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Properties of Resonance Wave Functions*

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Resonances of quantum systems are associated with poles of the Green's function which occur at complex energies. The wave functions corresponding to such poles increase exponentially at large distances and so are very badly divergent. Nevertheless, these resonance wave functions have useful properties which can be exploited in cases where only their behavior at small distances is relevant. In this paper we construct and study such resonance wave functions for several illustrative quantum systems of theoretical interest. It is shown that the wave functions may be considered *renormalized* in a sense analogous to that of quantum field theory. However, the renormalization which occurs here is entirely automatic and the theory has neither *ad hoc* procedures nor infinite quantities. In addition to other results, we obtain a representation of the Green's function in terms of the resonance wave functions; this representation appears likely to be useful because it has an energy dependence that is especially simple.

I. INTRODUCTION

There is an enormous literature dealing with resonances of quantum systems, and usually the resonances are described via continuum (scattering) theory. However, this description seems to miss the most striking characteristic of a narrow resonance. A narrow scattering resonance is always associated with a long-lived decaying state, a state which physically resembles a true discrete eigenstate. The resemblance is especially strong when the lifetime is long. Obviously one should choose a description in which this resemblance is clearly exhibited and emphasized. To this end it appears profitable to introduce and study a set of resonance wave functions.

With these wave functions (one for each resonance) we can see the general physical similarity of resonance states and bound states, and also the specific technical differences. The resonance wave functions will necessarily have some abnormal or anomalous properties which reflect the time dependence of the decaying state.

In this paper we have constructed and studied resonance wave functions for several illustrative models of theoretical interest. The definition of these wave functions was suggested by a perturbation theory of decaying states.[1-4] The most stubborn abnormality is their refusal to be normalized or mutually orthogonal. In fact we shall find that the resonance wave functions are *renormalized* in a sense described below. However, this renormalization is entirely automatic (there is no *ad hoc* step in the mathematics) and the theory has no infinite quantities. Actually, both renormalized and also nonrenormalized perturbation theories exist and are correct; they differ because they calculate different quantities. The situation is thus much simpler than the renormalization of quantum field theories.

The main object of this paper is then to identify and interpret the anomalous normalization properties of the resonance wave functions. The normalization is not at all arbitrary, but proves to have a definite physical significance. This interpretation is given in Sec. II.

Sections III and IV contain detailed discussions of two specific cases. The model of Sec. III is a two-level system which can decay into a continuum. Section IV deals with potential scattering resonances, which occur when the potential has a high barrier, so that a particle trapped inside can slowly tunnel out (e.g., the Gamow theory of α decay). The models warn us about certain special phenomena and give some substance to the general operator theory. The models are also used as examples to suggest typical analytic properties of resonance systems.

These model systems are both one-particle systems. The particle can be in either of two "channels," an *outer* channel with a continuous density of states (e.g., a free particle) and an *inner* channel, which originally had discrete states (the discrete states have become resonances because of the coupling between channels). In the two-level model of Sec. III, the inner channel is a two-component space based on the two original states. In the case of potential scattering, the inner channel is the interior of a fixed sphere.

The resonance wave functions of this paper are defined in terms of the *residues* of a Green's function $G(E)$ at its complex poles E_n. This choice of resonance parameters follows the resonance theory of Siegert, of Humblet and Rosenfeld, and others.[5–7] In Sec. II, we show the simple connection between these resonance wave functions and the *eigenfunctions* $\Phi_s(E)$ of the Green's function. For the potential scattering case, the latter functions correspond to the alternative resonance theory of Kapur and Peierls.[8,9]

The resonance energies E_n are defined as the exact complex poles of an appropriate Green's function $G(E)$. This Green's function is the projection of the total Green's function onto the inner channel; for the systems considered here it is a single-valued function of $k=E^{1/2}$. The resonance poles E_n normally occur on a second sheet of the energy plane (i.e., in the lower-half k plane); we denote them by $E_n=K_n^2$.

The resonance wave functions will be defined in terms of the residues of $G(k)$ at its poles:

$$|\phi_n\rangle\langle\tilde{\phi}_n| \equiv \lim_{k\to K_n}(k^2-K_n^2)G(k)\ . \tag{1.1}$$

[It will be shown that the residue factors in Sec. II. In Eq. (1.1), $|\phi_n\rangle$ is the nth resonance wave function, and $\langle\tilde{\phi}_n|$ is a related dual function (it is not simply the complex conjugate of $|\phi_n\rangle$). Detailed relations between $|\phi_n\rangle$ and $\langle\tilde{\phi}_n|$ are given below.]

The reader will note that a specific normalization is already *fixed* by this equation, i.e.,

$$\langle\tilde{\phi}_n|\phi_n\rangle = Z_n\ , \tag{1.2}$$

where the normalization factor Z_n is determined by Eq. (1.1) and is *not* necessarily unity (or even real). The inner product of Eq. (1.2) is taken over the inner channel (if it ran over the outer channel too, we should have $Z_n=\infty$). The fixed value of Z_n represents the most immediate anomalous property associated with $|\phi_n\rangle$. In Sec. II it is shown that the value of Z_n is determined by the energy dependence of an effective Hamiltonian $H_{\mathrm{eff}}(E)$ which governs the inner channel. The normalization of Eq. (1.2) is not at all arbitrary but has a definite physical significance.

When the system is perturbed, its complex energy eigenvalue changes from the original value E_n^0. In general, both the real and imaginary parts of E_n^0 change. Let us assume that the perturbation operator V acts only in the inner channel; in that case the perturbed complex energy will be seen to be

$$E_n = E_n^0 + \langle\tilde{\phi}_n^0|V|\phi_n^0\rangle + O(V^2)\ . \tag{1.3}$$

Now the surprising point is that this formula is correct as written, *with* the anomalous normalization of Eq. (1.2). The perturbation formula collects together changes in the line center and linewidth into a single expression. It shows the true significance of ϕ_n, for it shows that ϕ_n determines the dynamical response of the resonance state to an external perturbation. A complete perturbation theory of this type, containing the terms higher order in V, was constructed by More[4]; the first-order theory of Eq. (1.3) had been established earlier by Humblet[1] and Zel'dovich[2] for the case of potential scattering.

Often it is possible to write the Green's function in terms of its residues by virtue of the Mittag-Leffler expansion theorem. This gives an explicit representation of $G(k)$:

$$G(k)=\sum_n \frac{|\phi_n\rangle\langle\tilde{\phi}_n|}{2K_n(k-K_n)}\ . \tag{1.4}$$

When this representation is valid, it is very useful; for example, the higher-order perturbation theory is based on this representation.[4] Thus the convergence of this representation is a crucial question. We discuss the situation carefully for two specific cases in Secs. III and IV, and conclude that Eq. (1.4) may well converge in favorable specific cases.

A special feature of the representation (1.4) is that its energy dependence is very simple (recall that $k=E^{1/2}$). For this reason, it is especially easy to Fourier transform the representation (1.4) and thereby obtain the time-evolution operator $U(t)=e^{-iHt}$ in the form

$$U(t)=\sum_n |\phi_n\rangle u_n(t)\langle\tilde{\phi}_n|\ , \tag{1.5}$$

where $u_n(t)$ is a simple definite integral. With this *diagonalization* of $U(t)$ we can study various time-dependent phenomena, including the precise limitations on the validity of an exponential decay law. Such limitations (e.g., a $t^{-3/2}$ power law for large times t) have been studied by many authors, mainly for the case of a single isolated resonance.[18–21] The resonance wave-function formalism enables us to give a general discussion of the case of many resonances. That discussion will appear in a future paper.

We conclude this introduction with a survey of the literature. There are very many papers on resonances and decaying states, and no suitable recent review article exists. Our survey is doubtless incomplete, but it will point out the main fields being cultivated in the literature.

Resonance states were discussed in the context of nonrelativistic potential scattering by Siegert,[5] Humblet,[1] Humblet and Rosenfeld,[6] Newton,[10] and Goldberger and Watson[7,11]; these authors work from the analytic properties of the S matrix in the partial-wave representation. The Kapur–Peierls resonance theory is reviewed in modern textbooks of nuclear physics, for example, by McCarthy[12] and Jones.[13] Properties of the Kapur–Peierls functions are discussed by many authors.[8,9,14,15] Other definitions of resonance parameters occur in theoretical nuclear physics,[16] but these definitions seem to aim at special needs of nuclear theory.

Nuclei have many resonances (thousands per MeV), many channels for reaction scattering, and correspondingly many reaction thresholds and unphysical sheets. We believe that a Mittag–Leffler representation of this type (1.4) can be justified only if the complete analytic configuration of $G(E)$ is known, i.e., if it is possible to analytically continue $G(E)$ onto all of its unphysical sheets.[6] For this reason the methods of this paper are of little interest for many-channel systems, except as approximations.

Nuclear energy levels also have a certain imperturbability. For example, an external static magnetic field would have almost no effect on the width of a nuclear resonance (although certain extremely small effects of this category actually do exist, e.g., pressure dependence of K capture). Thus a perturbation theory of nuclear resonances has been termed unnecessary or uninteresting.[6]

Physical conditions are very different in atomic or solid-state physics; it is easy to imagine interesting problems which involve only a few resonance states, with only a few channels, and atomic or ionic energy levels are eminently subject to external perturbations which may move one resonance to within a linewidth of another.

