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UNSTABLE STATES WITH SIMPLE POTENTIALS

by

Robert Earl Kingman

A Dissertation Submitted to the Faculty of the
DEPARTMENT OF PHYSICS
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1971
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ABSTRACT

A method recently developed by K. Just which describes simple decay processes is presented. Explicit solutions of Schroedinger's equation are obtained for a certain class of potentials. The resulting decay laws display deviations from a purely exponential decay which might be observable. Bound states and resonances result from the assumption of a bare state and a continuum of eigenstates of the "unperturbed" Hamiltonian $H_0$ for certain potentials. These follow from the roots of the function $D(\omega)$ central to the theory. Explicit solutions are obtained for simple potentials and the poles and residues of $D(\omega)^{-1}$ are presented for more realistic potentials.
CHAPTER 1

INTRODUCTION

It is well known that the "stationary" states of a hydrogen atom as calculated from the Schroedinger theory are, except for the ground state, unstable. The spontaneous decay of an excited state is well described within the framework of Quantum Electrodynamics. An exponential decaying state may be obtained by the method of Weisskopf and Wigner (1) or by using perturbation theory approximations with complex energies. A method elaborated by K. Just describes simple decay processes by an explicit solution of Schroedinger's equation for a certain class of potentials. The decay is described by an integral involving a complex function of the energy, D(ω). The approximation of Weisskopf and Wigner is obtained if one takes this function as ω - k_0 + iγ/2. Better approximations to the function reveal considerably more structure to the decay.

The method is useful in describing resonant scattering for two level systems, in processes for which the ground state and one excited state are important. The ground state plus an incident particle form a continuum of states φ^k, where k is the energy of the states. The state φ resulting after the absorption is the excited state of 1
the two level system which subsequently decays by emission of a similar particle to the continuum states $\phi^k$. From the point of this paper the manner of formation of the excited state is unimportant; it might be formed by other mechanisms such as decay from another excited state or by collisions in the case of atomic physics. Hence we consider $\phi$ as the "prepared" state (in the usual sense of quantum mechanics). This means we consider explicitly only the right half of the diagram relevant for resonant scattering.

The ground and excited states are assumed to contain all the structure except for that relevant to the absorption and decay. Again for atomic physics this would include the nucleus, electrons, photons mediating the Coulomb interaction, and the Lamb shift photons. The states $\phi$ and $\phi^k$ are "bare" in the sense that they are eigenstates of that part $H_0$ of the Hamiltonian which does not contain the interaction $V$ responsible for the radiative transitions. However, $H_0$ shall contain all the energies relevant for the internal structure of the states $\phi^k$, including all the interactions within these states. Therefore the interaction $V$ considered as relevant for the radiative transitions will be assumed not to act among these states; $(\phi^k, V\phi^l) = 0$. This assumption makes it possible to obtain explicitly the stationary states, $\psi^w$,
of the total Hamiltonian $H = H_0 + V$. The only nonvanishing matrix elements of $V$ in the basis are $(\phi^k, \phi^l) \equiv V(k)$ and $V(k)^*$ corresponding to the excitation to the higher state, $\phi$. The vanishing of $(\phi, \phi^k)$ corresponds merely to a shift of the level $k_0$ of $\phi$. While a rigorous justification of the vanishing of $(\phi^k, \phi^k)$ would be inextricably connected with the decomposition of the Hamiltonian and the resulting eigenstates $\phi^k$ of $H_0$, the previous arguments make it physically reasonable.

The final results will contain $V(k)$ only quadratically. Therefore they will be valid also if $|V(k)|^2$ would be replaced by an integral $\int |V(k, \theta)|^2 d\theta$ over the states with the same eigenvalue $k$ of the bare energy $H_0$, distinguished by degeneracy parameters $\theta$ such as the direction of emitted photon. The phase space factors entering this integral will here be incorporated into an "effective" potential $V(k)$, analogous to that appearing in the radial Schrödinger equation. The square root appearing in our last example for $|V(k)|^2$ corresponds therefore to $S$ wave scattering.

In addition to the continuum of states with energies $\omega$ there may also be several discrete states, $\psi_{\Omega_i}$, with energies $\Omega_i$, $i = 1, 2, 3, \ldots$, the zeroes of $D$. These states correspond to bound states formed by the ground state and the incident particle. These well known results can in the present approach be discussed in detail.
Energy shifts are also obtained but they may be unrealistic since the contributions from the other excited and unbound states are not included in our two level model.

The Weisskopf and Wigner and other methods are described in the references (2-10).
CHAPTER 2

METHOD OF K. JUST

2-1 A Basis for the Hilbert Space

One begins as in perturbation theory by separating the Hamiltonian into two hermitian operators, $H_o + V$. The eigenstates of $H_o$ are taken to be orthonormal and are complete by the definition of our Hilbert space. For simplicity we assume that the spectrum of $H_o$ consists of a single discrete state $\phi$, and a continuous set of eigenvectors $\phi^k$. A decomposition of $H$ is sought such that the only nonzero matrix elements of $V$ occur between the states $\phi$ and $\phi^k$. Thus we have

\[
\begin{align*}
H_o \phi &= k \phi \\
H_o \phi^k &= k \phi^k \\
(\phi, \phi) &= 1 \\
(\phi, \phi^k) &= 0 \\
(\phi^k, \phi) &= 0 \\
(\phi^k, V \phi^k) &= 0 \\
(\phi^k, V \phi) &= V(k). 
\end{align*}
\]  

(2.1)
The method has been generalized to include the cases of degeneracy and many bound states. As these details are not pertinent to this study they have not been included.

2-2 Stationary States

We seek to express the eigenfunctions of the total Hamiltonian as linear combinations of the \( \phi \)'s. Denoting the energies of the states by \( \omega \) we have

\[
H \psi^w = \omega \psi^w
\]  

(2-2)

with

\[
\psi^w = \int \phi^\ell c(\ell,\omega) d\ell + \phi c(\omega).
\]  

(2-3)

The coefficients may be obtained by taking the inner products

\[
(\phi, H \psi^w) = \omega (\phi, \psi^w) = (\phi, (H_o + V) \psi^w)
\]

which with (2-3) give

\[
(\phi, [H_o - \omega + V] [\int \phi^\ell c(\ell,\omega) d\ell + \phi c(\omega)]) = 0.
\]

With equations (2-1) this expression simplifies to

\[
(k_o - \omega)c(\omega) + \int V(\ell)^* c(\ell,\omega) d\ell = 0.
\]  

(2-4)

Similarly from the inner products \( (\phi^k, H \psi^w) \) one obtains

\[
(k - \omega)c(k,\omega) + V(k)c(\omega) = 0.
\]  

(2-5)

