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Theory of Decaying States*

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This paper constructs a special perturbation theory which directly describes the alteration of decaying states by an external perturbation. The complex energies of the decaying states appear in this theory. When lifetime effects are taken into account, we find that the criteria for quantum degeneracy are slightly strengthened and sharpened. We also discuss the smooth merger of the properties of decaying states and those of true eigenstates in the case of long lifetimes.

I. INTRODUCTION

It is intuitively clear that a decaying state closely resembles a true eigenstate, even though the two are distinguished by certain differences of detail. The differences are worth careful study, for all the excited states of real atomic and nuclear systems actually decay. The energy of a decaying state is usefully regarded as a *complex* number, for example—and the associated wave functions cannot be normalized. Despite these technical differences, there is a systematic correspondence between the properties of true eigenstates and those of decaying states, and for long lifetimes the two merge smoothly. We study this correspondence in a simple context in which an elementary mathematical treatment is practical. Some results are new; others merely strengthen or beautify theorems long known in the very extensive literature.[1–19]

This paper presents a special perturbation theory which directly describes the alteration of decaying states by an external perturbation.[1] The complex energies of the decaying states appear in this theory. In this way, we can study the near degeneracy of two levels with finite widths. Do they become degenerate (and strongly coupled) as soon as their wings overlap? This question was raised by Casalese and Gerjuoy in a study[20] of the Stark quenching of hydrogen spectra, but obviously it is a very general and fundamental question.

In the context of this work, we find the opposite result. The criteria for quantum degeneracy are slightly strengthened or sharpened when lifetime effects are included. Two levels with different widths may behave as if nondegenerate even when their centers overlap. The perturbation theory is discussed in Sec. V; the mathematical derivation is given in Sec. IV. The earlier sections establish properties of the wave functions associated with the decaying states.

For physical reasons, these methods are primarily of interest in applications to atomic or solid-state physics; however, the general theory of decaying states has been most extensively developed in the literature of high-energy physics[2–15] and nuclear physics.[16–19]

In the present paper, as in much of the cited literature, the system decays by tunneling through a potential barrier (see Fig. 1). There are many advantages to studying this model problem.[21] There is a well-developed theory of potential scattering developed by Jost, Pais, Regge, and many others[3–10]; we take over this theory and apply it. There are no unnecessary or inconvenient quantum numbers; we express the theory in very simple notation. Most of the essential problems already arise in the tunneling model, and it is itself of direct physical interest because many important physical systems decay via tunneling.[22] However, it would be quite interesting to extend the present theory to cases where the decay mechanism is autoionization, radiation of light, radiation of phonons, or other processes.

To study the tunneling model, we may consider the scattering of particles by a potential having a barrier and an inner region (see Fig. 1). This is one fundamental view of the decaying state; in this *scattering viewpoint*, our initial wave function is a plane wave or wave packet approaching the potential. The particle has a continuous energy spectrum, but certain energies are singled out as resonance scattering peaks. These energies e_n are defined only to within their widths Γ_n. It is well known that the Green's function and S matrix have a pole at the nearby complex energy $E_n = e_n + i\Gamma_n$. This pole gives one precise definition of e_n and Γ_n.[21–24] It is well known that resonance scattering is associated with large time delays (of the order of $\hbar/\Gamma_n$) during which the particle is "captured" or trapped behind the potential barrier.[2–4]

Another fundamental approach to a theory of decaying states is the *bound-state* viewpoint. Here one introduces an unperturbed Hamiltonian H_0 which is assumed to have true discrete eigenstates. In the barrier penetration case, H_0 might have an infinitely high barrier; there are discrete states inside the barrier and a continuum of exterior states. The discrete interior states have normalized wave

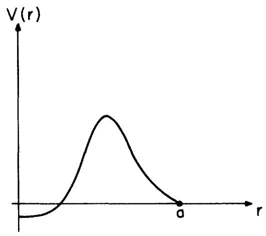

FIG. 1. A potential with a barrier.

functions ψ_n^0; from the bound-state viewpoint one of these is taken as the initial state of the system. The remainder of the Hamiltonian $H_1 = H - H_0$ causes a time dependence in the occupation of the state ψ_n^0; the particle is transferred outside with a characteristic time $T_n = \hbar / \Gamma_n$.

However there are technical difficulties with the bound-state viewpoint. In the tunneling problem, for example, H_1 cannot be a finite operator; it is the difference between the finite barrier of Fig. 1 and the infinite barrier of H_0. Also, there is a discontinuity in the description; even a tiny amount of tunneling formally causes a serious change in the mathematical nature of the eigenstates.

Ultimately the bound-state viewpoint is not as realistic as the scattering viewpoint. It deals with states ψ_n^0 which are not physically real, which are only defined with reference to the (arbitrary) choice of H_0. It is in the spirit of modern theoretical physics[25] to deal as far as possible with the physically real states, even when they are unknown or are mathematically complicated.[26] For all these reasons, the bound-state viewpoint is not mathematically or physically elegant.