There exists a considerable literature on resonances from a high-energy viewpoint, mainly concerned with the Lee model or with K_0-meson decay.[2,17,18] The time dependence of resonances was studied by Jacob and Sachs,[18] Schwinger,[19] Newton,[20] Goldberger and Watson,[11] Rosenfeld,[21] and others.[2,31] Most of these works aim at understanding the $t^{-3/2}$ power law, which dominates the decay from a single isolated resonance at long times. The papers listed work from scattering theory; Rosenfeld and Newton give particularly interesting discussions of the dependence of decay characteristics on the form of the incident wave packet.

Linewidth effects in perturbation theory have been studied many times: the classical work of Weisskopf and Wigner[22] or Heitler[23] is based on a special truncation of the exact quantum equations of motion. Lane[24] had discussed the implications (for nuclear isospin conservation) of the removal of degeneracy of nearby energy levels by lifetime effects; his discussion is based on the R-matrix resonance theory. There are probably many discussions of the phenomenon in the context of specific applications.[25] Although the approach of our paper is limited to a simpler category of quantum systems at present, we believe that the approach is considerably more satisfactory, because so many of the results emerge as exact statements.

II. EIGENFUNCTIONS OF GREEN'S FUNCTION

The resonance wave functions ϕ_n were defined above in terms of the *residues* of the Green's function $G(k)$ at its complex poles $k=K_n$. It is useful to relate these functions ϕ_n to another family of functions $\Phi_s(k)$ which are defined here as *eigenfunctions* of the Green's function $G(k)$ for arbitrary fixed k. This definition of the functions Φ_s is equivalent (for potential scattering) to the special boundary condition of Kapur and Peierls[8] as we show explicitly in Sec. IV, below. The relation between the resonance functions ϕ_n and the Kapur–Peierls functions $\Phi_s(k)$ is very simple, but is worth spelling out explicitly, because doing so clarifies the role of the anomalous normalization factor Z_n.

Recently Walker and Sternheim have constructed a decaying state perturbation theory for the discussion of "exotic" atoms containing an unstable meson.[14] In their theory, the meson decay is described by a non-Hermitian part of the Hamiltonian, which is chosen to be a constant, independent of meson energy. In that case, the resonance wave functions ϕ_n and the Kapur–Peierls functions Φ_s become entirely identical, a circumstance very convenient for further mathematical manipulation (see also Fonda *et al.*[15]).

However, in general, the decay-producing part of a Hamiltonian *is* energy dependent; indeed such energy dependence is probably required by causality. Certainly if the decay occurs by tunneling through a potential barrier, the decay rate shows a strong (exponential) dependence upon energy. In this more general case, the families ϕ_n and Φ_s are not identical; we consider the relation between them.

First it is necessary to give a more explicit description of the quantum system in question. We imagine there are two channels. In one channel, the "outer" channel, the particle has a continuous spectrum beginning at $E=0$. In the other channel (the "inner" channel) there are discrete states (bound states) which decay owing to the coupling to the outer channel.

The true complete Hamiltonian H is a fixed Hermitian operator, independent of particle energy. By using projection operators for the inner and outer channels, we may write H as an operator sum of four parts, as

$$H = H_{ii} + H_{i0} + H_{0i} + H_{00} \ .$$

In this equation the term H_{i0}, for example, consists of all matrix elements of H which would transfer the particle from a continuum (outer) state into an inner-channel state.

The resolvent operator $R(z) = (z-H)^{-1}$ also may be divided into four corresponding parts, and of these four the part corresponding to inner-channel matrix elements will be termed the *Green's function* $G(k)$; i.e., we set

$$G(k) = R_{ii}(k^2) \ .$$

This Green's function is the projection of the resolvent operator onto the set of states of the inner channel.

For example, in the case of potential barrier scattering we can choose a fixed radius R_c containing all of the potential; the inner channel then consists of the region inside this sphere and the outer channel consists of the exterior region. The Green's function $G(x, x'; k)$ is the usual Green's function, but with both x and x' *restricted* to be within the sphere. This Green's function includes both direct effects of the potential and also indirect effects associated with the loss of particles out through the sphere.

The Green's function $G(k)$ may be regarded as the resolvent of an *effective Hamiltonian* $H_{\text{eff}}(k)$ which operates in the inner channel only. The effective Hamiltonian contains the inner channel part H_{ii} of the true Hamiltonian, but also imitates the effects of loss of particles into the outer channel. $H_{\text{eff}}(k)$ is usually an energy-dependent operator and is of course non-Hermitian. It may be defined by the operator equation

$$k^2 - H_{\text{eff}}(k) = [G(k)]^{-1} \ ,$$

and is single valued as a function of k. We should emphasize that H_{eff} is defined to operate only in the inner channel. Such an effective Hamiltonian is often referred to as an optical-model Hamiltonian (the term self-energy refers to a very similar concept).

Because the effective Hamiltonian depends parametrically on the energy k^2, its eigenfunctions also depend on k:

$$H_{\text{eff}}(k) | \Phi_r(k) \rangle = e_r(k) | \Phi_r(k) \rangle \ .$$

This equation defines what we call Kapur–Peierls states Φ_r. The terminology is motivated by the fact that this definition is equivalent to that of Kapur and Peierls for the case which they studied (potential scattering). The reader will note that the energy k^2 is *not* the eigenvalue in the equation above; in fact the Kapur–Peierls eigenvalue $e_r(k)$ has no immediate physical significance.

Eigenfunctions of $H_{\text{eff}}(k)$ are also eigenfunctions of the Green's function itself. We distinguish between left and right eigenfunctions, although they are very closely related:

$$G(k) | \Phi_r(k) \rangle = [k^2 - e_r(k)]^{-1} | \Phi_r(k) \rangle \ , \tag{2.1}$$

$$\langle \tilde{\Phi}_s(k) | \, G(k) = [k^2 - \tilde{e}_s(k)]^{-1} \langle \tilde{\Phi}_s(k) | \ . \tag{2.1a}$$

Detailed relations between these functions are discussed in the Appendix; they originate in the fact that the Green's function is a *real* operator function of ik. In the Appendix it is shown that

$$\tilde{e}_s(k) = e_s(k) = [e_s(-k^*)]^* \tag{2.2}$$

and

$$\langle x | \tilde{\Phi}_s(k) \rangle = \langle x | \Phi_s(k) \rangle^* = \langle \Phi_s(k) | x \rangle = \langle x | \Phi_s(-k^*) \rangle \ . \tag{2.3}$$

Now consider the quantity $\langle \tilde{\Phi}_s(k) | G(k) | \Phi_r(k) \rangle$. It may be evaluated in two ways, letting $G(k)$ operate to the left and right; equating the results it follows that

$$\langle \tilde{\Phi}_s(k) | \Phi_r(k) \rangle = 0 \qquad \text{for} \qquad e_r \neq e_s \ ,$$

which shows that the Kapur–Peierls eigenfunctions $|\Phi_r\rangle$ can be chosen to belong to a biorthogonal family of vectors and dual vectors (the product in this equation, and in all the following equations, runs *only* over the state space of the inner channel).

As demonstrated by Peierls for the case of potential scattering,[9] for all but a few exceptional k values one may choose the functions to be members of a biorthonormal family:

$$\langle \tilde{\Phi}_r(k) | \Phi_s(k) \rangle = \delta_{rs} \ . \tag{2.4}$$

Also, the functions $\Phi_s(k)$ are usually a complete set.[9,15] At the risk of a slight oversimplification, we can say that the reason the functions Φ_s form a complete orthonormal set is that they are eigenfunctions of a *fixed* operator $G(k)$ or $H_{\text{eff}}(k)$. However, they depend parametrically upon k in a complicated way, and the functions $\langle\tilde{\Phi}_r(k)|$ are *not* generally orthogonal to the functions $|\Phi_s(k')\rangle$ associated with a different wave vector k'.

Using the completeness of the Kapur–Peierls functions, we may expand the Green's function $G(k)$ in terms of the set $|\Phi_r(k)\rangle$, and doing so gives

$$G(k)=\sum_r \frac{|\Phi_r(k)\rangle\langle\tilde{\Phi}_r(k)|}{k^2-e_r(k)} . \tag{2.5}$$

However, this formula is of very limited utility. For example, the time-evolution operator $U(t)$, which is a Fourier transform of $G(k)$, cannot be found from this formula, because the functions $|\Phi_s(k)\rangle$ and $e_s(k)$ are far too complicated. They are too complicated even in "simple" cases (e.g., Sec. III).

However, the *singularities* of $G(k)$ may easily be extracted from Eq. (2.5), and doing so connects the Kapur–Peierls functions to the resonance wave functions ϕ_n. $G(k)$ will have a pole whenever $k=K_n$ obeys the equation

$$K_n^2=e_s(K_n) \tag{2.6}$$

for some $s=s(n)$. This equation relates a Siegert resonance energy $E_n=K_n^2$ (for which there is a pole of the Green's function or S matrix) to the Kapur–Peierls eigenvalue $e_s(k)$.

Two technical points may be mentioned here. First, there may be more than one solution of (2.6) for fixed s; i.e., the correspondence between Kapur–Peierls eigenvalues and Siegert energies is not in general one-to-one. An example occurs in Sec. III, below. Second, there exists the unlikely possibility of a degeneracy of Kapur–Peierls eigenvalues. In that (exceptional) case, other difficulties would have already occurred in the completeness relation,[9] so we assume that the Kapur–Peierls eigenvalues are nondegenerate at the interesting values of k.