Henceforth \( V \) shall designate the function \( V(k) \).
Realistic potentials will have some threshold $\tau$, i.e., the minimum "energy" of the states $\phi^k$ below which $V(k)$ will vanish. As in solid state physics there may also exist a band structure so that $V(k)$ might be illustrated as in Figure 2-1. If $\omega$ lies in a region of nonzero $V$, i.e., in the support of $V$, $c(k,\omega)$ becomes singular at $k = \omega$. We consider this case first. The singularity in the distribution $c(k,\omega)$ may be handled by letting $\omega \rightarrow \omega_c \equiv \omega + i\epsilon$ where $\omega$, $\epsilon$ are real and $\epsilon > 0$. Since one can always add the zero distribution to (2-5) the general solution is

$$c(k,\omega) = \eta^\omega \delta(k-\omega) + (\omega_c - k)^{-1} V(k) c(\omega)$$

(2-6)

where $\eta^\omega$ is complex. Here $\epsilon$ is taken positive and in Appendix C the $\eta^\omega$ are shown to be arbitrary phase factors with the $\delta(k-\omega)$ term essential for the orthogonality and completeness of the $\psi$'s. As an alternate approach note that if the function $V(k)$ can be analytically continued near the singularity of $c(k,\omega)$ we can deform the integration path around the singularity. The most general way is to take a linear combination of paths deformed above and below the singularity. As indicated symbolically in Figure 2-2 this can be done in several ways. We choose the $b$ representation where the integration around the singularity corresponds to a delta function. With (2-6) we may solve (2-4). Thus
Figure 2-1. Simple potential forms.

(a) unphysical  (b) no band structure  (c) band structure

Figure 2-2. Integration contours for equation (2-5).
\[ [k_o - \omega + \int (\omega - \ell)^{-1} |V(\ell)|^2 d\ell] c(\omega) + \eta^w V(\omega)^* = 0, \]

or

\[ c(\omega) = \eta^w V(\omega)^*/D(\omega) \]  \hspace{1cm} (2-7)

with

\[ D(\omega) = \omega - k_o + \int (\ell-\omega)^{-1} |V(\ell)|^2 d\ell. \]  \hspace{1cm} (2-8)

As indicated symbolically in Figure 2-3 this last result may be written

\[ D(\omega) = \omega - k_o + \oint (\ell-\omega)^{-1} |V(\ell)|^2 d\ell + i\pi |V(\omega)|^2 \]  \hspace{1cm} (2-9)

so that \( D(\omega) \neq 0 \) for \( V(\omega) \neq 0 \).

Figure 2-3. The integral expressed by its principal part.

For \( \omega \) in a region of zero \( V \) note that \( c(k,\omega) \) has no singularities and (2-5) gives

\[ c(k,\omega) = (\omega-k)^{-1} V(k) c(\omega) \]  \hspace{1cm} (2-10)

which with (2-4) implies \( D(\omega) = 0 \). Taking the derivative of \( D \) we see that

\[ D'(\omega) = 1 + \oint (\ell-\omega)^{-2} |V(\ell)|^2 d\ell \geq 0 \]  \hspace{1cm} (2-11)
since the integrand is never negative. Note the $\varepsilon$ need not be retained here because $V(\omega) = 0$. Thus $D(\omega)$ is a monotonic increasing function of $\omega$ in regions of $V(\omega) = 0$, and hence cannot vanish more than once in each of these regions. $D(\omega)$ vanishes once below the bare state level $k_o$ if $\tau_1 > k_o$, since $D(-\infty) \to -\infty$ and $D(k_o) = \int_{-\infty}^{\infty} (\ell - k_o)^{-1} |V(\ell)|^2 \, d\ell > 0$, while it may vanish once for $\omega < \tau_1$ if $\tau_1 < k_o$. Thus we see that there are only discrete solutions $\omega = \omega_a$ to (2-10) giving discrete energy eigenstates $\psi_{\omega_a}$. For the potentials we consider in numerical detail there will be at most one discrete state $\psi$ with energy $\Omega$, since our potentials are of types (a) and (b) in Figure 2-1.

Since any vector of a basis is determined up to an arbitrary phase we are free to set $\eta^w$ to unity. Thus (2-3) becomes

$$\psi = \int \phi^* \, c(\ell, \Omega) \, d\ell + \phi \, c(\Omega)$$

$$\psi^w = \int \phi^* \, c(\ell, w) \, d\ell + \phi \, c(w)$$

with

$$(\psi, \psi) = 1$$

$$(\psi, \psi^w) = 0$$

$$(\psi^w, \psi^\sigma) = \delta(w-\sigma),$$

(2-13)
where \[ c(k,\omega) = \delta(k-\omega) + (\omega - k)^{-1} V(k) \ c(\omega) \]
\[ c(\omega) = V(\omega)^* / D(\omega) \]
\[ D(\omega) = \omega - k_0 + \int (\ell - \omega)^{-1} |V(\ell)|^2 \ d\ell \]
\[ (2-14a) \]
for \( \omega \in \text{supp } V \), and
\[ c(k,\Omega) = (\Omega - k)^{-1} V(k) \ c(\Omega) \]
\[ c(\Omega) = [D'(\Omega)]^{-1/2} \]
\[ = [1 + \int (\ell - \Omega)^{-2} |V(\ell)|^2 \ d\ell]^{-1/2} \]
\[ D(\Omega) = 0 \]
\[ (2-14b) \]
for \( \Omega \notin \text{supp } V \). The result for \( c(\Omega) \) follows from the normalization of the state \( \Psi \) as shown in Appendix C, equation (C-11). The orthogonality and completeness of the states \( \Psi^w, \Psi \) shown there allow us to invert (2-12) and obtain
\[ \phi = \int \Psi^w c(\omega)^* d\omega + \Psi c(\Omega)^* \]
\[ \phi^{\ell} = \int \Psi^w c(\ell,\omega)^* d\omega + \Psi c(\ell,\Omega)^* . \]
\[ (2-15) \]

**2-3 Transition Amplitudes**

With these relations and defining the time translated counterparts of the eigenstates of \( H_0 \)
\[ \phi(t) \equiv U_t \ \phi \]
\[ \phi^k(t) \equiv U_t \ \phi^k \]
\[ (2-16) \]
where the unitary operator $U_t$ is

$$U_t = e^{iHt}$$

we calculate the transition amplitudes from the states $\psi^k$, $\psi$ to $\phi(t)$ and $\phi^k(t)$. With the help of (2-15), (2-16), (2-13), and the fact that

$$U_y^Y = e^{iHt} = e^{i\Omega t}$$

$$U_y^w = e^{iwt}$$

we obtain

$$\varphi(t' - t) = (\phi(t'), \phi(t))$$

$$= (\int e^{iwt} \phi^*(w) dw + e^{i\Omega t} \phi^*(\Omega))$$

$$= \int e^{-i\omega(t' - t)} |c(\omega)|^2 dw + e^{-i\Omega(t' - t)} |c(\Omega)|^2.$$

