}\,')}{\partial n}\right]dS\,, \tag{9}$$

$$\Sigma^{(\infty)}(\vec{r})=\lim_{R\to\infty}\int_{S_R}\left[\psi_E(\vec{r}\,')\,\frac{\partial G_E(\vec{r},\vec{r}\,')}{\partial n_R}-G_E(\vec{r},\vec{r}\,')\,\frac{\partial\psi(\vec{r}\,')}{\partial n_R}\right]dS\,, \tag{10}$$

with $S_R$ in (10) denoting a sphere of radius $R$ centered at any convenient point in the region $V$. Further, $\partial/\partial n$ in Eq. (9) denotes differentiation along the outward normal to $S$ and $\partial/\partial n_R$ in (10) denotes differentiation along the outward radial direction. In Ref. 7, where the energy $E$ was assumed to be real, $k$ in Eq. (8) represents the positive root of the right-hand side of Eq. (2) when $E>0$ and the root with positive imaginary part when $E<0$. However, the relations (4)–(7) retain their validity whether or not $E$ is real. When $E$ is complex we interpret $k$ in Eq. (8) as that root of the expression on the right-hand side of (2) that has a non-negative real part.

By analogy with classical electromagnetic theory we may define *natural modes* of our system (particle + potential) as those solutions of the Schrödinger equation that are well behaved throughout the whole space and that are outgoing at infinity. The natural modes may be either radiative (in which case $E$ is complex) or nonradiative (in which case $E$ is real). We will identify the radiative natural modes with *resonances*[8] and the nonradiative ones with *bound states* of the system. Let us consider the implications of Eqs. (4)–(7) when $\psi_E(\vec{r})$ is a natural mode.

The requirement that natural modes are solutions of the Schrödinger equation that are outgoing at infinity implies that $\Sigma^{(\infty)}(\vec{r})$, defined by Eq. (10), identically vanishes (cf. Ref. 7), i.e., that for all points $\vec{r}$

$$\Sigma^{(\infty)}(\vec{r})=0\,. \tag{11}$$

The relation (5) then reduces to

$$\Sigma(\vec{r}_<)=0\,, \tag{12a}$$

or more explicitly

$$\int_S\left[\psi_E(\vec{r}\,')\,\frac{\partial G_E(\vec{r}_<,\vec{r}\,')}{\partial n}-G_E(\vec{r}_<,\vec{r}\,')\,\frac{\partial\psi_E(\vec{r}\,')}{\partial n}\right]dS=0\,. \tag{12b}$$

We interpret the formula (12b), which must be satisfied for every point $\vec{r}_<$ situated in the volume $V$, as a *boundary condition for natural modes*. More precisely *the natural modes of our system are those well-behaved solutions of the Schrödinger equation that satisfy the constraint expressed by Eq. (12b) for every point* $\vec{r}_<$ *in the volume* $V$. For similar reasons that we gave in Ref. 7 in connection with a boundary condition of this kind, we may refer to Eq. (12b) as the *extinction theorem for natural modes*.

We will see shortly that the Schrödinger equation (1) can be solved subject to our (nonlocal) boundary condition (12b) only for certain values of $E$, i.e., we are dealing with an *eigenvalue problem*. According to our classification, those eigenvalues $E$ that are real are associated with bound states and those that are complex are associated with resonances. Since we have already discussed bound states from the present standpoint in Ref. 7 we may from now on confine our attention to resonance states, though our main results apply to both cases.

Our boundary condition (12b) may be used to solve the interior problem, i.e., to determine the (unnormalized) wave functions at all points $\vec{r}_<$ in $V$. The solution will provide, as a by-product, the complex energies of the resonance states.[9] The solution to the "exterior problem," i.e., determination of the wave function at points $\vec{r}_>$ outside $V$ may then be written down at once in a closed form by the use of Eq. (6), as simplified by the requirement (11)

$$\psi_E(\vec{r}_>)=\frac{1}{4\pi}\,\Sigma(\vec{r}_>)\,, \tag{13a}$$

or, more explicitly,

$$\psi_E(\vec{r}_>)=\frac{1}{4\pi}\int_S\left[\psi_E(\vec{r}\,')\,\frac{\partial G_E(\vec{r}_>,\vec{r}\,')}{\partial n}-G_E(\vec{r}_>,\vec{r}\,')\,\frac{\partial\psi_E(\vec{r}\,')}{\partial n}\right]dS\,. \tag{13b}$$

It is clear that the boundary values $\psi_E(\vec{r}\,')$ and $\partial\psi_E(\vec{r}\,')/\partial n$ on $S$ that enter the integrand on the right-hand side of (13b) may be obtained from the solution of the interior problem by letting $\vec{r}_<$ move to the boundary surface $S$.

Up to now we have only made use of two of our four relations (4)–(7), namely of Eqs. (5) and (6) and we have seen that, together with the time-independent Schrödinger equation (1), they provide the complete specification of the (unnormalized) wave functions of resonance states and of bound states, as defined in the present paper. We will now make use of some of the implications of Eqs. (5) and (6) in the remaining two relations (4) and (7) and will see that they reduce to a more familiar pair of equations that our wave functions must satisfy. On substituting from (12a) into (4) we obtain the equation

$$\psi_E(\vec{r}_<) = -\frac{1}{4\pi}\int_V \psi_E(\vec{r}')U(\vec{r}')G_E(\vec{r}_<, \vec{r}')d^3r' , \qquad (14)$$

and on substituting from (13a) into (7) we find that

$$\psi_E(\vec{r}_>) = -\frac{1}{4\pi}\int_V \psi_E(\vec{r}')U(\vec{r}')G_E(\vec{r}_>, \vec{r}')d^3r' . \qquad (15)$$

These two formulas will be recognized as the "interior" and the "exterior" forms of the equation to which the integral equation of the conventional theory of nonrelativistic potential scattering reduces in the absence of the incoming wave.[10] This is as it should be, since the property of "no incoming wave" is considered to be characteristic of resonance states and of bound states.[11]

We will next show that when the particle interacts with a central potential $[U(\vec{r}) \equiv U(r), r = |\vec{r}|]$ which vanishes outside a sphere of radius $r = a$, our nonlocal boundary condition (12b) reduces to a set of local boundary conditions previously obtained for this case by other authors.