When k approaches K_n, the residue of $G(k)$ in the energy plane is then

$$\lim_{k\to K_n}(k^2-K_n^2)G(k)=\frac{|\Phi_s(K_n)\rangle\langle\tilde{\Phi}_s(K_n)|}{1-e_s'(K_n)} , \tag{2.7}$$

where $e_s'(K_n)$ is the energy derivative

$$e_s'(K_n)\equiv\frac{1}{2K_n}\left(\frac{de_s}{dk}\right)_{k=K_n} .$$

This equation connects the Kapur–Peierls functions and the resonance wave functions ϕ_n, and gives an explicit formula for the normalization factor Z_n. Comparing Eq. (2.7) with our definition (1.1) of ϕ_n, we see that we may choose

$$|\phi_n\rangle=[1-e_s'(K_n)]^{-1/2}\,|\Phi_s(K_n)\rangle . \tag{2.8}$$

Because of relations (2.3) we further see that

$$\langle\tilde{\phi}_n|x\rangle=\langle x|\phi_n\rangle \tag{2.9}$$

for the resonance wave functions defined by Eq. (2.8).

Can we alter the normalization of the resonance wave functions? The only freedom to do so, without altering Eq. (1.1), consists of the possibility of multiplying $|\phi_n\rangle$ by some number Y, and then dividing $\langle\tilde{\phi}_n|$ by the same number. Such an alteration would *spoil the symmetry* evinced in Eq. (2.9), and is therefore evidently undesirable. In this sense, the theory assigns a fixed normalization to the resonance wave functions, and *not even the phase* is arbitrary. But the normalization constant is not unity.

Instead we have

$$Z_n=\langle\tilde{\phi}_n|\phi_n\rangle=[1-e_s'(K_n)]^{-1} \tag{2.10}$$

and this shows that the normalization constant Z_n is explicitly determined by the energy dependence of the effective Hamiltonian, since

$$e_s(k)=\langle\tilde{\Phi}_s(k)|H_{\text{eff}}(k)|\Phi_s(k)\rangle$$

and therefore

$$e_s'(K_n)=\frac{1}{2K_n}\langle\tilde{\Phi}_s(K_n)|\frac{dH_{\text{eff}}}{dk}|\Phi_s(K_n)\rangle \tag{2.11}$$

[Eq. (2.11) is proven by using the fact that Eq. (2.4) is true for each k]. This equation shows why the anomalous normalization does not arise in the approximate method of Walker and Sternheim[14] or Fonda *et al.*,[15] for in those theories the operator H_{eff} is assumed to be independent of energy.

To slightly anticipate the argument, formula (2.10) already begins to exhibit a suggestive similarity to formulas of field theory or many-body theory, where a quasiparticle renormalization constant is expressed in terms of the energy derivative of the self-energy operator. This "renormalization" interpretation is further discussed after Eq. (2.15).

Because of the relation $e_s^*(k)=e_s(-k^*)$, it is clear that if K_n solves Eq. (2.6), then so also does $-K_n^*$. Thus the resonance poles occur in pairs, reflected with respect to the axis of imaginary k. Wherever possible we label the poles so that

$$K_{-n}=-K_n^* . \tag{2.12}$$

We can easily use this labeling if there is no more than one pole on the imaginary k axis, i.e., no more than one bound state or virtual state. If there were more than one such state, we could introduce alphabetical symbols to label them, and thereby preserve Eq. (2.12) for the true resonance poles. With this understood, we also have

$$\langle x|\phi_{-n}\rangle=\langle x|\phi_n\rangle^* \tag{2.13}$$

as a consequence of Eqs. (2.2) and (2.3).

To recapitulate, the resonance functions ϕ_n are special values of the Kapur–Peierls functions $\Phi_s(k)$

for those values of k corresponding to the resonance poles. The anomalous normalization factor Z_n is determined by the energy dependence of the effective Hamiltonian; Z_n will differ from unity if the decay rate is strongly energy dependent. The resonance wave functions are not (usually) orthogonal, because

$$\langle \tilde{\phi}_n | \phi_m \rangle = (Z_n Z_m)^{1/2} \langle \tilde{\Phi}_r(K_n) | \Phi_s(K_m) \rangle$$

and the right-hand side is not (usually) zero.

If we use the Kapur–Peierls functions we have the advantages of their orthonormality; for work at a single fixed energy this is an important advantage. For other purposes the resonance functions ϕ_n will prove more useful. A suggestion of this utility is contained in the following discussion of the first-order perturbation theories.

Imagine that the system discussed above is perturbed by a weak perturbation V, which operates *only* in the inner channel ($V = V_{ii}$). We introduce a superscript zero to identify the unperturbed quantities.

Just to make sure this situation is clear, we should point out that we are *not* treating the decay-producing Hamiltonian H_{0i} as a perturbation; our intention is always to treat it (formally) exactly. Instead the perturbation is the slight change V in H_{ii}; this perturbation induces slight changes in the resonance energies and widths.

It is easy to show that the Kapur–Peierls eigenvalues change to

$$e_r(k) = e_r^0(k) + \langle \tilde{\Phi}_r^0(k) | V | \Phi_r^0(k) \rangle + O(V^2) \qquad (2.14)$$

in the presence of the perturbation V. This formula is proven in the usual manner of textbook perturbation theory, using the orthonormality of the Kapur–Peierls functions. However, while this equation tells the change of the Kapur–Peierls eigenvalue $e_r(k)$, it does *not* tell the change of the true pole position E_n. That must be found by solving the equation

$$K_n^2 = e_r(K_n) = e_r^0(K_n) + \langle \tilde{\Phi}_r^0(K_n) | V | \Phi_r^0(K_n) \rangle + \cdots \ .$$

This equation should be solved *consistently* to first order in V. Setting $K_n = K_n^0 + K_n^{(1)} + \cdots$, we see that the right-hand side contains two terms which are first order in V, i.e.,

$$(K_n^0)^2 + 2K_n^0 K_n^{(1)} + \cdots$$

$$= e_r^0(K_n^0) + K_n^{(1)} \left(\frac{de_r^0}{dk} \right)_{k=K_n^0} + \langle \tilde{\Phi}_r^0(K_n^0) | V | \Phi_r^0(K_n^0) \rangle + \cdots$$

and so

$$K_n^{(1)} = \frac{\langle \tilde{\Phi}_r^0(K_n^0) | V | \Phi_r^0(K_n^0) \rangle}{2K_n^0 - (de_r^0/dk)_{K_n^0}} \ .$$

This implies Eq. (1.3) which we repeat here for convenience:

$$E_n = E_n^0 + \langle \tilde{\phi}_n^0 | V | \phi_n^0 \rangle + O(V^2) \ . \qquad (1.3)$$

This is the first-order decaying-state perturbation theory.

It is clearly essential to this result that the resonance wave function ϕ_n *not* be normalized to unity. The normalization of ϕ_n can actually be most clearly understood as containing a "feedback" effect. Suppose we apply a perturbation V in an effort to change the energy of the resonance state. We may imagine that the perturbation V itself immediately produces a direct energy shift $\Delta^{(0)} = \langle \tilde{\Phi}_r^0(K_n^0) | V | \Phi_r^0(K_n^0) \rangle$ equal to the original expectation value of V (taken with wave functions normalized to unity).

However, this direct energy shift alters the energy at which the resonance system is coupled to the continuum. In the tunneling case, it thereby alters the tunneling rate, which is strongly dependent upon energy. If the continuum coupling had produced a level shift, that too would be altered by the direct energy shift. Thus there is an indirect energy shift which is, to first order in $\Delta^{(0)}$, given by $\Delta^{(1)} = \Delta^{(0)} e_r'(K_n^0)$. But this first indirect energy shift likewise induces a second indirect energy shift $\Delta^{(2)} = \Delta^{(1)} e_r'(K_n^0)$, and so on. All these indirect terms are of first order in V. The successive shifts are given by the expansion of the geometric series implicit in the normalization of ϕ_n in Eq. (1.3). Such a geometric series is the usual mathematical representation of a *feedback coupling*.

Another description of the result (2.15) is to say that the matrix elements of V which enter are renormalized. They are not computed with the normalized wave functions $\Phi_r^0(K_n^0)$ but rather with renormalized wave functions ϕ_n. Off-diagonal renormalized matrix elements $\langle \tilde{\phi}_n | V | \phi_m \rangle$ enter into the higher-order terms of the perturbation theory.[4]

There is a striking similarity between this calculation and the general field-theory technique of renormalization, although our situation is much simpler. We need introduce no "counterterms" (extra additive terms in the Hamiltonian) and the renormalization parameters Z_n cannot be factored out of the Green's function (except very near a pole). Also, in our case there is no mystery about finding a complex value of Z_n. By comparing the renormalization interpretation with the "feedback" discussion above, we obtain some intuitive insight into the general meaning of renormalization.

In fact, *both* the renormalized perturbation theory of Eq. (2.15) and also the original (nonrenormalized) perturbation theory of Eq. (2.14) are equally *correct*. They differ because they compute different quantities. The renormalized perturbation theory computes the new location of the pole of the Green's function (or S matrix) whereas the original perturbation theory computed the perturbed Kapur–Peierls eigenvalue.