In this way one obtains

$$(\phi(t'), \phi(t)) = \varphi(t' - t)$$

$$(\phi(t'), \phi^k(t)) = \varphi(k, t' - t)$$

$$(\phi^k(t'), \phi^l(t)) = \varphi(k, l, t' - t)$$

(2-18)
where

\[ \varphi(t) = \int e^{-i\omega t}|c(\omega)|^2d\omega + e^{-i\Omega t}|c(\Omega)|^2 \]

\[ \varphi(k, t) = \int e^{-i\omega t}c(\omega)c(k, \omega)^*d\omega + e^{-i\Omega t}c(\Omega)c(k, \Omega)^* \]

\[ \varphi(k, \ell, t) = \int e^{-i\omega t}c(k, \omega)c(\ell, \omega)^*d\omega + e^{-i\Omega t}c(k, \Omega)c(\ell, \Omega)^* \]

(2-19)

The physical problem is defined when states \( \phi, \phi^k \) are given with their inner products and the operator \( V \) is specified by its nonvanishing matrix elements \( V(k) = (\phi^k, V\phi) \). In practice the form of \( V(k) \) may not be known or the function \( D(\omega) \) may be too complicated for practical computation. In Chapter 4 approximation techniques are discussed which allow \( D(\omega) \) to be replaced by approximations suited to computation. In the case that \( V(k) \) is unknown it is worthy to note that \( |V(k)|^2 \) and \( k_0 \) may be recovered from a given \( D(k) \). This follows from (2-9) because

\[ D(k) - D(k)^* = 2\pi i |V(k)|^2 \]

\[ k_0 = \int (\ell - i\epsilon)^{-1} |V(\ell)|^2d\ell - D(0). \]  

(2-20)
CHAPTER 3

STATES FOR SIMPLE POTENTIALS

In order to demonstrate the nature of the method and its solutions we now consider several simple forms for the potential \( V \).

3-1 Square "Barrier" Potentials

Consider potentials of the form

\[
V(k) = v[\Theta(k-T_1) - \Theta(k-T_2)]
\]

then from (2-8) for \( w \in \text{supp } V \)

\[
D(w) = w - k_0 + v^2 \int_{T_1}^{T_2} (\ell - w)^{-1} d\ell
\]

\[
= w - k_0 + v^2 \lim_{\epsilon \to 0} \left[ \ln(\ell - w) \right]_{T_1}^{T_2}
\]

\[
+ \ln(\ell - w) \bigg|_{T_1}^{T_2} + i\pi v^2
\]

\[
D(w) = w - k_0 + v^2 \ln \frac{T_2 - w}{T_1 - w}
\]

which is also valid for \( w /\notin \text{supp } V \). From (2-14) we obtain

\[
c(w) = 0 \quad w /\notin \text{supp } V
\]

\[
c(k, w) = 0
\]
while
\[ c(w) = v[w - k_o + v^2 \ln \frac{\tau_2 - w}{\tau_1 - w}] - 1 \]
\[ c(k, w) = \delta(k-w) + (w - k)^{-1} \left[ v^2 (w-k_o) + \ln \frac{\tau_2 - w}{\tau_1 - w} \right] \]

As discussed on page 10 the discrete states occur for
\[ D(\Omega) = 0 \quad \Omega \notin \text{supp } V. \]

Let us assume \( k_o < \tau_1 \); then looking for a root for \( \Omega < \tau_1 \) we have
\[ \Omega - k_o + v^2 \ln \frac{\tau_2 - \Omega}{\tau_1 - \Omega} = 0 \quad (3-2) \]

Since the log term is positive we see as illustrated in Figure 3-2 that a single state exists with \( \Omega < k_o \). Taking
The origin at $k_0$ and measuring the energy in units of $v^2$, we get

$$\Omega + \ln \frac{\tau_2 - \Omega}{\tau_1 - \Omega} = 0 \quad (3-3)$$

For $\Omega > \tau_2$ we again obtain the equations (3-2) and (3-3). As an ansatz for an approximation solution to (3-3) write

$$\tau_2 = \tau_1 + \Delta$$

which for

$$\Delta \ll \tau_1 - \Omega$$

gives

$$\Omega + \frac{\Delta}{\tau_1 - \Omega} = 0 \quad (3-4)$$
or

\[ \Omega^2 - \tau_1 \Omega - \Delta = 0 \]

which gives

\[ \Omega = \frac{\tau_1}{2} - \sqrt{\frac{\tau_1^2}{4} + \Delta \frac{\Delta}{\tau_1}} \]  

consistent with (3-4). This form is useful for the \( \Omega < \tau_1 \) solution which requires the negative radical.

For the \( \Omega > \tau_2 \), write (3-3)

\[ \tau_2 - \Omega = (\tau_1 - \Omega) e^{-\Omega} \]

\[ \Omega = \frac{\tau_2 - \tau_1 e^{-\Omega}}{1 - e^{-\Omega}} \]  

which for \( \tau_2 \gg 1 \) gives

\[ \Omega = \tau_2 + \Delta e^{-\Omega} \]

or

\[ \Omega \approx \tau_2 + \Delta e^{-\tau_2}. \]  

Note that these results depend only on the separations \( \tau_1 - k_0, \tau_2 - k_0 \).

The constants \( c(\Omega), c(k, \Omega) \) are given by (2-14) and (3-1), with
\[ c(\Omega)^{-2} = D'(\Omega) = 1 + \frac{v^2(2\Omega - \Omega_1 - \Omega_2)}{(\Omega_2 - \Omega)(\Omega_1 - \Omega)} \]

or

\[ c(\Omega)^2 = \frac{(\Omega_2 - \Omega)(\Omega_1 - \Omega)}{\Omega^2 + (2v^2 - \Omega_1 - \Omega_2)\Omega + \Omega_1 \Omega_2 - v^2(\Omega_1 + \Omega_2)} \quad (3-8) \]

thus we obtain the two discrete eigenstates of the total Hamiltonian from (2-12) to be

\[ \psi_{1,2} = [\int_{\tau_1}^{\tau_2} \phi^L v(\Omega_1,2,2 - \xi) - \xi d\xi + \phi] c(\Omega_{1,2}) \quad (3-9) \]

and the continuum states

\[ \psi^w = \phi^w + [\int_{\tau_1}^{\tau_2} \phi^L v(w,2 - \xi) - \xi d\xi + \phi] c(w) \quad (3-10) \]

with

\[ c(w) = V(w)^*/D(w) = v \frac{Q(w - \Omega_1) - Q(w - \Omega_2)}{w - k_o + v^2 \ln \frac{\Omega_2 - w}{\Omega_1 - w}} \]