We therefore adopt the scattering viewpoint. Working exactly in the scattering formalism, we attempt to identify features of the bound-state viewpoint hidden in the scattering theory. These features become especially clear and prominent in the case of long lifetimes, and we give close attention to that limiting case.

II. DECAYING-STATE WAVE FUNCTIONS

In order to know the real nature of anything, we must understand its resistance to changes. For example, when a decaying state of the complex energy E_n^0 is perturbed by a weak potential $\lambda u(r)$, then its energy is altered to[1]

$$E_n = E_n^0 + \lambda \int_0^\infty [\phi_n^0(r)]^2 \, u(r)\, dr + O(\lambda^2). \qquad (1)$$

The formula suggests that we consider the function $\phi_n^0(r)$ as a wave function for the (unperturbed) decaying state.

In Ref. 1, we have shown that the function $\phi_n(r)$ is related to the Jost function $f(k;r)$ by the formula (we omit superscripts to distinguish unperturbed quantities in this section)

$$\phi_n(r) = N_n f(K_n; r), \qquad (2)$$

where K_n is the (complex) wave vector of the decaying state, obtained as a solution of $f(K_n; 0) = 0$. In Eq. (2), the factor N_n is determined by

$$N_n^2 = -i f(-K_n)/f'(K_n), \qquad (3)$$

where $f'(k) \equiv (d/dk) f(k; 0)$. Equations (1)–(3) were derived in Ref. 1.

The Jost function $f(k;r)$ is that solution of the s-wave radial Schrödinger equation

$$\left(-\frac{d^2}{dr^2} + v(r) - k^2\right) f(k; r) = 0, \qquad (4)$$

specified by the boundary conditions

$$f(k; r) = e^{-ikr} \quad \text{for } r \geq a \qquad (5)$$

Here, as always, we assume that the potentials vanish beyond a finite fixed radius a. The general theory of Jost functions is reviewed by Newton[3] and by Goldberger and Watson.[4]

Our objective is to extend the perturbation formula (1) to higher-order terms. Although the result is simple, the derivation is distinctly difficult, because the decaying-state wave functions cannot be normalized nor are they mutually orthogonal. In fact the absolute value of $\phi_n(r)$ grows for large r (the imaginary part of K_n is positive). The integral which appears in (1) is finite, but only due to the properties of the potential.

The perturbation theory will have a characteristic non-Hermitian character. The wave function $\phi_n(r)$ is not real, and its complex square appears in (1) rather than the squared absolute value. This is perfectly proper and correct; the perturbation may alter the lifetime (and hence Γ_n) in first order. What is in a sense remarkable about the decaying state perturbation theory is the unification or integration of changes in the real and imaginary parts of the complex energies.

Formula (3) for the factor N_n is very similar to the Heisenberg expression for the bound-state normalization constant.[11] However, the significance is quite different. Whereas the bound-state normalization can be verified by integrating the absolute square of the wave function over the range $(0, \infty)$, in the case of a decaying state such an integral certainly diverges and the wave function cannot be normalized.

All the anomalous properties of decaying states gradually disappear in the limit in which their lifetimes become long. The wave function $\phi_n(r)$ defined above becomes real, normalized and even orthogonal to the wave functions of other decaying states. These are the properties we will now establish; they depend crucially (of course) on the choice (3) for the factor N_n.

Before considering the general case, we give a simple soluble example. In addition to providing general orientation, this example will aid us to anticipate the analytic properties of the quantities of the theory. We consider the special potential

$$v(r) = V_0\,\delta(r-b). \tag{6}$$

For this potential it is easy to determine $f(k;r)$ and $f(k) = f(k;0)$:

$$f(k) = 1 + (V_0/2ik)\,(1 - e^{-2ikb}). \tag{7}$$

The decaying-state wave vectors K_n are the solutions of the equation $f(K_n) = 0$. When V_0 is much larger than K_n, we have an expansion

$$K_n = \frac{\pi}{b}n - \frac{\pi}{b^2V_0}n + \frac{\pi}{b^3V_0^2}n + i\frac{\pi^2n^2}{b^3V_0^2} + O(V_0^{-3}). \tag{8}$$

Here the integer n may be positive or negative. The K_n appear in symmetrically placed pairs in the upper half k plane, as in general.

For the particular decaying state specified by K_n, we obtain

$$\phi_n(r) = \left(\frac{2}{b}\right)^{1/2} \frac{\sin K_n r}{[1 + (bV_0 + 2iK_nb)^{-1}]^{1/2}} \quad (r \leq b). \tag{9}$$

This is obtained by straightforward substitution into Eqs. (2 and 3) and is exactly true. In the limit in which V_0 approaches infinity, the K_n will become real [see Eq. (8)] and $\phi_n(r)$ will approach

$$\phi_n(r) = (2/b)^{1/2}\sin(n\pi r/b) \quad (r \geq b), \tag{9'}$$

which *is* the normalized (real) rigid-box wave function.