In order to extend the theory to higher-order terms, even to second order in V, it is apparently necessary to prove the representation (1.4) for the Green's function.[4] Since that representation is true only by virtue of the detailed analytic properties of the Green's function, we must now turn to a few specific example systems.

III. TWO-STATE RESONANCE MODEL

We now turn to a special resonance model, a two-level system which decays into a continuum. The model is exactly soluble and any property of the resonances can be examined in as much detail as desired. Certain of the results are surprising or unexpected; for example, there are five resonance wave functions ϕ_n, corresponding to five distinct poles of the Green's function. Since these five functions occur in a two-component space, it is quite clear that they could not be orthonormalized by any method. This illustrates the very real differences between the set ϕ_n and the Kapur–Peierls states $\Phi_n(k)$, for there are only two of the latter (for each k).

The set of five resonance wave functions ϕ_n is an overcomplete set, and may be used for expanding wave functions or operators. The expansion of the Green's function $G(k)$ is easily established; in this case the expansion is merely a finite partial-fractions decomposition. Thus the model of this section illustrates the possible behavior of resonance systems in a case of maximum mathematical simplicity.

We then consider a single electron which can be in either of two channels. In the inner channel, the electron can occupy any linear combination of two basic orbitals, $|a\rangle$ and $|b\rangle$, which have real unperturbed energies e_a and e_b. The unperturbed Hamiltonian of the inner channel is

$$H_i^{(0)} = |a\rangle e_a \langle a| + |b\rangle e_b \langle b| \ . \tag{3.1}$$

The resolvent of $H_i^{(0)}$ is

$$R_{ii}^{(0)}(z) = |a\rangle\langle a|/(z-e_a) + |b\rangle\langle b|/(z-e_b) \ . \tag{3.2}$$

In the outer channel, the electron is assumed to be free to move in one space direction (on the full open interval $-\infty < x < \infty$). The unperturbed outer-channel Hamiltonian is accordingly taken to be

$$H_0^{(0)} = -\frac{d^2}{dx^2} \tag{3.1a}$$

and its well-known resolvent is

$$\langle x| R_{00}^{(0)} |x'\rangle = \frac{1}{2ik}\, e^{ik|x-x'|} \ . \tag{3.2a}$$

This operator depends (in a single-valued way) upon $k = z^{1/2}$, where z is the complex energy.

The coupling Hamiltonian H_c causes transitions between the channels. It allows an electron in an inner-channel state to decay into the outer channel. Alternatively, if an electron in the outer channel approaches the origin ($x=0$), the coupling Hamiltonian H_c transfers this electron into the inner channel, where it may remain for some time.

We assume that the coupling Hamiltonian removes the electron from the origin of the outer channel and injects it into a specific (fixed) linear combination state $|\xi\rangle = \alpha|a\rangle + \beta|b\rangle$ in the inner channel (α and β are assumed to be *real* numbers in the sequel). Temporarily letting the symbol $\hat{Q}$ denote the operator which changes the channel from outer to inner, the coupling Hamiltonian H_c is

$$H_c = \lambda|\xi\rangle \hat{Q}\delta(x) + \lambda\delta(x)\hat{Q}^+\langle\xi| \ . \tag{3.3}$$

The number λ is a coupling-strength parameter. If the coupling Hamiltonian H_c operates on an arbitrary wave function $\psi(x)$ of the outer channel, the result is $\lambda\psi(0)$ times the inner-channel state $|\xi\rangle$.

The complete Hamiltonian is

$$H = H_i^{(0)} + H_0^{(0)} + H_c \ .$$

We shall study the resolvent of this operator, formally defined by

$$R(z) = 1/(z-H) \ .$$

The resolvent is constructed by solving the formal equation

$$R(z) = R^{(0)}(z) + R^{(0)}(z) H_c R(z) \ .$$

This equation is easily solved. The matrix elements of $R(z)$ between outer-channel states are, for example,

$$\langle x| R_{00}(z) |x'\rangle = \frac{e^{ik|x-x'|}}{2ik} + \frac{e^{ik|x|}}{2ik}\, \frac{\lambda^2 F(k^2)}{1-(\lambda^2/2ik)F(k^2)} \times \frac{e^{ik|x'|}}{2ik} \ , \tag{3.4}$$

where it is convenient to define the function

$$F(k^2) \equiv \langle\xi| R_{ii}^{(0)} |\xi\rangle = \alpha^2/(k^2-e_a) + \beta^2/(k^2-e_b) \ . \tag{3.5}$$

In the sequel we are primarily interested in $R_{ii}(z)$, the projection of the resolvent $R(z)$ onto the inner channel. This will be called $G(k)$ and has the form

$$G(k) = R_{ii}^{(0)}(k^2) + \lambda^2 \hat{R}_{ii}^{(0)}(k^2)\, \frac{|\xi\rangle\langle\xi|}{2ik-\lambda^2 F(k^2)}\, \hat{R}_{ii}^{(0)}(k^2) \tag{3.6}$$

or, in greater detail,

$$\langle a| G(k) |a\rangle = \frac{1}{k^2-e_a} + \frac{\alpha^2\lambda^2}{(k^2-e_a)^2[2ik-\lambda^2 F(k^2)]} \ ,$$

$$\langle a|G|b\rangle=\langle b|G|a\rangle$$

$$=\frac{\lambda^2\alpha\beta}{(k^2-e_a)(k^2-e_b)[2ik-\lambda^2F(k^2)]}\ ,$$

$$\langle b|G|b\rangle=\frac{1}{k^2-e_b}+\frac{\beta^2\lambda^2}{(k^2-e_b)^2(2ik-\lambda^2F)}\ . \qquad (3.7)$$

Although these equations constitute a complete solution for the model, the properties of the resonances are not exhibited explicitly in this representation. To learn about the resonances, we examine the Green's function $G(k)$ for its singularities. As a function of k, the Green's function $G(k)$ has only poles, and no other singularities. If the inner-channel states are not degenerate ($e_a \neq e_b$) and if both α and β are nonzero, then it is easily verified that there is no singularity of $G(k)$ at the unperturbed energies e_a, e_b for finite λ. The poles of $G(k)$ occur whenever $k=K_n$ obeys

$$2iK_n=\lambda^2F(K_n)=\frac{\lambda^2\alpha^2}{K_n^2-e_a}+\frac{\lambda^2\beta^2}{K_n^2-e_b}\ . \qquad (3.8)$$

The resonance wave functions, defined as in Secs. I and II, are given by

$$|\phi_n\rangle=N_n\left(\frac{\alpha|a\rangle}{E_n-e_a}+\frac{\beta|b\rangle}{E_n-e_b}\right)\ , \qquad (3.9)$$

where $E_n=K_n^2$ and (in this section only)

$$N_n=\left(\frac{i}{\lambda^2K_n}-F'(E_n)\right)^{-1/2}\ , \quad F'(E)=\frac{dF}{dE}\ . \qquad (3.10)$$

The normalization factor Z_n for the resonance wave functions is determined in terms of $F(E)$ by

$$Z_n=\langle\tilde{\phi}_n|\phi_n\rangle=-N_n^2F'(E_n)=(1-F(E_n)/2E_nF'(E_n))^{-1}\ . \qquad (3.11)$$

In general, Eq. (3.8) is equivalent to a fifth-order algebraic equation, and it has *five* solutions. Thus there are five poles of $G(k)$ and five corresponding resonance wave functions. Their significance becomes clear in the case of long lifetimes. Thus we expand all the above quantities in powers of λ.

First, consider the two solutions associated with the unperturbed state $|a\rangle$. These may be denoted $|\phi_{\pm a}\rangle$ and $E_{\pm a}$. The expansion with respect to λ is then

$$E_{\pm a}=e_a\pm\frac{\lambda^2\alpha^2}{2i\sqrt{e_a}}+\frac{\lambda^4\alpha^2}{4e_a}\left(\frac{\alpha^2}{2e_a}-\frac{\beta^2}{e_a-e_b}\right)+\cdots \qquad (3.12)$$

for the complex energy, and

$$|\phi_{\pm a}\rangle=|a\rangle\mp\frac{\lambda^2}{2i\sqrt{e_a}}\,\frac{\alpha^2}{4e_a}\,|a\rangle\pm\frac{\lambda^2\beta\alpha}{2i\sqrt{e_a}\,(e_a-e_b)}|b\rangle+\cdots \qquad (3.13)$$

for the resonance wave function.

This pair of poles of $G(k)$ originates in the unperturbed level e_a. The first term of the complex energy E_a is just the decay rate ω as evaluated in the "Golden Rule" perturbation theory, i.e.,

$$E_a=e_a\pm\tfrac{1}{2}i\omega\ , \quad \omega=2\pi|M|^2\rho(e_a)$$

where the matrix element M between the inner state $|a\rangle$ and a continuum state $L^{-1/2}e^{ikx}$ is

$$M=\alpha\lambda/L^{1/2}$$

(L is an arbitrary large quantization length). The density of states in a range of length L is then $\rho(e_a)=L/2\pi\sqrt{e_a}$ and thus $\omega=\lambda^2\alpha^2/\sqrt{e_a}$.

The second term in E_a, proportional to λ^4, is an energy *level shift* resulting from the coupling to the continuum and the induced coupling to state $|b\rangle$. In more general or realistic models, this energy shift is not necessarily an order smaller than the decay rate.