We see from (3-10) that the \( \psi^w \) and \( \phi^k \) states have the same spectral range. Furthermore we see that \( \psi^w = \phi^w \) for \( w \notin \text{supp } V \), i.e., the interaction does not affect these states. The relative contributions of \( \phi^L \) to \( \psi^w \) are illustrated in Figure 3-3.
The transition probabilities follow from the square of the amplitudes (2-18),

\[ \varphi(t) = \sqrt{2} \int_{\tau_1}^{\tau_2} e^{-i\omega t} \left[ (w-k_0 + \nu^2 \ln \frac{\tau_2 - w}{\nu^2 \tau_1} + \frac{\nu^4 \pi}{2} \right]^{-1} \]

\[ + \sum_{j=1,2} e^{-i\Omega_j t} \left( c_j \right)^2 \]  

and similarly for the other amplitudes. The complicated integral can be evaluated with contour integration by approximating the \( R(w) \equiv D(w)^{-1} \) appearing in the integrand, by a single valued complex function which essentially vanishes on the real axis outside the support of \( V \). In the case in which \( \tau_2, - \tau_1 \rightarrow \infty \) from (3-1) we see that

\[ D(w) \rightarrow w - k_0 + i \gamma/2 \]
with

$$\gamma = 2\pi v^2$$

and the integral of (3-11) reduces to

$$v^2 \int_{-T}^{T} e^{-i\omega t} \left[ (\omega-k_o)^2 + \gamma^2/4 \right]^{-1} d\omega$$

$$= v^2 \int_{-T}^{T} e^{i\omega t} \left[ (\omega-k_o+i\gamma/2)^{-1}[\omega-k_o-i\gamma/2]^{-1} d\omega$$

$$= e^{-ik_o t} - \gamma t/2$$

which gives for (3-11)

$$\varphi(t) = e^{-\gamma t/2-ik_o t}$$

(3-13)

Figure 3-4. Contour integration evaluation of (3-12) -- In the lower half plane $R(-i\omega) < 0$. 
Note that $\Omega_k \rightarrow \tau_k$ and $c(\Omega_k)$ become negligible. Thus we see that the state $\phi$ is unstable with a component decaying at a rate $\gamma$. Note that the results of this approximation correspond to the approximation of Weisskopf and Wigner (1). See also page 311 of reference (2).

### 3-2 Inverse Square Root Potentials

With $V$ given by

$$V(k) = v \Theta(k-\tau)(k-K)^{-1/2}$$

it is

$$\tau > K$$

one obtains

$$D(w) = w - k_0 + v^2 \int_{\tau}^{\infty} (\ell-w)^{-1}(\ell-K)^{-1} d\ell + i\pi v^2(w-K)^{-1}$$

$$= w - k_0 + v^2(w-K)^{-1}(p \int_{\tau}^{\infty}[(\ell-w)^{-1}(\ell-K)^{-1}]d\ell + i\pi)$$

$$= w - k_0 + v^2(w-K) \ln \frac{\tau-K}{\tau-w}.$$  \hspace{1cm} (3-15)

Figure 3-5. States of $H_0$ with the potential (3-14) where $L$ is the lowest energy of the states $\phi^k$. 
Using the units of (3-1) we find that a bound state occurs for

\[ \Omega(\Omega - K) + \ln \frac{\tau - K}{\tau - \Omega} = 0 \] (3-16)

which is satisfied for \( \Omega < 0 \) corresponding to the discussion of page 7. The root \( \Omega = K \) of (3-16) comes from the multiplication of (3-15) by \( \Omega - K \) and is extraneous since \( D(K) = K + (\tau - K)^{-1} \neq 0 \).

\[ \begin{align*}
\text{Figure 3-6. Bound states for equation (3-16).}
\end{align*} \]

### 3-3 Hyperbolic Potentials

As a third example we consider potentials of the form

\[ V(k) = \nu \theta(k - \tau) (k - K)^{-1}, \tau > K \]

which gives for \( \omega \in \text{supp } V \)
\[ D(w) = w - k_0 + v^2 \int_{\tau}^{\infty} (\ell - w)^{-1}(\ell - K)^{-2} d\ell + i\pi v^2(\omega - K)^{-2} \]

\[ = w - k_0 + v^2(\omega - K)^2 \left[ \int_{\tau}^{\infty} (\ell - w)^{-1}(\ell - K)^{-1} + (\omega - K)(\ell - K)^{-2} d\ell + i\pi \right] \]

\[ D(w) = w - k_0 + v^2(\omega - K)^2 \left[ \ln \frac{\tau - K}{\tau - \omega} + \frac{\omega - K}{\tau - K} \right]. \quad (3-17) \]

Again the same expression is valid for \( w < \tau \). The bound state occurs for

\[ (\Omega - K)^2(2\Omega - K) + \ln \frac{\tau - K}{\tau - \Omega} = 0. \quad (3-18) \]

Eliminating the extraneous roots at \( \Omega = K \) this again gives a discrete state at \( \Omega < 0 \).

### 3-4 Sawtooth Potentials

We now consider the form

\[ V(k) = v[\theta(k - \tau_1) - \theta(k - \tau_2)] (\tau_2 - k)/\Delta \]

with \( \Delta \equiv \tau_2 - \tau_1 \). Then for \( w < \tau_1 \)

\[ D(w) = w - k_0 + \frac{v^2}{\Delta^2} \int_{\tau_1}^{\tau_2} \frac{(\tau_2 - \ell)^2}{\ell - w} d\ell \]

which gives

\[ D(w) = w - k_0 - y^2 + \frac{v^2}{\Delta} (\tau_2 - w)^2 \ln \frac{\tau_2 - w}{\tau_1 - w}. \quad (3-19) \]
This expression is valid for all \( w \), as can easily be verified. For this \( V \), bound states occur if

\[
\Omega - 1 + \left( \frac{\tau_2 - \Omega}{\tau_2 - \tau_1} \right)^2 \ln \frac{\tau_2 - \Omega}{\tau_1 - \Omega} = 0
\]

for

\[ \Omega \not\in [\tau_1, \tau_2]. \]
CHAPTER 4

NUMERICAL EXAMPLES

From the preceding examples we have seen that complicated expressions for \( D \) arise from simple forms for \( V \) making difficult the calculations for the transition amplitudes (2-9). We now consider a potential for which the amplitudes can readily be obtained.

4-1 Lorentzian Potentials

For potentials of the form

\[
V(\ell) = v(\ell - c + i \gamma/2)^{-1}
\]

and assuming the continuum states \( \phi^k \) extend from \(-\infty \leq k \leq \infty\) we obtain for \( D \)

\[
D(\omega) = \omega - k_o + v^2 \int_{-\infty}^{\infty} (\ell - \omega)_{\ell}^{-1} [(\ell - c)^2 + \gamma^2/4]^{-1} d\ell.
\]

Using contour integration in the lower half plane we obtain

\[
D(\omega) = \omega - k_o - \frac{2\pi v^2}{\gamma(\omega - c + i\gamma/2)}
\]

with no possibility for bound states since \( V \) does not vanish. In order to calculate \( \varphi(t) \) from (2-19) we first look at \( c(\omega) \),

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Figure 4-1. Lorentzian potential.