We argue that this simple behavior occurs generally, for an arbitrary potential $v(r)$. We begin with the differential equation (4) and the similar equation for a different wave vector k'. We multiply each equation by the Jost solution of the other equation, subtract, and then integrate from $r=0$ to $r = R \geq a$. The result is

$$(k^2 - k'^2)\int_0^R f(k;r)\,f(k';r)\,dr = \left(f(k;r)\frac{d}{dr}f(k';r) - f(k';r)\frac{d}{dr}f(k\,r)\right)\Bigg|_0^R. \tag{10}$$

Now we set $k' = K_n$, so that $f(k';0)$ is zero, and use the condition (5) to evaluate the contributions from $r=R$. The result is further simplified using a relation

$$\frac{d}{dr}f(K_n;0) = -\frac{2iK_n}{f(-K_n)} \tag{11}$$

proven in the Appendix of Ref. 1. We then obtain

$$\int_0^R \phi_n^2(r)dr = 1 + N_n^2\,(e^{-2iK_nR}/2iK_n), \tag{12}$$

which is exactly true for all $R \geq a$.

Note that the right-hand side of (12) becomes large as R grows. If we fix $\mathrm{Im}K_n$, i.e., fix the lifetime, and let R grow, then the integral of (12) diverges. Thus the decay state cannot be normalized on the interval $(0,\infty)$ for fixed K_n.

However, the limit taken in the other yields unity. If we *fix R*, and then let $\mathrm{Im}K_n$ become zero by raising the barrier height, the decaying state is ultimately "normalized" on the (arbitrary) finite interval $(0, R)$.

To establish this result, we must show that N_n^2 becomes zero in the limit of long lifetimes. This is the case in the example above. Our demonstration for the general case is plausible but not quite rigorous.[27] For k near K_n, we expand the Jost function $f(k)$ in a power series

$$f(k) = \alpha(k-K_n) + \beta(k-K_n)^2 + \cdots. \tag{13}$$

We assume that the linear term of this series dominates within the (small) circle of radius $2\mathrm{Im}K_n$, and so obtain the estimate

$$f(K_n^*) \cong -2i\alpha\,\mathrm{Im}K_n. \tag{13'}$$

We then recall the general theorem[3,4]

$$f(-k) = f^*(k^*), \tag{14}$$

and using this we obtain

$$N_n^2 \cong (2\alpha^*/\alpha)\,\mathrm{Im}K_n \tag{15}$$

for the factor N_n^2, which thus approaches zero linearly with $\mathrm{Im}K_n$. When this argument is correct,[27] the integral of Eq. (12) becomes unity in the limit of long lifetimes (for fixed arbitrary R). Thus the decaying-state wave function is *normalized* in that limit.

Again using Eq. (13'), we may show that the wave function $\phi_n(r)$ becomes *real*. In the long-life limit, when $\mathrm{Im}K_n$ is small, the differential equation has real coefficients. Thus if $\phi_n(r)$ begins being real near the origin, it can remain real out to $r=R$. Actually, $\phi_n(0)$ is zero, so we must examine $(d/dr)\phi_n(0)$. We compute this quantity from Eqs. (11) and (15). The result *is* real, whatever the phase of α.

If we return to Eq. (10) and let $k = K_n$ and $k' = K_m$, we can simply show that the wave functions of two decaying states exactly obey

$$\int_0^R \phi_n(r)\,\phi_m(r)\,dr = -N_nN_m\,[e^{-i(K_n+K_m)R}/i(K_n+K_m)] \tag{16}$$

for $n \neq m$.

Again using the estimate (15) we find the decaying-state wave functions to be *orthogonal* in the limit of long lifetime on a fixed interval $(0, R)$. The limit taken in the other order, i.e., on $(0,\infty)$ for finite lifetime, again yields infinity.

To summarize this discussion, we have shown that the decaying-state wave functions become real orthonormal wave functions for the limiting case of long lifetimes. This correspondence is scarcely surprising; it implies that the decaying-state perturbation theory which we will ultimately construct merges smoothly into the ordinary perturbation theory of discrete eigenstates in the appropriate limit.

III. DECAY OF A PREPARED STATE

In this section we show the existence of an initial state $\psi_n(0)$ which begins localized behind the barrier but in time decays out into the exterior region. Calculations of this type have often been given in the literature[2,4,7]; our approach differs in certain technical details. This section is a digression from the main theme of the paper.

The state $\psi_n(0)$ is normalizable. It is intimately connected with $\phi_n(r)$, but not the same. $\psi_n(0)$ is essentially concentrated or localized behind the potential barrier. However, it is not the eigenstate of some unperturbed Hamiltonian, but rather is a certain superposition of the real-energy continuum wave functions of the actual Hamiltonian.

Our initial state $\psi_n(0)$ is not alleged to be unique. In fact, it is a very subtle and interesting question how much ambiguity does exist in an "initial" state of a decaying system.[7] However we do not attempt to study these questions here, but content ourselves to exhibit the *one* initial state $\psi_n(0)$.