The two states $\phi_{\pm a}$ are linearly independent for finite λ. However, they are closely interconnected by relations like

$$\langle a|\phi_a\rangle^*=\langle a|\phi_{-a}\rangle\ .$$

As becomes clear below (see the discussion of the time-evolution operator in Sec. V) one of these two states is the decaying-state wave function and the other is the wave function of a corresponding growing state, whose presence guarantees time-reversal symmetry.

It is interesting to examine the normalization factor Z_n for the case of long lifetimes (small λ). The expansion is

$$Z_a=\langle\tilde{\phi}_a|\phi_a\rangle=1+i\,\frac{\lambda^2\alpha^2}{4e_a\sqrt{e_a}}+\cdots\cong 1+\frac{i}{2}\left(\frac{\mathrm{Im}E_a}{\mathrm{Re}E_a}\right)\ . \qquad (3.14)$$

A similar result holds whenever the level shift may be neglected, so that the Kapur–Peierls eigenvalue may be approximately represented by

$$e_r(k)\cong e_0+\tfrac{1}{2}i\omega\ , \quad \omega\ll e_0$$

and the resonance energy E_n is approximately

$$E_n\cong e_0\pm\tfrac{1}{2}i\omega_0\ ,$$

where ω_0 is the decay rate evaluated at the unperturbed energy e_0. If we have

$$\frac{d\omega}{dE}\cong s\,\frac{\omega_0}{e_0}$$

(this will be the case if the decay rate ω depends on the sth power of the energy), then the formula for Z_n is approximately

$$Z_n\cong\frac{1}{1-is\omega/2e_0}\cong 1+is\left(\frac{\mathrm{Im}E_n}{\mathrm{Re}E_n}\right)\ .$$

This gives a general approximate expression for the normalization factor.

A second pair of solutions of Eq. (3.8) is associated with the unperturbed state $|b\rangle$ in exactly analogous fashion.

The *fifth* solution of Eq. (3.8) has a different character. Its significance also becomes clear in the case of small coupling. In that case its wave vector K_0 is very small and has the expansion

$$K_0=\frac{i\lambda^2}{2}\left(\frac{\alpha^2}{e_a}+\frac{\beta^2}{e_b}\right)\left(1+\frac{\lambda^2\alpha^2}{e_a^2}+\frac{\lambda^2\beta^2}{e_b^2}+O(\lambda^4)\right) \quad (3.15)$$

and the corresponding wave function is

$$|\phi_0\rangle=\frac{\lambda^2}{\sqrt{2}}\left(\frac{\alpha^2}{e_a}+\frac{\beta^2}{e_b}\right)^{1/2}\left(\frac{\alpha|a\rangle}{e_a}+\frac{\beta|b\rangle}{e_b}\right)+O(\lambda^4)\ . \quad (3.16)$$

In order to interpret this state, it is useful to reexamine the outer-channel resolvent operator given in Eq. (3.4). This resolvent corresponds to free propagation plus scattering at the origin. The T-matrix operator for the scattering may be defined by the operator equation

$$R_{00}(z)=R_{00}^{(0)}(z)+R_{00}^{(0)}(z)T(z)R_{00}^{(0)}(z)\ , \quad (3.17)$$

where the T matrix is given by

$$\langle x|\,T(k^2)\,|x'\rangle=\frac{\lambda^2F(k^2)}{1-\lambda^2F(k^2)/2ik}\,\delta(x)\,\delta(x')\ . \quad (3.18)$$

This operator describes the scattering as seen in the outer channel. It is the T matrix of a one-dimensional scattering problem, with an energy-dependent effective potential

$$\lambda^2F(k^2)\delta(x)\ .$$

This potential can be *attractive*, for small k^2, if e_a and e_b are positive (which we have assumed, in order to have decaying states). When the effective potential is negative (attractive), it may produce a bound state in the outer channel.

This bound state is not a resonance, but a true (negative-energy) bound state. Its wave function is largest at the origin, and dies away exponentially from the origin. The outer-channel wave function may be extracted from Eq. (3.17) and is

$$\psi_0(x)=A_0e^{-\gamma_0|x|}\ , \quad (3.19)$$

where

$$\gamma_0=|K_0|\ ,$$
$$A_0=-\frac{F(-\gamma_0^2)}{2\gamma_0[1/\gamma_0\lambda^2-F'(-\gamma_0^2)]}\ . \quad (3.20)$$

The state $|\phi_0\rangle$ given by Eq. (3.16) is the part of this bound state which appears in the inner channel. Thus the extra (fifth) pole of $G(k)$ is the inner-channel part of a true bound state; this shows why the wave vector K_0 is purely imaginary, for the associated energy is real and negative.

The complete wave function for the bound state is normalized to unity. This is expressed by the statement, easily proven from Eqs. (3.11), (3.19), and (3.20), that

$$\langle\tilde{\phi}_0|\phi_0\rangle+\int_{-\infty}^{\infty}|\psi_0(x)|^2dx=1\ . \quad (3.21)$$

This last equation supplies a further interpretation, *for this special case*, of the "renormalization" Z_0 of the state $|\phi_0\rangle$. Z_0 is the probability that a particle known to be in the bound state will be found in the inner channel. This interpretation is similar to the interpretation of real renormalization constants of quantum field theories, which describe the renormalization factor as the probability of finding the physical quasiparticle in a "bare particle" state.

However, this interpretation is *only* valid for bound states. It is by no means correct for resonances. The resonances are not associated with real renormalization factors Z_n, and the outer-channel parts of the resonance wave functions cannot be normalized at all (except by *ad hoc* modifications of the mathematical definitions). It is our opinion that the only correct interpretation of the factors Z_n for the resonances is the feedback interpretation given in Sec. II above.

For the model of this section it is entirely trivial to establish the Mittag–Leffler representation of the Green's function. The Green's function $G(k)$, given in Eq. (3.7), is a meromorphic function of k, with only the five singularities at $k=K_n$. As mentioned above, there are no singularities at the unperturbed energies, and no branch cuts (in the k plane). For large values of k, it can easily be shown that

$$G(k)=\frac{1}{k^2}\,\underline{1}+O(k^{-5}) \quad (3.22)$$

(the symbol $\underline{1}$ in the first term denotes the unit matrix). Thus the decomposition of $G(k)$ into partial fractions may be carried out, and the result is

$$G(k)=\sum_{n=-2}^{+2}|\phi_n\rangle\langle\tilde{\phi}_n|/2K_n(k-K_n)\ . \quad (3.23)$$

By comparing this relation with the asymptotic form of the Green's function for large k, a number of relations between the ϕ's can be read off. The most interesting one is

$$\frac{1}{2}\sum_{n=-2}^{+2}|\phi_n\rangle\langle\tilde{\phi}_n|=\underline{1}\ ,$$

which expresses the fact that the resonance wave functions form an over-complete set.

It is possible to construct the eigenfunctions of the Green's function $G(k)$ for the model of this section, and by explicit construction one may verify the statements of Sec. II above. We urge the reader to convince himself that the k dependence of these eigenfunctions is quite complicated (it includes branch cuts). For this reason the representation of Eq. (3.23) is especially impressive, because of the simplicity of its k dependence.

IV. POTENTIAL SCATTERING RESONANCES

The simplest type of resonance occurs when a particle moves under the influence of a potential which has a high (but finite) barrier; if the particle approaches the barrier it may be trapped for some time behind the barrier before it escapes by tunneling. Since the mathematical theory of potential scattering is very highly developed, it is possible to give a very general discussion and still the results are exact.

In an earlier paper[4] a resonance perturbation theory was constructed for potential scattering. Here that theory is reviewed and recast in the language of Sec. II, a language more suitable for comparison with the Kapur–Peierls theory. In this case, the comparison reveals the unsatisfactory nature of the Kapur–Peierls wave functions $\Phi_s(r)$, for the Φ_s do not always go over smoothly into bound-state wave functions in the appropriate limit. On the other hand, the resonance wave functions $\phi_n(r)$ will automatically become real, orthonormal bound-state wave functions if the barrier becomes very high. In this sense they are more suitable for use in the limit of long lifetimes. The present section concludes with a detailed discussion of the representation of the Green's function $G(k)$ in terms of the ϕ_n, for a simple special case.

The tunneling model involves a spherically symmetric potential $v(r)$ which contains a barrier. It is convenient to consider only the solutions having s-wave symmetry (the extension to higher angular momentum should present no difficulty), and in order that the solutions have the simplest analytic properties, it is convenient to require that the potential $v(r)$ be zero beyond a fixed radius a. It is assumed that there are no bound states.

The usual solutions of the Schrödinger equation for such a potential are the real energy continuum scattering solutions $w(k;\, r)$. These are defined (following Goldberger and Watson[7]) by the boundary conditions

$$\begin{aligned} &w(k;\, 0)=0\ , \\ &w(k;\, r)=(2/\pi)^{1/2}\sin(kr+\delta) \qquad \text{for} \quad r\geq a \end{aligned} \tag{4.1}$$

for any real energy $E=k^2$ [here $\delta(k)$ is the real s-wave phase shift].

The functions $w(k;\, r)$ form a complete set, assuming that there are no bound states, and are thus adequate for any quantum-mechanical calculation. There is a continuum perturbation theory for the functions $w(k;\, r)$; this perturbation theory tells how they change when the potential $v(r)$ is slightly altered. The continuum wave functions in principle describe all properties of the resonance phenomena.