Figure 4-2. Contour of integration for $D(\omega)$. 
$v^2 |c(w)|^{-2} = [(w-c)^2 + \gamma^2/4] |D(w)|^2$

$= [(w-k_0)(w-c) - 2\pi v^2/\gamma]^2 + (w-k_0)^2 \gamma^2/4. \quad (4-3)$

A contour integration gives $\varphi(t)$ in terms of the roots of (4-3), i.e., the poles of $D(w)^{-1}$ in (4-2),

$v^2 |c(w)|^{-2} = (w-w_1)(w-w_1^*)(w-w_2)(w-w_2^*) \quad (4-4)$

with

$w_K = r_K - i \gamma_K/2 \quad K = 1, 2.$

Then

$\varphi(t) = v^2 \int e^{-i\omega t} \frac{dw}{(w-w_1)(w-w_1^*)(w-w_2)(w-w_2^*)}$

$= v^2 \int e^{-i\omega t} \left( \frac{1}{w-w_1} - \frac{1}{w-w_2} \right) \frac{dw}{(w-w_1)(w-w_2)(w-w_1^*)(w-w_2^*)}$

or

$\varphi(t) = \frac{2\pi v^2}{(w_1-w_2)} \left[ \frac{e^{-\gamma_1 t/2} - i r_1 t}{\gamma_1(w_1-w_2^*)} - \frac{e^{-\gamma_2 t/2} - i r_2 t}{\gamma_2(w_2-w_1)^*} \right] \quad (4-5)$

for $t > 0$. From (4-2, 3, 4) we see that

$(w-w_1)(w-w_2) = (w-k_0)(w-c) - 2\pi v^2/\gamma + i(w-k_0)\gamma/2$

$= (w-r_1+i\gamma_1/2)(w-r_2+i\gamma_2/2)$
which gives

\[ r_1 + r_2 = c + k_o \quad r_1 r_2 - \gamma_1 \gamma_2 / 4 = k_o c - 2\pi v^2 / \gamma \]

\[ \gamma_1 + \gamma_2 = \gamma \quad \gamma_1 r_2 + r_1 \gamma_2 = k_o \gamma. \quad (4-6) \]

To solve for the real constants \( r_K, \gamma_K \) note that these equations imply

\[ (r_1 - r_2)(\gamma_1 - \gamma_2) = (r_1 + r_2)(\gamma_1 + \gamma_2) - 2(r_1 \gamma_2 + r_2 \gamma_1) \]

\[ = (c+k_o)\gamma - 2k_o \gamma = (c-k_o)\gamma \equiv b \]

\[ (r_1 - r_2)^2 - (\gamma_1 - \gamma_2)^2 / 4 = (r_1 + r_2)^2 - (\gamma_1 + \gamma_2)^2 / 4 - 4r_1 r_2 \]

\[ + \gamma_1 \gamma_2 = b^2 / \gamma^2 - \gamma^2 / 4 + 8\pi v^2 / \gamma - 4k_o c \equiv a \]

which in turn give

\[ (r_1 - r_2)^4 - a(r_1 - r_2)^2 - b^2 / 4 = 0 \]

\[ (\gamma_1 - \gamma_2)^4 / 4 + a(\gamma_1 - \gamma_2)^2 - b^2 = 0 \]
or

\[ 2(r_1-r_2)^2 = \sqrt{a^2+b^2} + a \]

\[ (\gamma_1-\gamma_2)^2/2 = \sqrt{a^2+b^2} - a. \]  

(4-7)

Then the constants follow from (4-6) and (4-7), while (4-5) becomes

\[ \varphi(t) = \frac{2\pi v^2}{r_1-r_2+i(\gamma_1-\gamma_2)/2} \left[ \frac{-\gamma_1 t/2-ir_1 t}{\gamma_1(r_1-r_2)-i\gamma/2} - \frac{-\gamma_2 t/2-ir_2 t}{\gamma_2(r_2-r_1)-i\gamma/2} \right] \]

(4-8)

with \( t > 0 \).

Choosing \( k_0 \) as the zero point of the energy and its unit such that \( 8\pi v^2/\gamma^2 = 1 \), corresponding to a decay rate of 1 in the W. W. (Weisskopf and Wigner) approximation we see that (4-8) depends only on two real parameters, say for instance the center \( c \) of the potential, and its width \( \gamma \).

In Figures A-1 to A-6 the values of \( r_K, \gamma_K \), and the differences of the residues \( p_1 - p_2, q_1 - q_2 \) of \( R(w) \equiv 1/D(w) \) are shown by contours in the \( \gamma, c \) plane. Since
\[ R(w) = \frac{w-c+i\gamma/2}{(w-w_1)(w-w_2)} = \frac{w-w_1-w_2}{(w-w_1)(w-w_2)} \]

\[ = \frac{w_2}{(w_2-w_1)(w-w_1)} + \frac{w_1}{(w_1-w_2)(w-w_2)} \]

\[ p_1+iq_1 = \frac{w_2}{w_2-w_1} = \frac{r_2-i\gamma/2}{r_2-r_1-i(y_2-y_1)/2} \]

\[ = \frac{r_2(r_2-r_1)+y_2(y_2-y_1)/4+i\gamma r}{(r_2-r_1)^2+(y_2-y_1)^2/4} \]

\[ p_2+iq_2 = \frac{w_1}{w_1-w_2} \]

\[ p_1+p_2+i(q_1+q_2) = 1 \]

\[ p_1 = (1+p_1-p_2)/2 \]

\[ p_2 = [1-(p_1-p_2)]/2 \]

\[ q_1 = -q_2 = (q_1-q_2)/2, \quad (4-9) \]

the \( p_k, q_k \) are immediately recoverable from the differences. Furthermore simple checks are provided by (4-6), for example the \( r_1 = -1, r_2 = 2 \) contours intersect at \( r_1 + r_2 = c = 1, \gamma = .53 \). Only positive \( \gamma, c \) are needed because \( \gamma < 0 \) is not needed and for \( c > -c, r_1 > -r_2, r_2 > -r_1, \gamma_K > \gamma_K \) as is seen from (4-6) and (4-7), while equation (4-9) shows that \( p_1 > p_2, p_2 > p_1, q_1 > -q \frac{r_1}{r_2}, \)
q_2 \Rightarrow -q \frac{r_2}{r_1^2}. The dependence upon c reflects the influence of the discrete eigenstate \phi since c is the difference between the potential center and k_o, while the k's were assumed to range from negative to positive infinity. For \gamma \gg 2\pi v^2 = 1, V is essentially flat and in this region Figures A-3, A-4 show that \gamma_1 \approx 1 while \gamma_2 \gg 1 causing (4-8) to reduce to the W.W. result (3-13). For \gamma = 2 the state \phi decays at about half the W.W. rate. From (2-12), and Figure 4-4, we see that the state \phi makes its largest contribution to the resulting stationary states y^w at w = r_1, r_2. The energy "shifts" become quite large, especially that of r_2, which varies slowly with \gamma.