We introduce the continuum eigenstates of the actual radial Schrödinger equation (4) with real energy, following a notation of the textbook of Goldberger and Watson[3]; these states $w(k;r)$ obey

$$w(k;0)=0, \tag{17}$$

$$\lim_{r\to\infty} w(k;r)=(2/\pi)^{1/2}\sin(kr+\delta), \tag{17'}$$

where $\delta(k)$ is the s-wave phase shift. The limit in (17') is assumed for $r \geqq a$, since $v(r)=0$ for $r \geqq a$. The functions $w(k;r)$ are formally orthonormal in the sense that

$$\int_0^\infty w(k;r)w(k';r)\,dr=\delta(k-k'), \tag{18}$$

and are complete for a potential without bound states In order to abbreviate the notation, we assume that the potential has no bound states.

The phase shift $\delta(k)$ is related to the Jost function $f(k)=f(k;0)$ through the formula

$$e^{2i\delta(k)}=f(k)/f(-k). \tag{19}$$

In the sequel we will need to recall two properties of the Jost function, which are well known[3,4]: (i) $f(k)$ is entire, i.e., analytic for all finite k, and (ii) if there are no bound states, then $f(k)$ is nonzero for $\mathrm{Im}(k)$ negative, i.e., throughout the lower half k plane. These properties hold for a finite range bounded potential $v(r)$ with no bound states.

We concentrate on one decay state specified by the wave vector $K_n=K'+iK''$ which corresponds to a zero of $f(k)$ in the upper half-plane. Because these zeros appear in symmetrical pairs, we may assume both K' and K'' are positive.

Consider the function

$$A_0(r)\equiv\frac{1}{(2\pi)^{1/2}}\int_0^\infty \frac{e^{i\delta(k)}}{k-K_n}\,w(k;r)dk. \tag{20}$$

We shall show that this function is a suitable "prepared state" for the decay calculation. In order to develop its properties we consider first

$$A(r)\equiv A_0(r)+A_1(r)\equiv\int_{-\infty}^{\infty}\frac{\bar{A}(k)w(k;r)}{(2\pi)^{1/2}}\,dk$$

$$\equiv\frac{1}{(2\pi)^{1/2}}\int_{-\infty}^{\infty} e^{ika}\frac{e^{i\delta(k)}}{k-K_n}\,w(k;r)dk\,. \tag{21}$$

In this equation, we define $A(r)$, $A_1(r)$, and $\bar{A}(k)$. $A(r)$ is zero when $r\geq a$. In that case, $w(k;r)$ assumes the asymptotic form (17′) and we obtain

$$-A(r)=\frac{1}{2\pi i}\int_{-\infty}^{\infty} e^{ika}\,\frac{e^{-ikr}}{k-K_n}\,dk$$

$$-\frac{1}{2\pi i}\int_{-\infty}^{\infty} e^{ika}\,\frac{e^{2i\delta(k)}e^{ika}}{(k-K_n)}\,dk\,. \tag{21'}$$

The first integral is clearly zero, as we may displace its contour down into the lower half-plane. The second integral is also zero. Writing it

$$-(1/2\pi i)\int_{-\infty}^{\infty}[e^{ikr}e^{ika}/(k-K_n)][f(k)/f(-k)]\,dk\,,$$

we see that we are free to displace the contour into the upper half-plane. The integrand has no pole at K_n because $f(k)$ is zero there; and $f(-k)$ is nonzero throughout the upper half-plane. Thus we have shown

$$A(r)=0 \quad \text{for } r\geqq a. \tag{22}$$

Next, we show that $A_0(r)\gg A_1(r)$ in a certain sense. This result only holds when $K'\gg K''$ (i.e., in the case of a long-lived state). It is no surprise, because $A(k)$ is large in the region of integration of $A_0(r)$. Using the formal orthonormality relation (18), we compute

$$|A_0|^2\equiv\int_0^\infty |A_0(r)|^2dr=\frac{1}{2\pi}\int_0^\infty\frac{dk}{|k-K_n|^2}$$

$$=\frac{1}{2\pi K''}\left(\frac{\pi}{2}+\arctan\frac{K}{K''}\right),$$

$$|A_1|^2\equiv\int_0^\infty |A_1(r)|^2dr$$

$$= \frac{1}{2\pi K''} \left(\frac{\pi}{2} - \arctan \frac{K'}{K''} \right) .$$

Calling $x = K''/K'$, and assuming $x \ll 1$, it is clear that

$$|A_1|^2/|A_0|^2 = (x/\pi)\,[1 - O(x)] . \qquad (23)$$

In this sense $A_1(r)$ is small. When this limit $x \ll 1$ holds, we further have