However, when the barrier is high, then the decaying states trapped behind it have very long lifetimes and we expect that the continuum theory misses the point. The continuum scattering wave functions $w(k;\, r)$ are nothing like discrete bound-state wave functions. It is to be expected that certain linear combinations of the $w(k;\, r)$ are physically more like bound states trapped behind the barrier.

The resonance wave functions $\phi_n(r)$ are such linear combinations. In the special case of long-lived resonances the wave functions $\phi_n(r)$ tend to resemble bound-state wave functions more and more closely, and hence they are more natural or appropriate than the functions $w(k;\, r)$.

The functions $\phi_n(r)$ are solutions of the radial Schrödinger equation with complex eigenvalue K_n^2:

$$\left(-\frac{d^2}{dr^2}+v(r)\right)\phi_n(r)=K_n^2\phi_n(r)\ . \tag{4.2}$$

The boundary conditions they satisfy may be written

$$\begin{aligned} &\phi_n(0)=0\ , \\ &\frac{d\phi_n}{dr}=iK_n\phi_n\ , \quad r\geq a \end{aligned} \tag{4.3}$$

but these statements do not yet specify the normalization of the resonance wave function, and as asserted several times, the normalization is their most interesting property. The normalization may be imposed as in Sec. I, completely defining $\phi_n(r)$ in terms of the residue of the Green's function $G(k)$ at its complex pole K_n, i.e.,

$$\lim_{k\to K_n}(k^2-K_n^2)G(r,\, r';\, k)\equiv\phi_n(r)\phi_n(r')\ . \tag{4.4}$$

This gives the same definition of $\phi_n(r)$ as was used in Ref. 4, with two technical provisions. In Ref. 4, the Green's function $G(k)$ was denoted $\Gamma(k)$ and had its poles at $k=-K_n$, a systematic notational change from the usage here. The other proviso concerns the separation into bound and free channels.

In the analysis of Ref. 4, no channel radius was introduced; the solutions $\phi_n(r)$ were considered on the entire range $0<r<\infty$. Of course they cannot be normalized on that range, because their absolute value grows exponentially with r.

Although special mathematical techniques (Zel'dovich,[2] Gyarmati,[26] and Bergren[27]) can be developed to normalize the functions on the range $(0,\, \infty)$ these techniques are not perfectly satisfactory. These techniques introduce ways of regularizing the divergent normalization integral of $\phi_n(r)$ either by introducing a cutoff factor $e^{-\epsilon r^2}$ or by deforming the contour of integration to complex r. In fact these methods lead to results quite similar to those of this paper. However, the regularization techniques are slightly unsettling. Consider for example the regularized integral[28]

$$\lim_{\epsilon\to 0^+}\int_0^\infty e^{-\epsilon r^2}e^{\beta r}\,dr=-1/\beta\ .$$

In the special case of positive real β, this regularization of the integral gives a negative result, even though the integrand is always positive. While this may not be completely incorrect, it is certainly dangerous.[29]

One entirely avoids such unpleasantness by introducing a channel radius R_0 which separates the inner "bound channel" region ($0<r<R_0$) from the outer "free channel" region ($r>R_0$). The normalization integrals are defined to run only from zero to R_0. Although the channel radius R_0 is itself arbitrary and unphysical, no final physical result should depend upon R_0. It is always assumed that $R_0\geq a$ in this paper (recall that a is the radius beyond which the potential is zero).

We now review some formulas from Ref. 4, in order to set up the comparison with Sec. II. In Ref. 4, the wave functions $\phi_n(r)$ were constructed in terms of the Jost function $f(k;r)$; in the extensive list of references given in Ref. 4 one will find detailed treatments of the analytic properties of the Jost function for complex k. For any value of k, $f(k;r)$ is defined to be that solution of the radial Schrödinger equation (4.2) which obeys the special boundary condition

$$f(k;r)=e^{-ikr}\quad\text{for}\quad r\geq a\ . \tag{4.5}$$

There is no boundary condition imposed upon $f(k;0)=f(k)$, and so $f(k;r)$ alone does not always constitute an acceptable solution of the Schrödinger equation. However, for certain values Q_n of k we have

$$f(Q_n)=f(Q_n;0)=0 \tag{4.6}$$

and this equation defines the zeros Q_n of the Jost function. These values are the negatives of the K_n, i.e., the Green's function $G(k)$ has a pole at $k=K_n=-Q_n$.

The resonance wave function $\phi_n(r)$ is proportional to $f(Q_n;r)$:

$$\phi_n(r)=N_nf(Q_n;r)\ , \tag{4.7}$$

where the proportionality constant N_n is determined by

$$N_n^2=-i[f(-Q_n)/f'(Q_n)]\ . \tag{4.8}$$

In Ref. 4 it was shown that formulas (4.7) and (4.8) determine the same function $\phi_n(r)$ as does the residue definition (4.4). It was further shown that

$$N_n^2\propto \operatorname{Im}K_n\ , \tag{4.9}$$

and hence that this quantity approaches zero for states of very long lifetime. This fact implies an approximate orthogonality and normalization of the $\phi_n(r)$, for it was demonstrated that

$$\int_0^{R_0}\phi_n^2(r)\,dr=1-N_n^2(e^{-2iQ_nR_0}/2iQn) \tag{4.10}$$

and

$$\int_0^{R_0}\phi_n(r)\phi_m(r)\,dr=-N_nN_m[e^{-i(Q_n+Q_m)R_0}/i(Q_n+Q_m)] \tag{4.11}$$

for any choice of $R_0\geq a$. Relations (4.10) and (4.11) are exact; we shall demonstrate below the equivalence of (4.10) to the normalization factor Z_n of Secs. I and II. It was also shown in Ref. 4 that the normalization of $\phi_n(r)$ is such that it becomes real for the case of long lifetimes. Thus the states $\phi_n(r)$ become real, normalized, and orthogonal for long lifetimes; the behavior of the Kapur–Peierls functions is not necessarily so pleasant.

In order to construct Kapur–Peierls functions, we shall seek the eigenfunctions of the Green's function, for arbitrary fixed k. Let

$$\int_0^{R_0}G(r,r';k)\Phi_s(r')\,dr'=[k^2-e_s(k)]^{-1}\Phi_s(r)\ , \tag{4.12}$$

where $\Phi_s(r)\equiv\Phi_s(k;r)$. Imagine that $\Phi_s(r)$ is a solution to this equation; let us discover its properties. First, it obeys the Schrödinger equation with complex eigenvalue $e_s(k)$, throughout the bound channel ($r\leq R_0$). This is demonstrated from the basic fact that, for both r and r' in the bound channel,

$$\left(-\frac{d^2}{dr^2}+v(r)-k^2\right)G(r,r';k)=\delta(r-r')\ .$$

Using this relation, it is easily shown that

$$\left(-\frac{d^2}{dr^2}+v(r)\right)\Phi_s(r)=e_s(k)\Phi_s(r) \tag{4.13}$$

for each $r<R_0$. Since $G(0,r';k)=0$, it is evident from Eq. (4.12) that $\Phi_s(0)=0$. The boundary condition at $r=R_0$ is slightly more difficult to extract. Assume temporarily that R_0 is slightly larger than a, and choose $a<r<R_0$. The Green's function may be represented in terms of the Jost function $f(-k;r)$ and an arbitrary solution $g(k;r)$ which is required to be zero at the origin. This representation is

$$G(r,r';k)=\begin{cases}Af(-k;r)g(k;r')\ , & r>r'\\ Af(-k;r')g(k;r)\ , & r<r'\ .\end{cases} \tag{4.14}$$

In this representation, A^{-1} is the Wronskian of f and g:

$$1/A=g(r)f'(-k;r)-g'(r)f(-k;r)\ . \tag{4.15}$$

Using this representation, and performing the differentiations carefully, we can show that

$$\frac{\Phi'(r)}{\Phi(r)}=\frac{f'(-k;r)\int_0^r g(r')\Phi(r')\,dr'+g'(r)\int_r^{R_0} f(-k;r')\Phi(r')\,dr'}{f(-k;r)\int_0^r g(r')\Phi(r')\,dr'+g(r)\int_r^{R_0} f(-k;r')\Phi(r')\,dr'}\;.$$

Now if r approaches R_0, the second integral in the numerator and demoninator becomes very small, and so

$$\frac{\Phi'(R_0)}{\Phi(R_0)}=\frac{f'(-k;R_0)}{f(-k;R_0)}=ik\;. \qquad (4.16)$$

This equation is the desired Kapur–Peierls boundary condition. The above derivation is slightly informal; a much more formal discussion is given by McCarthy.[12] McCarthy introduces a boundary-condition operator involving a δ function of $(r-R_0)$; this operator is the non-Hermitian addition to $G(k)$, and serves to enforce the same result (4.16). Although this more elaborate treatment may seem more satisfactory to some, it leads to no different result. To summarize, it is appropriate to refer to the eigenfunctions of $G(k)$ as Kapur–Peierls functions, for they obey the special boundary condition of the Kapur–Peierls resonance theory. Although the eigenvalue in the Schrödinger equation (4.13) for $\Phi_s(k;r)$ is $e_s(k)$, the boundary condition involves k.