Figure 4-4. Contribution of the bare state \phi to y^w for a Lorentzian potential.
A Smoothed "Barrier" Potential

While (4-1) is unrealistic it might be useful as an approximation for the interaction of radiation with atoms. A more realistic potential would be a smoothed version of Figure 3-5. One such form is

\[ V(\ell) = \nu \frac{(\ell-\tau)^{1/4}}{(\ell-\tau+\gamma)^{1/2}} \Theta(\ell-\tau) \quad (4-10) \]

which has a lower threshold at \( \tau \), "width" \( \gamma \), a maximum value at \( \tau + \gamma = \infty \), the "center" of the potential, and tends to zero as \( \ell^{1/4} \) for \( \ell \to \infty \). With it

\[ D(\nu) = \nu - k_o + \nu^2 \int_\tau^\infty \frac{\sqrt{\ell-\nu}}{(\ell-\nu)(\ell-\tau+\gamma)} d\ell \]

for \( \nu < \tau \). Rationalizing the integrand with \( k^2 = \ell - \tau \) we have

\[ D(\nu) = \nu - k_o + 2\nu^2 \int_0^{\infty} \frac{k^2}{(k^2+\tau-\nu)(k^2+\gamma)} \frac{dk}{k^2+\tau-\nu} \]

\[ = \nu - k_o + \frac{2\nu^2}{\nu-\tau+\gamma} \int_0^{\infty} \left[ \frac{\nu-\tau}{k^2+\tau-\nu} - \frac{\gamma}{k^2+\gamma} \right] dk \]

\[ D(\nu) = \nu - k_o + \frac{2\nu^2}{\nu-\tau+\gamma} \left[ -\sqrt{\nu-\tau} \tan^{-1} \frac{k}{\sqrt{\nu-\tau}} + \sqrt{\gamma} \tan^{-1} \frac{k}{\sqrt{\gamma}} \right]_0^{\infty} \]
Figure 4-5. Smoothed potential barrier.

\[ D(w) = w - k_o + \frac{\pi v^2}{\sqrt{\gamma} + \sqrt{\tau-w}} \]  

(4-11)

which is valid for all \( w \). We assume that the states \( \phi^k \) exist over interesting regions of \( k \). Taking \( w > \tau \) and \( \gamma \gg 1 \) and evaluating the denominator term at the maximum of \( V, \tau + \gamma \), gives

\[ D(w) \approx w - k_o + \left(1 - \frac{i}{2}\right) \frac{\pi}{\tau} \frac{v^2}{\sqrt{\gamma}}. \]

If we choose our origin at \( k_o = 0 \), and our scale such that \( V(\ell_{\text{max}}) = V(\tau+\gamma) = 1/\sqrt{2\pi} = \frac{v}{\sqrt{2}} \frac{1}{\sqrt{\gamma}} \), then \( v^2 = \sqrt{\gamma}/\pi \) and

\[ D(w) \approx \omega + \frac{1}{1 + \frac{\tau-w}{\sqrt{\gamma}}} \]

corresponding to a \textit{W.W.} rate of 1 and (4-11) becomes

\[ D(w) = w + \frac{1}{1 + \sqrt{\tau-w}/\gamma} = w + (1+z)^{-1} \]  

(4-12)
with \( z^2(w) = (\tau - w) / \gamma \). The zeros of \( D \) are given by

\[
\omega^2(\tau - w) / \gamma = \omega^2 + 2\omega + 1
\]

or

\[
\omega^3 + (\gamma - \tau)\omega^2 + 2\gamma \omega + \gamma = 0 \quad (4-13)
\]

and the residues of \( R(\omega) = 1/D(\omega) \) become

\[
P_K + i q_K = \frac{1}{2\pi i} \oint \frac{dz}{D(z)} = \frac{1}{2\pi i} \oint \frac{dz}{D'(\omega_K)(z - \omega_K)} + ... = 1/D'(\omega_K).
\]

Since \((4-12)\) with \( D(\omega) = 0 \) gives \( z = -(\omega + 1) / \omega \), hence

\[
D'(\omega) = 1 + \frac{1}{(z+1)^2} \left( \frac{1}{2\gamma z} = 1 - \frac{\omega^3}{2\gamma(\omega+1)}, \right.
\]

and we obtain

\[
P_K + i q_K = \frac{2\gamma(\omega_K+1)}{2\gamma(\omega_K+1) - \omega^3}. \quad (4-14)
\]

If we replace the discontinuous \( D \) of \((4-12)\) with the continuous function on two sheets

\[
D_I(\omega) = \omega + \left[ 1 + \sqrt{\frac{\tau - w}{\gamma}} \right]^{-1} \quad \text{first Riemann sheet}
\]

\[
D_{II}(\omega) = \omega + \left[ 1 - \sqrt{\frac{\tau - w}{\gamma}} \right]^{-1} \quad \text{second Riemann sheet}
\]

we can evaluate the functions of \((2-19)\) by approximating \( R(\omega) = D^{-1}(\omega) \) as described below and performing a contour
integration. For $t > 0$ the $I^+$, $II^-$ complex plane is needed. We assume here that the zeros of $D$ lie far from the branch point. Then the important root lies in the $II^-$ plane, lying nearest the contour of integration. Thus

$$D(w) \approx w - (w_2 - i\gamma_2/2)$$

gives

$$\varphi(t) \approx v^2 \int_{-\infty}^{\infty} e^{-iw t} \frac{(w-\tau)^{1/2} Q(w-\tau)}{(w-\tau+\gamma)(w-w_2+i\gamma_2/2)(w-w_2-i\gamma_2/2)} \, \mathrm{d}w$$

$$+ e^{-i\Omega t} |c(\Omega)|^2$$

$$\approx -\frac{iv^2}{\gamma} \frac{\sqrt{w_2-\tau-i\gamma_2/2}}{w_2-\tau+\gamma-i\gamma_2/2} e^{-\gamma_2 t/2-iw_2 t} + e^{-i\Omega t} |c(\Omega)|^2,$$  \hspace{1cm} (4-17)

if the bound state $\Omega$ exists, i.e., if $D(\Omega) = 0$ in the first sheet, where
\[ |c(\Omega)|^2 = \frac{1}{D'(\Omega)} = \text{residue of } D(\Omega)^{-1} \]

otherwise

\[ |c(\Omega)|^2 = 0. \]