$$\int_0^\infty |A_0(r)|^2 dr = (1/2K'')\,[1 - O(x)] . \qquad (24)$$

Now consider the properties of $A_0(r)$. (i) It is normalizable [see Eq. (24) above] unlike $\phi_n(r)$. (ii) It is primarily *localized* within the range $(0, a)$. This follows from the fact that for $r > a$, $A(r) = 0$ implies $A_0(r) = -A_1(r)$ and thus

$$|A_1|^2 = \int_0^\infty |A_1(r)|^2\, dr \geq \int_a^\infty |A_1(r)|^2\, dr$$

$$= \int_a^\infty |A_0(r)|^2\, dr.$$

Using (23) it follows that

$$\int_0^\infty |A_0(r)|^2\, dr \gg \int_a^\infty |A_0(r)|^2\, dr , \qquad (25)$$

and thus $A_0(r)$ is large only for $r < a$. (iii) Note also that $A_0(r)$ contains a *Lorenz state distribution*:

$$|\bar{A}(k)|^2 = [\, (k - K')^2 + K''^2]^{-1}.$$

We thus regard $A_0(r)$ as a suitable prepared state. We assume it is the initial state of a particle obeying the time-dependent Schrödinger equation

$$\Psi_n(r, 0) \equiv A_0(r) . \qquad (26)$$

We compute the portion remaining in this state at a later time t, given by $|R(t)|^2$, where

$$R(t) \equiv (1/|A_0|^2)\int_0^\infty \Psi_n^*(r, 0)\, \Psi_n(r, t)\, dr. \qquad (27)$$

Now it is evident that

$$\Psi_n(r,t) = (2\pi)^{-1/2}\int_0^\infty \bar{A}(k) w(k;r)\, e^{-ik^2 t}\, dk$$

and again using the formal orthogonality of the w's we see that

$$R(t) = \frac{1}{2\pi |A_0|^2} \int_0^\infty \frac{e^{-ik^2 t}}{(k - K')^2 + (K'')^2}\, dk. \qquad (28)$$

This formula is *exact*. It does not neglect contributions from other possible decaying states. The evaluation (or rather estimation) of this integral is straightforward. We swing the contour to run along the lower half-plan diagonal, and obtain the usual pair of contributions[2,4,7]: a decaying exponential and a nonexponential term which dominates at very short or very long times, but which is small compared to unity,

$$|R(t)|^2 = e^{-2\Gamma t} + O(x), \qquad (29)$$

where $\Gamma = 2K'K''$.

Thus $\Psi_n(0)$ is an acceptable localized initial state and decays according to the usual decay law. This state was constructed from the eigenfunctions of the *actual* Hamiltonian, with no artificial separation into perturbed and unperturbed parts. Our result is exact and does not neglect contributions from other decaying states. Both these features slightly extend the usual derivations of this result.

It can be shown (by a contour deformation) that

$$e^{iK_n a} f(K_n ; r) = A(r) + B(r) + C(r), \qquad (30)$$

where $A(r)$ is the function discussed above, $B(r)$ is zero when there are no bound states, and $C(r)$ is defined by a contour integral over a large semicircle in the upper half k plane

$$C(r) = \lim_{|k| \to \infty} \frac{1}{2\pi i} \int' e^{ika}$$

$$\times [f(k; r) - f(-k; r) f(k)/f(-k)]\, \frac{dk}{k - K_n} , \qquad (31)$$

On the contour of integration, we have $k = |k| e^{i\theta}$, where θ ranges over $(0, \pi)$. The separation indicated in Eq. (30) is evidently the removal of an "infinite frequency" portion of $f(K_n; r)$, in a sense suggested by Weiner.[28] It may be regarded as a projection of $f(K_n; r)$ into the Hilbert space of the continuum wave functions $w(k; r)$. The nonuniqueness of the initial state $\Psi_n(0)$ can be studied in this fashion, but we do not pursue this interesting question here.

To summarize, one may describe the decaying state by the wave function $\phi_n(r)$, which obeys a definite differential equation but cannot be normalized. Alternatively, one may describe it by the initial state $\Psi_n(0)$, which may be normalized but does not obey a differential equation and which is time dependent.

IV. DECAYING-STATE PERTURBATION THEORY

We now develop the perturbation theory for decaying states. At this point, it should be clear how *not* to proceed. One should not merely imitate the elementary derivation of eigenstate perturbation theory, for the required orthogonality and normalization theorems are not true.[29] They are approximately true (Sec. II) and by imitating the elementary derivation one could establish an approximate perturbation theory. It is possible to do better.

We begin with the *continuum* perturbation theory for the scattering wave functions $w(k; r)$. Through a technique of analytic continuation, we show that the continuum theory implies the decaying-state perturbation theory. The decaying-state theory is merely a recasting of continuum perturbation theory into a different form.

It is tempting to say that nothing new is obtained in this fashion, and that is perhaps logically correct. However, the decaying-state perturbation theory has the advantage of dealing with discrete states. An approximation, such as limiting the intermediate state sum to nearby states, is better defined and more appropriate in such a discrete theory. More important, for long-lived decaying states one is able to work directly with the resonance parameters of interest. Finally, the decaying state theory may be more generally valid.