With a central potential the wave function $\psi(\vec{r}_<)$ may be expanded in a series of partial waves[12]

$$\psi_E(\vec{r}_<) = \sum_{l=0}^{\infty} \chi_l(\vec{r}_<; k)P_l(\cos\theta) , \qquad (16)$$

where

$$\chi_l(r; k) = \frac{u_l(r;k)}{r} , \qquad (17)$$

and $u_l(r;k)$ is a regular solution of the radial equation

$$\left[\frac{d^2}{dr^2} + \left(\epsilon - U(r) - \frac{l(l+1)}{r^2}\right)\right]u_l(r;k) = 0 \qquad (18)$$

$$(l = 0, 1, 2, \ldots)$$

$(\epsilon = k^2 = 2mE/\hbar)$. The Green's function may be expanded as (cf. Ref. 13)

$$G_E(\vec{r}_<, \vec{r}') = k \sum_{l=0}^{\infty} (2l+1)j_l(kr_<)\hbar_l^{(+)}(kr') \times P_l(\cos\Theta) , \qquad (19)$$

valid with $r_< < r'$, where $h_l^{(+)}$ is the spherical Hankel function of the first kind and order $l$ and $\Theta$ is the angle between the directions of the vectors $\vec{r}_<$ and $\vec{r}'$. If we now substitute from (16) and (19) into our boundary condition (12b) we find (cf. Appendix A of Ref. 7) that it implies that

$$\sum_{l=0}^{\infty} \alpha_l j_l(kr_<)P_l(\cos\theta) = 0 , \qquad (20)$$

where

$$\alpha_l = (ka)^2[\phi_l(a;k)h_l^{(+)\prime}(ka) - (1/k)\phi_l'(a;k)h_l^{(+)}(ka)] , \qquad (21)$$

the prime denoting differentiation with respect to the radial argument. Because of the orthogonality of the Legendre polynomials $P_l(\cos\theta)$, it follows from (20) that we must have $\alpha_l = 0$ for all $l$. If we express these conditions in terms of the functions $u_l(r;k)$, they are seen to imply that

$$[h_l^{(+)\prime}(ka) + (1/ka)h_l^{(+)}(ka)]u_l(a;k) - (1/k)h_l^{(+)}(ka)u_l'(a;k) = 0 \qquad (l = 0, 1, 2, \ldots) . \qquad (22)$$

Equation (22) is a set of (local) boundary conditions on the radial wave functions $u_l$ of the resonance states. These boundary condtions can only be satisfied for certain values of $k$ [that then give the complex resonance energies via the relation (2)], so that we are dealing with an eigenvalue problem. More specifically, the eigenvalue problem is that of determining, for each $l$, the solutions of Eq. (18) which are well behaved throughout the range $0 \leq r \leq a$ and which satisfy the boundary conditions (22) when $r = a$. These solutions must, of course, also satisfy the usual boundary conditions $u_l(0;k) = 0$ $(l = 0, 1, 2, \ldots)$ when $r = 0$.

The set of equations (22) is, except for notation, precisely the set of boundary conditions for the radial wave functions of resonance states obtained previously by Humblet [Ref. 3, Eq. (11.1)] and Humblet and Rosenfeld [Ref. 4, Eq. (1.33)] by entirely different methods. For the special case when $l = 0$ the boundary condition was derived eariler by Siegert[2] and it is also implicit in the well-known derivation of Kapur and Peierls,[5] of the dispersion formula for nuclear reactions, by the technique of perturbation of boundary conditions.

We may summarize our analysis by saying that we derived, on the basis of a new definition of a resonance state (of a system consisting of a particle interacting with a finite-range potential) a general boundary condition that the wave function of such a state must satisfy. Our definition of a resonance state is independent of the notion of scattering, and our derivation of the boundary condition is entirely based on two identities that follow from the Schrödinger equation. We also showed that our definition of a resonance implies that the wave function of such a state is a solution of the homogeneous integral equation to which the usual integral equation of potential scattering reduces in the absence of any incoming wave. With a central potential our nonlocal boundary condition reduces to a set of local ones for the radial wave functions of the resonance states, which are in agreement with those obtained previously for this special case by other techniques.

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[8] The resonances so defined may be subdivided into "proper resonances" and "virtual states," according to whether the real part of $E$ is positive or negative.

[9] As is customary, we speak of a solution of the Schrödinger equation as representing a state of the system, even when the energy eigenvalue is complex. However, such language must be used with caution [cf. H. M. Nussenzveig, *Causality and Dispersion Relations* (Academic, New York, 1972), p. 160].

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[12] A. Messiah, *Quantum Mechanics* (North-Holland, Amsterdam, 1961), Vol. 1, p. 385.

[13] J. D. Jackson, *Classical Electrodynamics* (Wiley, New York, 1962), p. 541 and p. 68. The function $h_l^{(1)}$ of that reference corresponds to $-ih_l^{(+)}$ of the present paper.