Now it is possible to explicitly construct the Kapur–Peierls functions. We set $q^2=e_s(k)$ for arbitrary fixed k, although neither q nor $e_s(k)$ is yet known. The general solution of Eq. (4.13) may be written

$$\Phi_s(k;r)=Af(q;r)+Bf(-q;r)\;.$$

The ratio of A and B is determined by the condition $\Phi(0)=0$, so that

$$A/B=-f(-q)/f(q)\;.$$

The discrete (quantized) value of q is then determined by the other boundary condition:

$$ik=\frac{\Phi'(R_0)}{\Phi(R_0)}=-iq\,\frac{Ae^{-iqR_0}-Be^{iqR_0}}{Ae^{-iqR_0}+Be^{iqR_0}}$$

or

$$-\frac{k}{q}=\frac{f(-q)e^{-iqR_0}+f(q)e^{iqR_0}}{f(-q)e^{-iqR_0}-f(q)e^{iqR_0}}\;. \qquad (4.17)$$

The actual values of A and B would be determined by the requirement that

$$\int_0^{R_0}\Phi^2(r)\,dr=1\;,$$

but this condition will not be worked out here.

Poles of the Green's function occur whenever $K_n^2=e_s(K_n)$, as shown in Sec. II. This means that $k^2=q^2$ in Eq. (4.17), i.e., either

$$q=-k \text{ and } f(q)=0 \text{ (case i)}$$

or

$$q=k \text{ and } f(-q)=0 \text{ (case ii)}\;,$$

a set of alternatives which follows from Eq. (4.17). Since Q_n was defined by the equation $f(Q_n)=0$, both cases (i) and (ii) give a pole of $G(k)$ at $k=K_n=-Q_n$. The solutions of cases (i) and (ii) are actually identical; thus the Kapur–Peierls condition $e_s(K_n)=K_n^2$ is equivalent to the criterion $f(-K_n)=0$.

We shall now determine the derivative dk/dq at the points of type (i) where $f(q)=0$. This will enable us to evaluate the normalization factor Z_n of Secs. I and II, from the Kapur–Peierls point of view [see Eq. (2.10)]. That evaluation is then to be compared to Eq. (4.10).

Starting with Eq. (4.17) we may differentiate each side with respect to q and then set $f(q)=0$ to obtain

$$-\frac{dk}{dq}=1+2q\,\frac{f'(q)}{f(-q)}\,e^{2iqR_0} \quad \text{with} \quad q=Q_n\;.$$

That gives us

$$e_s'(K_n)=\frac{Q_n}{K_n}\left(\frac{dq}{dk}\right)_{q=Q_n}=\left(1+\frac{2Q_nf'(Q_n)}{f(-Q_n)}\,e^{2iQ_nR_0}\right)^{-1} \qquad (4.18)$$

for the energy derivative of the Kapur–Peierls eigenvalue, and hence

$$Z_n=[1-e_s'(K_n)]^{-1}=1+\frac{f(-Q_n)}{2Q_nf'(Q_n)}\,e^{-2iQ_nR_0} \qquad (4.19)$$

for the renormalization factor Z_n. The value (4.19) should be compared with the result in Eq. (4.10), which may be rewritten as

$$\int_0^{R_0}\phi_n^2(r)\,dr=1-\left(\frac{-if(-Q_n)}{f'(Q_n)}\right)\frac{e^{-2iQ_nR_0}}{2iQ_n}\;.$$

The exact agreement is clear.

This gives us an explicit check of the general theory of Sec. II for the potential scattering case, and shows how all the quantities are constructed from the Jost function $f(k;r)$, for an arbitrary potential. Although the quantity Z_n does depend explicitly upon the channel radius, the desired agreement between (4.10) and (4.19) holds for any channel radius. Incidentally, the regularization procedure of Bergren[27] and Gyarmati and Vertse[26] is equivalent to asserting that

$$\operatorname*{Lim\,Reg}_{R_0\to\infty} Z_n=1\;,$$

where Lim Reg is the "regularized limit." For finite values of R_0, the absolute value $|Z_n|$ grows exponentially with R_0, and so this regularized limit procedure (while consistent) is strange.

We now consider the Kapur–Peierls functions a little more closely, to show how they behave for long lifetimes. While a general investigation is undoubtedly possible, it is simpler to examine a special soluble case, already discussed in Ref. 4. This case is the extremely simple barrier potential

$$v(r)=V_0\delta(r-b)\ , \tag{4.20}$$

where $b<R_0$. For this potential, the Jost function $f(k)$ is

$$f(k)=1+(V_0/2ik)(1-e^{-2ikb}) \tag{4.21}$$

and there is an expansion of the K_n for the long-lifetime limit of the form

$$-K_n=Q_n=\frac{\pi n}{b}-\frac{\pi n}{b^2V_0}-\frac{\pi n}{b^3V_0^2}+i\,\frac{\pi^2n^2}{b^3V_0^2}+\cdots\ . \tag{4.22}$$

In this case, the limit of long lifetime is simply the limit $V_0\rightarrow\infty$. The resonance wave function is exactly given by

$$\phi_n(r)=\left(\frac{2}{b}\right)^{1/2}\frac{\sin Q_nr}{[1+(bV_0+2iQ_nb)^{-1}]^{1/2}}\ , \tag{4.23}$$

and it is easily seen, by inserting the expansion of (4.22) into Eq. (4.23), that for $V_0\rightarrow\infty$ this wave function becomes the real, normalized box-quantization wave function appropriate to the range $(0,\ b)$.

For long lifetimes, the Kapur–Peierls eigenvalues are determined by the limit of Eq. (4.17), but this limit must be taken very carefully. First, if b is not equal to R_0, the condition upon $e_s(k)=q^2$ is

$$-\frac{k}{q}=i\,\frac{\cos q(R_0-b)}{\sin q(R_0-b)}\ . \tag{4.24}$$

This condition is necessary even if it is also true that $qb=n\pi$, as is seen by carefully applying l'Hopital's rule to Eq. (4.17). The eigenvalues q determined by Eq. (4.24) still depend upon k, and are complex. They seem to have no simple physical interpretation, and in this sense the Kapur–Peierls theory does not behave in a sensible way for high barriers.

It is evident from Eq. (4.24) that the Kapur–Peierls eigenvalues are still dependent upon the channel radius R_0, even in the limit $V_0\rightarrow\infty$. This extremely unsatisfactory feature is not shared by the Siegert poles $E_n=K_n^2$.

However, a second case arises for the special choice of channel radius $R_0=b$. In that case, the limit of Eq. (4.17) must be taken differently, and in that case the ultimate Kapur–Peierls eigenvalues approach the correct limiting values $q=n\pi/b$ for large V_0. Thus for this potential there exists a "correct" choice of channel radius for which the Kapur–Peierls theory behaves correctly in the long-lifetime limit.

Next we examine the solution for the same potential $v(r)=V_0\delta(r-b)$ for the case of *finite* potential V_0 and large energy k^2. For any $r<b$, one has

$$f(k;\,r)=(1+V_0/2ik)e^{-ikr}-(V_0/2ik)e^{-ik(2b-r)}\ . \tag{4.25}$$

Equation (4.21) is a special case of this formula. Defining $S(k)=f(k)/f(-k)$, the Green's function is then (for $0<r'<r<b$)

$$G(r,\,r';\,k)=(1/2ik)f(-k;\,r)[f(k;\,r')-S(k)f(-k;\,r')]\ . \tag{4.26}$$

This formula is a consequence of Eqs. (4.14) and (4.15). We shall examine the limiting behavior of $G(k)$ as $k\rightarrow\infty$.

If k approaches infinity in the upper half-plane, with large positive imaginary part, then $f(k;\ r)$ and $S(k)$ become finite while $f(-k;\ r)$ becomes zero. The dominant exponential behavior of $f(k;\ r')-S(k)f(-k;\ r)$ is then

$$f(k;\,r')-S(k)f(-k;\,r')\rightarrow\frac{1}{1-V_0/2ik}\,e^{-ikr'}$$

and therefore

$$G(r,\,r';\,k)\rightarrow\frac{1}{2ik}\,e^{ik(r-r')}+\frac{V_0}{1-V_0/2ik}\,e^{ik(b-r)}e^{ik(b-r')}\ .$$

All the exponentials decrease, because we have assumed $r>r'$, $b>r$, and $b>r'$; thus we have shown that

$$G(r,\,r';\,k)\rightarrow 0\ ,\quad \text{as } k\rightarrow\infty \text{ in the upper half-plane}\ . \tag{4.27}$$

If k is in the lower half-plane, $G(k)$ may have resonance poles near the real axis [at these poles $S(k)$ is infinite]. But if we examine the asymptotic values for large (negative) values of $\mathrm{Im}(k)$, we find

$$G(r,\,r';\,k)\rightarrow-(1/2ik)\,e^{-ik(r-r')}\rightarrow 0,\qquad \text{as } k\rightarrow\infty \text{ in the lower half-plane} \tag{4.27a}$$

and thus the Green's function $G(k)$ is *bounded* by its values near the real axis under the conditions $0<r'<r<b$.

If r or r' were outside the barrier, the situation would be quite different; the Green's function would approach infinity for large values of k.