The continuum perturbation theory is expressed in terms of a Green's function $G(r,r';q)$ defined by

$$G(r,r';q) \equiv \int_0^\infty w(k;r)\,w(k;r')\;\frac{dk}{q^2-k^2}\,. \tag{32}$$

This is the exact Green's function associated with the total potential $v(r)$. The continuum wave functions $w(k;r)$ are defined for real wave vector k only [see Eq. (17) above], whereas q is an arbitrary complex number. For complex q, no further boundary conditions are needed to define $G(q)$. Since there are two ways for q to become real, we should need boundary conditions to distinguish them; that will not prove necessary in this work. For each q, we formally have

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

The Green's function $G(q)$ has a *branch cut* along the real axis of the q plane. Since we continue to assume that there are no bound states for the potentials of interest, the branch cut is the only singularity of $G(q)$. The discontinuity of $G(q)$ across the cut is

$$\lim_{\beta\to 0}\left[G(q+i\beta)-G(q-i\beta)\right]=(-i\pi/q)w(q;r)w(q;r')\,, \tag{33}$$

where q is real. We wish to continue $G(q)$ to obtain a function with no branch cut, but with possible poles. In order to accomplish this, we recall the connection between $w(k;r)$ and the Jost function

$$w(k;r)=\frac{f(k)f(-k;r)-f(-k)f(k;r)}{i(2\pi)^{1/2}|f(-k)|}$$

$$\equiv\left(\frac{2}{\pi}\right)^{1/2}\frac{k\,g(k;r)}{|f(-k)|}\,. \tag{34}$$

This formula is valid for real k.[3,4] The function $g(k;r)$ defined above is often called $\phi(k;r)$ in the literature.[3,4] It is an entire function of k for each fixed r. Because of the absolute value appearing in (34), the integrand of Eq. (32) does not seem to be an analytic function of k. However, on the line of integration (i.e., for all real k) it is numerically true that

$$|f(k)|^2=|f(-k)|^2=f(k)f(-k),$$

which follows from Eq. (14). Thus the expression (32) is numerically equal to

$$G(r,r';q)=\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{k^2g(k;r)g(k;r')}{f(k)f(-k)}\;\frac{dk}{q^2-k^2} \tag{35}$$

but here the integrand is *meromorphic*. It is analytic but for poles at the zeros of $f(-k)$. Now it is possible to perform the analytic continuation of $G(q)$ by deforming the contour of integration in Eq. (35). The problem is soluble only because we have an explicit representation of $G(q)$ as the integral of a *meromorphic* function.

We define $\Gamma(q)$ to be the meromorphic function which agrees with $G(q)$ in the upper half q plane. The value $\Gamma(q)$ in the lower half q plane is obtained by deforming the contour in Eq. (35). We find that

$$\Gamma(r,r';q)=G(r,r';q)\quad(\mathrm{Im}\,q>0)\,, \tag{36}$$

$$\Gamma(r,r';q)=G(r,r';q)-2iq\,\frac{g(q;r)\,g(q;r')}{f(q)f(-q)}\quad(\mathrm{Im}\,q<0). \tag{37}$$

The result may be confirmed directly by comparison with Eq. (33). $\Gamma(q)$ is analytic in the upper half q plane, has no branch cut along the real axis, but has poles in the lower half q plane at $q=-K_n$, where K_n is a decaying-state wave vector. The poles are the only singularities. The residue at the nth pole is easily computed

$$\lim_{q\to -K_n}(q+K_n)\,\Gamma(r,r';q)=-(1/2K_n)\;\phi_n(r)\,\phi_n(r'). \tag{38}$$

We invoke the Mittag-Leffler theorem to write $\Gamma(q)$ as an infinite sum of partial fractions[30,31]:

$$\Gamma(r,r';q)=\sum_n[\phi_n(r)\;\phi_n(r')/(-2K_n)\;(q+K_n)]\quad(r<a,\,r'<a). \tag{39}$$

The convergence of such a representation depends upon the distribution of the larger K_n. If the potential vanishes beyond a finite radius a, then the K_n are distributed appropriately so that the Mittag-Leffler representation converges.[30,31]

It is *reassuring* to make a slight heuristic digression at this point in order to convince ourselves that the representation (39) *is* sensible in the case of long lifetimes.

The decaying states occur in mirror-image pairs, and we label them so that $K_{(-n)}=-K_n^*$. See Eq. (8) above for an example of this labeling. Then from Eqs. (2) and (3), it follows that

$$\phi_{(-n)}(r) = \phi_n^*(r) \ . \tag{40}$$

These symmetries occur in general. Now we consider $\Gamma(q)$ or $G(q)$ for long lifetime and for *both* $r, r' < a$. In that case, both ϕ_n and K_n become real. For positive Imq, $\Gamma(q)$ and $G(q)$ agree by Eq. (36); they are

$$G(r, r'; q) \cong \sum_{n>0} \frac{\phi_n(r)\,\phi\,(r)}{q^2 - K_n^2} \tag{41}$$

in the limit of long lifetimes. This is the expected result; each decaying state is correctly counted *once*. Note that the sum in (41) is over positive n only; that in Eq. (39) ran over all poles (positive or negative n).