Motivated by these results we discuss the poles and residues of \( D(\omega)^{-1} \) as implied by (4-13). Depending on \( \gamma, \tau \) we get a real root \( \omega_1 \) and a conjugate pair \( \omega_K = r_2 \pm iy_2/2 \), or three real roots. The real root \( \Omega \) lies in the first sheet if in (4-12) \( z = -1 - 1/\Omega > 0 \). Thus we have a bound state if the root \( \omega = \Omega \) satisfies \(-1 < \Omega < 0 \). Otherwise the roots lie in the second sheet. This is consistent with the general property that \( D(\omega) \) can vanish in the first sheet only for \( \omega \) real, and \( \not\in \text{supp } V \) as can be seen from the analytic continuation of (2-8). Because \( D(\omega) \) can vanish only once in each connected region of vanishing \( V \), we can here have at most a single bound state, \( \Psi \) as discussed on page 7. In Figures B-1 to B-12 we display the solutions \( \omega_K = r_K - iy_K/2 \) of (4-13) and the corresponding residues of \( D^{-1} \) as contour lines in the \( \gamma, \tau \) plane. While only \( \gamma > 0 \) is relevant, \( \tau < 0 \) and \( \tau > 0 \) must both be considered and give quite different results as would be expected from Figure 4-5. The real roots in the first sheet are indicated in Figures B-1, B-7 by solid lines, those in the second sheet by dotted lines, in Figures B-2-B-3, B-8-B-9 while the real parts in Figures B-2, B-8 and the imaginary parts in B-3, B-9 of the conjugate root pairs are dashed. The residues
are indicated correspondingly. We proceed to discuss these graphs. For real roots, (4-13) gives

\[ \gamma = \frac{w^2(\tau - w)}{(w+1)^2} \]  

so that the \( w = \) constant contours are linear with slopes \((w+1)^2/w^2\) and intercepts \( w \). Therefore the bound states \((-1 < w < 0)\) fill the upper \( \gamma \), \( \tau \) plane above \( \tau = -1 \) and the "anti" bound states for \( w < -1 \) fill the \( \gamma \), \( \tau \) plane below \( \tau = -1 \), and extend into the right \( \tau > -1 \), \( \gamma \) region. At the boundary between real and complex solutions, \( D \) has a repeated root,

\[ D(w) = (w-r_1)(w-r_2)^2 \]

so that \( D(w) = 0 \) implies \( D'(w) = 0 \), or from (4-13)

\[ 3w^2 + 2(\gamma - \tau)w + 2\gamma = 0. \]

From (4-18) for real roots we obtain

\[ w^3 + \gamma^2 + 2\gamma w + \gamma = 0 \]

Elimination of \( w \) between the last two equations gives the equation

\[ (\tau+1)\gamma^2 - (2\tau^2 + 9\tau + 27/4)\gamma + \tau^3 = 0 \]

or

\[ \gamma = \frac{2\tau^2 + 9\tau + 27/4}{2(\tau+1)} \left[ 1 \pm \sqrt{1 - \frac{4\tau^3(\tau+1)}{(2\tau^2 + 9\tau + 27/4)^2}} \right] \]  

(4-19)
for the boundary between the real and complex solutions, as shown by the O curve in B-3. The cusp, corresponding to the double root of (4-19), occurs for

\[(\tau + \frac{3}{8})^3 = 0\]

or

\[\tau = -\frac{9}{8}, \gamma = \frac{27}{8}, w = -\frac{3}{2}. \quad (4-20)\]

Figures B-7 to B-12 show the behavior of the roots and residues near the cusp. For large \(\tau\) boundaries go as

\[\gamma = (\tau + 7/2)(1 \pm \sqrt{8/\tau})\]

or

\[\gamma_\pm \approx \tau \pm \sqrt{8\tau} \quad \tau \gg 1\]

and we see that the upper right region of complex solutions continues to widen as \(\tau\) increases. For small \(\tau\)

\[\gamma_\approx \approx 4\tau^3/27 \quad \tau << 1.\]

A second set of real zeroes in the second sheet appears in the upper left hand \(\gamma, \tau\) plane, with \(w \geq \tau \geq 0\). In order to avoid contour intersections for the 3 real roots, they are plotted as follows. For \(-1.5 < w < -1\) the contours extend from \(\gamma = 0\) to the point at which they become tangent to the lowest boundary curve, for \(w < -1.5\) the contours are drawn to the intersection of the lowest boundary in B-1, and continue in B-3 to the point of tangency with the
intermediate boundary, while in B-2 the contours are continued from the point of tangency through the upper right \( \gamma, \tau \) plane. For \( \psi > 0 \) the contours are plotted to the point of tangency from below in B-3 and continued upward in B-2.

For \( \gamma = -\tau > 0 \) the potential is centered above the bare state, \( \phi \). In this case we obtain a decay rate about that of the W.W. rate, and energies of the resonance at about -.5 [see our normalization of (3-12)]. When \( \tau \geq 0 \), we get \( r_2 < \tau \), so that there the resonance poles lie to the left of the branch point as is also the case for all the real roots displayed in B-1. For \( \gamma \approx \tau \) the bound state poles lie at about -.5.
APPENDIX A

NUMERICAL RESULTS FOR LORENTZIAN POTENTIALS

In the following six graphs the poles $w_K = r_K - i\gamma_K/2$ and residues $p_K + iq_K$ of the complex function $R(\omega) \equiv D(\omega)^{-1}$ in equation (4-2), are given as contours in the $\gamma, c$ plane. Figures A-1 and A-2 give the real part of the poles $r_K$, A-3 and A-4 the imaginary parts $\gamma_K$, while A-5 and A-6 give only $\Delta p = p_1 - p_2$, $\Delta q = q_1 - q_2$. As shown in equation (4-9b), $p_K$ and $q_K$ are immediately recoverable from the differences. Thus once the width $\gamma$ and the center $c$ of the Lorentzian potential equation (4-1) are specified the transition amplitudes such as $\varphi(t)$ of equation (4-8) are determined. Only the first quadrant is plotted since $\gamma > 0$ and the discussion of page 27 shows that the $c < 0$ solutions follow from this quadrant.
Figure A-1. The real part, $r_1$, of the first pole of $R(w)$ from equation (4-2).
Figure A-2. The real part, \( r_2 \), of the second pole of \( R(\omega) \) from equation (4-2).
Figure A-3. The imaginary part, $\gamma_1$, of the first pole of $R(\omega)$ from equation (4-2).
Figure A-4. The imaginary part, $\gamma_2$, of the second pole of $R(\omega)$ from equation (4-2).
Figure A-5. The differences, $\rho_1 - \rho_2$, of the real parts of the residues of $R(w)$ from equation (4-2).
Figure A-6. The differences, $q_1 - q_2$, of the imaginary parts of the residues of $R(\omega)$ from equation (4-2).
APPENDIX B