Now the finite asymptotic values of Eq. (4.27) implies that $G(r,\ r';\ k)$ will be bounded on a set of concentric circles which avoid (pass between) the poles at $k=Q_n$. Then, according to the Mittag-Leffler theorem (quoted by Whittaker and Watson[30]), the Green's function may be represented as a sum

$$G(r,\,r';\,k)=\sum_n b_n(r,\,r')/k-K_n\ ,$$

where $b_n(r,\ r')$ is the residue at the pole K_n. This representation is of course the desired formula, expressing $G(k)$ in terms of the decaying-state wave functions $\phi_n(r)$. Occasionally it would be necessary to ensure convergence of the sum by reexpressing it in the "subtracted" form

$$G(r, r'; k) = G(r, r'; 0) + \sum_n b_n(r, r')\left(\frac{1}{k - K_n} + \frac{1}{K_n}\right),$$

as the latter form is more strongly convergent than the original form.

To summarize the discussion, it has been shown in some detail that for the special potential model of Eq. (4.20), the Mittag-Leffler representation of the Green's function exists for both r and r' within the barrier region.

V. CONCLUSION

In the preceding sections we have compared resonance wave functions obtained from the Siegert and Kapur-Peierls definitions of the resonance energies. The comparison especially clarifies the meaning of the normalization constant Z_n of the resonance wave functions ϕ_n. The factor Z_n contains a geometrical series which represents the feedback stabilization of the resonance state due to the coupling to the exterior continuum. In the model of Sec. III, we encountered a bound-state wave function which also had an anomalous normalization coefficient Z_0; in that case the real number Z_0 represented the *probability* that a particle known to be in the bound state would be found in the inner channel. For a true resonance, Z_n is not real and such a probability interpretation is not available.

The model of Sec. III was also an example for which the Siegert and Kapur-Peierls resonances were not in a one-to-one correspondence. In the potential scattering model discussed in Sec. IV, we showed that the Kapur-Peierls resonances do not necessarily behave properly in the limit of long lifetimes (unless one has made a specific felicitous choice of the channel radius). The Siegert resonances behave correctly in the limit whatever the channel radius, and this is an argument for the Siegert definition. However, the two resonance theories together seem more powerful than either would be separately.

In Sec. IV we explicitly constructed the Kapur-Peierls eigenvalue $e_r(k)$ and the normalization factor Z_n in terms of the Jost function for potential scattering. Finally we examined a specific simple barrier potential and showed that the analytic properties of the Green's function were suitable for the Mittag-Leffler expansion according to Eq. (1.4):

$$G(k) = \sum_n \frac{|\phi_n\rangle\langle\tilde{\phi}_n|}{2K_n(k - K_n)} . \tag{1.4}$$

In the remainder of this section we wish to indicate some implications of this expansion formula. We give only very abbreviated arguments, without any of the interesting details; our purpose is merely to underscore the potential utility of the resonance functions ϕ_n discussed in this paper.

One application is to the development of the complete "renormalized" perturbation theory. This theory is extracted from the representation (1.4) in a straightforward manner.[4] We introduce superscript zeros to distinguish the unperturbed quantities K_m^0 and ϕ_m^0, and again we assume that the perturbation operator V operates *only* in the inner channel. Then the complete (perturbed) Green's function G is related to the unperturbed Green's function G_0 by the usual operator equation

$$G(k) = G_0(k) + G_0(k)VG(k) .$$

There will be a pole of $G(k)$ whenever there is a solution eigenvector for the formal equation

$$1 = G_0(K_n)V ,$$

i.e., whenever there exists a state ϕ_n obeying

$$|\phi_n\rangle = \sum_n \frac{1}{2K_m^0} \frac{\langle\tilde{\phi}_m^0|V|\phi_n\rangle}{(K_n - K_m^0)} |\phi_m^0\rangle . \tag{5.1}$$

A more detailed derivation of this result appears in Ref. 4. The equation for ϕ_n has essentially the form of a Brillouin-Wigner perturbation expansion; i.e., K_n and ϕ_n appear on the right-hand side. Of course it is possible to expand them in terms of the unperturbed quantities and thereby obtain an explicit expression for K_n and ϕ_n to any given order.[4]

A second interesting application of the representation (1.4) for $G(k)$ is to study the time dependence of resonances. Such a study may be based upon the time-evolution operator $U(t) = e^{-iHt}$. This operator may be projected onto the state space of the inner channel, and the projection will also be denoted $U(t)$. This latter operator can be expressed as a Fourier transform of the Green's function as follows:

$$U(t) = -\frac{1}{2\pi i}\int_{-\infty}^{\infty} 2k\,dk\,G(k)e^{-ik^2t}$$

(if there are bound-state poles, the expression must be slightly altered). Applying expansion (1.4) for the Green's function, we can express $U(t)$ in the form

$$U(t) = \sum_n |\phi_n\rangle\, U_n(t)\, \langle\tilde{\phi}_n| , \tag{5.2}$$

which contains the function $U_n(t)$ defined by

$$U_n(t) = -\frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{k\,dk}{K_n} \frac{e^{-ik^2t}}{(k - K_n)} . \tag{5.3}$$

Thus, the time-evolution operator $U(t)$ has a very simple *diagonal* form in terms of the resonance wave functions.

However, the simple form (5.2) conceals some complex behavior. We shall mention two aspects of this behavior, without giving the mathematical details. First, the function $U_n(t)$ in Eq. (5.3) describes the nonexponential decay which holds at large time t. The function $U_n(t)$ may be evaluated by a contour deformation, which represents $U_n(t)$ as the sum of an exponential $e^{-iK_n^2 t}$ and a contour integral. The contour integral gives rise to the well-known $t^{-3/2}$ power law.[4,18–21] Second, and more interesting, the formula for $U(t)$ describes the mutual influence of two resonance states. Thus one can study the detailed dependence of decay characteristics on the choice of initial state. For this study, the nonorthogonality of the $|\phi_n\rangle$ appears to be an important special feature.

A discussion of the decay properties of such resonance systems would be quite interesting, but we do not pursue the topic further in this paper. However, the possibility of constructing detailed and exact formulas for the case of several resonances seems to us to provide a suitable justification for the further study of resonance wave functions.

APPENDIX: SYMMETRIES IN k PLANE

In this appendix we derive various symmetry relations for the resonance wave functions ϕ_n or Kapur–Peierls functions $\Phi_s(k)$ which were mentioned in Sec. II. Perhaps the best starting point is the familiar formula

$$G^{+}(k) = G(-k^*) \ . \tag{A1}$$

This formula, which may be verified in detail for the specific Green's functions of the models of Secs. II and IV, follows more generally from the Hermiticity of the total Hamiltonian and the nature of the inner-channel boundary conditions. A further argument tending to confirm the general validity of (A1) is the fact that the Green's function is a real operator for negative energies (i.e., it is real for real values of ik). By an operator analog of the Schwartz reflection principle, the relation (A1) then follows for any k.

Our first task is to relate the left and right Kapur–Peierls functions, which were defined in Eq. (2.4). We start from

$$\langle \tilde{\Phi}_s(k) | G(k) | x \rangle = [k^2 - \tilde{e}_s(k)]^{-1} \langle \tilde{\Phi}_s(k) | x \rangle$$

and take the complex conjugate, which is

$$\langle x | G^{+}(k) | \tilde{\Phi}_s(k) \rangle = [k^{*2} - \tilde{e}_s^{*}(k)]^{-1} \langle x | \tilde{\Phi}_s(k) \rangle \ . \tag{A2}$$

In this equation, as usual, $\langle \tilde{\Phi}_s(k) | x \rangle^* = \langle x | \tilde{\Phi}_s(k) \rangle$. Now, Eq. (A2) implies that $|\tilde{\Phi}_s(k)\rangle$ is a right eigenfunction of $G(-k^*)$, with the eigenvalue $[k^{*2} - \tilde{e}_s^{*}(k)]^{-1}$. Assuming the Kapur–Peierls states are nondegenerate, it thus is possible to label them in such a way that

$$\begin{aligned} |\tilde{\Phi}_s(k)\rangle &= |\Phi_s(-k^*)\rangle \ , \\ \tilde{e}_s^{*}(k) &= e_s(-k^*) \ . \end{aligned} \tag{A3}$$

Now just as the Green's function can be chosen to be real for negative real energies, so also can the eigenvalue and eigenfunction; again using the Schwartz reflection principle we deduce

$$\begin{aligned} e_s(-k^*) &= e_s^{*}(k) \ , \\ \langle x | \Phi_s(-k^*) \rangle &= \langle x | \Phi_s(k) \rangle^* \ . \end{aligned} \tag{A4}$$

From this it follows that

$$\begin{aligned} e_s(k) &= \tilde{e}_s(k) \ , \\ \langle x | \tilde{\Phi}_s(k) \rangle &= \langle x | \Phi_s(k) \rangle^* \ . \end{aligned} \tag{A5}$$

The second relation of Eq. (A5) shows the nature of the inner product:

$$\langle \tilde{\Phi}_s | \Phi_s \rangle = \int_0^{R_0} [\Phi_s(k;x)]^2 dx \ . \tag{A6}$$

This integral involves the complex square of the wave function, rather than the absolute square (here, R_0 is the channel radius).

The relations exhibited above differ only in notation from relations given in the original papers of Kapur and Peierls[8] and Peierls.[9] However, those authors advocate a different normalization of the function Φ_r.

The symmetry relation (2.9) now follows immediately from Eq. (A4).

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