The Green's function G and its continuation Γ refer to the exact potential $v(r)$. We denote all the corresponding unperturbed quantities by super- or subscript zeros and set

$$v(r) = v_0(r) + \lambda u(r), \tag{42}$$

and then we formally have

$$G = G_0 + \lambda G_0 u G. \tag{43}$$

Equation (43) is the continuum perturbation theory. The second term is an operator product. The equation may be continued into the lower half q plane, so that

$$\Gamma(r, r'; r) = \Gamma_0(r, r'; q) + \lambda \int_0^\infty \Gamma_0(r,s;q)\, u(s)\Gamma(s,r';q)\, ds. \tag{44}$$

We now extract and equate the residues of the two sides of this equation at the point $q = -K_n$. The resulting equation is

$$\phi_n(r) = \lambda \sum_m \frac{\phi_m^0(r)}{2K_m^0(K_n - K_m^0)} \int_0^\infty \phi_m^0(s) u(s)\, \phi_n(s)\, ds. \tag{45}$$

We may also extract and equate residues at $q = -K_n^0$, and this leads to a slightly different equation

$$\phi_n^0\,(r) = \lambda \sum_m \frac{\phi_m(r)}{2K_m(K_m - K_n^0)} \int_0^\infty \phi_n^0\,(s) u(s)\, \phi_m(s) ds. \tag{45$'$}$$

These equations form the basis for our perturbation theory. However they must be expanded carefully, as the term in the summations with $m = n$ will behave slightly differently from the other terms.

We write

$$K_n = K_n^0 + \lambda K_n^{(1)} + \lambda^2 K_n^{(2)} + \cdots,$$
$$\phi_n = \phi_n^0 + \lambda\, \phi_n^{(1)} + \cdots \ .$$

Expanding (45) and (45′) to first order in λ, we obtain the first- and second-order corrections to K_n^0. The first result is [see Eq. (1) above]

$$2 K_n^{(1)}\, K_n^0 = U_{nn}, \tag{46}$$

where we define

$$U_{nm} \equiv \int_0^\infty \phi_n^0(r)\, u(r)\, \phi_m^0(r)\, dr. \tag{47}$$

From Eq. (45) alone, we cannot determine $\phi_n^{(1)}(r)$ completely. But we can show that

$$K_n^{(2)} = {\sum_m}' \left[U_{nm}^2 / 4K_n^0 K_m^0\, (K_n^0 - K_m^0)\right], \tag{48}$$

where the prime on the summation indicates omission of the term with $m = n$. It is important that the (well-behaved) term with $m = -n$ be included in the summation.

Using Eq. (45) in conjunction with (45′), we find the first-order change in $\phi_n(r)$. The result is

$$\phi_n^{(1)}(r) = N_n^{(1)}\ \phi_n^0\ (r) + {\sum_m}' \left[U_{nm}\, \phi_m^0(r) / 2K_m^0\, (K_n^0 - K_m^0)\right], \tag{49}$$

where

$$N_n^{(1)} \equiv K_n^{(2)} / 2K_n^{(1)} + K_n^{(1)} / 2K_n^{(0)}. \tag{50}$$

Now we examine the "energies" $E_n = K_n^2$. The results are

$$E_n^{(1)} = U_{nn} = \int_0^\infty [\,\phi_n^0(r)]^2 u(r) dr, \tag{51}$$

which is Eq. (1) above, and

$$E_n^{(2)} = 2K_n^0\, K_n^{(2)} + [\,K_n^{(1)}]^2 = \frac{U_{nn}{}^2}{4E_n^0} + {\sum_m}' \frac{U_{nm}^2}{2K_m^0(K_n^0 - K_m^0)} \ . \tag{52}$$

This equation, which looks somewhat strange, may be shown to reduce to the usual result in the long lifetime limit. For in that case the quantities U_{nm} become real as do the K_n. The sum in Eq. (52) runs over both signs of m; we rearrange the sum to obtain

$$E_n^{(2)} \cong {\sum_{m>0}}' \left[U_{nm}^2 / (E_n^0 - E_m^0)\right] \tag{53}$$

in the long lifetime limit. Equation (53) is of course correct. The decaying-state perturbation theory reduces to eigenstate perturbation theory in the limit of long lifetimes.

V. DISCUSSION

We now review and discuss our results. We have introduced wave functions $\phi_n(r)$ to describe decaying states. These functions solve a complex-energy Schrödinger equation, but are not "proper" wave functions because they cannot be normalized. However in the limit of long lifetimes, we have shown that they become real, normalized, and mutually orthogonal on any appropriate fixed interval. Thus they reduce to eigenstate wave functions in the limit of long lifetimes.

We have studied a "projection" of $\phi_n(r)$ onto the scattering states of real energies. The result is an interesting initial state $\Psi_n(r;0)$ which begins localized behind the barrier but gradually decays out into the continuum.

We have constructed a perturbation theory which gives the changes in $\phi_n(r)$ and the associated complex energies E_n caused by a weak perturbation.

The simplest practical application of the resulting theory is to avoid the use of the WKB approximation in a discussion of tunneling problems. This is already an important application, we believe. One can compute the tunneling through the true potential $v(r)$ by choosing a simpler approximate potential $v_0(r)$ and then using the perturbation theory.

However, a much more general and more interesting application is to the near degeneracy of two decaying states. This will not normally occur in problems of the type we have been discussing, and there is no doubt that further mathematical analysis is required before absolutely reliable results can be obtained. Nevertheless we *can* suggest the implications of the work of Sec. IV, for these implications are quite clear.

As we see in Eqs. (48) and (52), it is the *differences* of two K_n's which appear in the "energy denominators" of the theory. The small denominators which signal degeneracy or near degeneracy cannot occur unless *both* real and imaginary parts of the complex energies of the two states are equal.

Thus we are led to a sharpening of the concept of degeneracy of two quantum states. Two energy levels will strongly mix for a weak perturbation only if both their centers and lifetimes coincide. The case where the centers coincide but the widths are very different should be considered a sort of "false" degeneracy, not associated with strong mutual influence (for weak perturbations).

This conclusion is very easily understood from rate-equation arguments.[32] Consider a very narrow (long-lived) state E_1 and a broad state E_2, and suppose the line centers coincide. Is the long-lived state strongly mixed with the short-lived state? No, for instead of resonating between the two states, a system transferred from state E_1 to state E_2 will probably decay before being transferred back to E_1. This conclusion obviously depends on the strength of the perturbation relative to the lifetimes of E_1 and E_2.

In this way a large difference in lifetimes can make states behave as if nondegenerate even when their centers overlap. This conclusion is probably very well known in other contexts (e.g., theory of electric circuits) and follows from rate equation arguments for quantum systems. The present derivation is more convincing.

We conclude with a number of technical comments on the decaying-state perturbation theory. We have already mentioned the *non-Hermitian* character of the theory. This is seen in the definition (47) of the matrix elements U_{nm}, in the appearance of U_{nm}^2 in (48) instead of an absolute square, and in the complexity of the K_n.

A very interesting point is the unambiguous expression (50) for the amount of $\phi_n^0(r)$ contained in $\phi_n^{(1)}(r)$. In this respect the decaying-state perturbation theory differs from elementary eigenstate perturbation theory.[29] The usual ambiguity of this overlap is associated with an ambiguity in the phase of an eigenstate. In the decaying-state theory, there is no such ambiguity.

This apparently formal difference has probably a deep and subtle physical content. It is intimately connected with the separation of "unlinked" diagrams of many-body perturbation theory, for that separation is connected with a manipulation of the phase of the "vacuum" state.[33]

Another related open question is the relation of this theory to adiabatic perturbation theory.[33] A time-dependent perturbation theory, with adiabatic switching of the perturbation $u(r)$, is not permissible when the system decays. It is well known that the adiabatic perturbation theory differs from elementary perturbation theory in the values of the ambiguous "overlap" phases mentioned above.

There is one unsatisfactory feature of the decaying-state perturbation theory worth further study. If the perturbation $u(r)$ is located *outside* the barrier, it appears to have a strange effect on the decaying states. Here again, one has a question of correct of limits. If we fix the barrier height and move $u(r)$ to larger values of r, we obtain a strange or confusing result. If instead we *fix* the location of $u(r)$ and then raise the barrier height, the influence of $u(r)$ upon the decaying-state parameters becomes weaker and weaker as N_n approaches zero.

It will be interesting to attempt to extend the present theory to the general case. Low has given a general treatment of decaying states in quantum electrodynamics, from a different viewpoint.[34] The rate equation approaches give interesting indications for the general case.[32] In the case of systems decaying through a *weak* coupling, the decaying-state perturbation theory may be obtained by performing the perturbations in other order, although this approach is subject to the difficulties discussed in the Introduction.

There are many other interesting aspects of decaying-state theory. For example, all the present work has been conditioned on the Jost-function approach to defining the resonance parameters.[3,4] There is another (slightly different) definition due to Kapur and Peierls[24] and a perturbation theory may also be constructed for that case. There exist also interesting variational theorems for decaying-state wave functions.[35] These variational theorems strengthen further the correspondence between the properties of decaying states and those of true eigenstates.

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[27]This argument is not rigorous. For long lifetimes, α itself approaches infinity. That alone does not affect the estimate given in Eq. (15); but it is not obvious without proof that the second term of the expansion (13) remains negligible in the limit. For the example of Eqs. (6)–(9), the approximation (13′) *is* justified.

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