NUMERICAL RESULTS FOR A SMOOTHED POTENTIAL

The poles \( w_k = r_k - i\gamma_k/2 \) and residues \( p_k + iq_k \) of \( R(w) = D(w)^{-1} \) for the potential equation (4-10) are given as contours in the \( \gamma, \tau \) plane in the following 12 graphs. Figure B-1 shows the real roots \( w = r_1 \), B-2 the real roots \( w = r_2 \) or the real part of the complex pair of roots \( w = w_k + i\gamma_k/2 \) and B-3 the real roots \( w = r_3 \) or the complex part of \( w \). Figure B-4 shows the real residues \( p_1 \), B-5 the real residues, or the real part of complex residues \( p_2 + iq_2 \), and B-6 the complex part of the residues. Figures B-7 to B-12 give an enlarged plot near the cusp occurring at \( \tau = -1.125, \gamma = 3.375, w = -1.5 \), where the functions vary rapidly. The boundstate quantities are illustrated by solid lines and the resonance pole quantities by dashed lines. The dotted lines represent the real poles and residues in the second sheet.

From these graphs for a particular potential width \( \gamma \) and threshold \( \tau \), the transition amplitudes such as \( \varphi(t) \), equation (4-17), are determined.
Figure B-1. Real poles of $R(\omega)$ from (4-10) -- The solid lines represent the bound state poles, $\omega = r_1$, in the first sheet while the dotted lines give the real poles, $\omega = r_1$, in the second sheet.
Figure B-1. Real poles of $R(w)$ from (4-10).
Figure B-2. Poles of \( R(w) \) from (4-10) -- The dashed lines represent the real parts of the complex poles, while the dotted lines give the real poles, \( w = r_2 \), in the second sheet.
Figure B-2. Poles of $R(w)$ from (4-10).
Figure B-3. Poles of $R(\omega)$ -- The dashed lines represent the imaginary parts of the complex poles, while the dotted lines give the real poles, $\omega = r_3$, in the second sheet.
Figure B-3. Poles of $R(w)$. 
Figure B-4. Residues of the real poles of $R(w)$ from (4-10) -- The solid lines represent the bound state residues of $R(w)$, while the dotted lines give the residues for the real poles, $r_1$, in the second sheet.
Figure B-4. Residues of the real poles of $R(w)$ from (4-10).
Figure B-5. Residues of the complex poles of $R(\omega)$ from (4-10) -- The dashed lines represent the real parts of the residues of $R(\omega)$ from the complex poles, while the dotted lines give the residues for the real poles, $r_2$, in the second sheet.
Figure B-5. Residues of the complex poles of $R(w)$ from (4-10).
Figure B-6. Residues of the complex poles of $R(w)$ — The dashed lines represent the imaginary parts of the residues of $R(w)$ from the complex poles, while the dotted lines give the residues for the real poles, $r_3$, in the second sheet.
Figure B-6. Residues of the complex poles of $R(\omega)$. 
Figure B-7. Real poles of $R(uu)$ in the second sheet near the cusp.
Figure B-8. Poles of $R(w)$ from (4-10) near the cusp -- The dashed lines represent the real parts of the complex poles, while the dotted lines give the real poles, $w = r_2$, in the second sheet.
Figure B-8. Poles of \( R(u) \) from (4-10) near the cusp.
Figure B-9. Poles of $R(\omega)$ near the cusp — The dashed lines represent the imaginary parts of the complex poles, while the dotted lines give the real poles, $\omega = r_3$, in the second sheet.
Figure B-9. Poles of $R(\omega)$ near the cusp.
Figure B-10. Residues of the real poles of $R(w)$ in the second sheet near the cusp.
Figure B-11. Residues of the complex poles of $R(\omega)$ from (4-10) near the cusp -- The dashed lines represent the real parts of the residues of $R(\omega)$ from the complex poles, while the dotted lines give the residues for the real poles, $r_2$, in the second sheet.
Figure B-11. Residues of the complex poles of $R(\omega)$ from (4-10) near the cusp.
Figure B-12. Residues of the complex poles of $R(\omega)$ near the cusp -- The dashed lines represent the imaginary parts of the residues of $R(\omega)$ from the complex poles, while the dotted lines give the residues for the real poles, $r_j$, in the second sheet.
Figure B-12. Residues of the complex poles of $R(\omega)$ near the cusp.
APPENDIX C

COMPLETENESS AND NORMALIZATION

C-1 Completeness of the States

We shall use the Dirac notation to show the completeness of the transformation (2-3), which for a single bound state $|\Psi\rangle$ of energy $\Omega$, becomes

$$|\Psi^w\rangle = \int |\phi^L\rangle\langle\phi^L|\Psi^w\rangle d\ell + |\phi\rangle\langle\phi|\Psi^w\rangle$$

$$|\Psi\rangle = \int |\phi^L\rangle\langle\phi^L|\Psi\rangle d\ell + |\phi\rangle\langle\phi|\Psi\rangle$$

and is equivalent to the operator equation

$$\int |\phi^L\rangle\langle\phi^L| d\ell + |\phi\rangle\langle\phi| = 1.$$  \hspace{3cm} (C-1)

To show completeness for the $\Psi$'s we need only prove the corresponding operator equation for them,

$$\int |\Psi^w\rangle\langle\Psi^w| dw + |\Psi\rangle\langle\Psi| = 1.$$  \hspace{3cm} (C-2)

Then B-1 may be inverted to give

$$|\phi^L\rangle = \int |\Psi^w\rangle\langle\Psi^w|\phi^L\rangle dw + |\Psi\rangle\langle\Psi|\phi^L\rangle$$

$$|\phi\rangle = \int |\Psi^w\rangle\langle\Psi^w|\phi\rangle dw + |\Psi\rangle\langle\Psi|\phi\rangle$$  \hspace{3cm} (C-3)

which in the notation of (2-3) gives
To verify (C-2) we operate with it on the state $|\varphi^k\rangle$ and $|\varphi\rangle$ and then proceed to recover them. Thus

$$|\chi^l\rangle \equiv \left[ \int |\varphi^l\rangle \langle \varphi^l | \varphi^w \rangle \langle \varphi^w | d\omega + |\varphi\rangle \langle \varphi | |\varphi^l\rangle \right] |\varphi^k\rangle$$

$$= \int |\varphi^l\rangle c(\ell,\omega)^* d\omega + |\varphi\rangle c(\ell,\Omega)^*$$

$$|\chi\rangle \equiv \left[ \int |\varphi^l\rangle \langle \varphi^l | \varphi^w \rangle \langle \varphi^w | d\omega + |\varphi\rangle \langle \varphi | |\varphi\rangle \right] |\varphi\rangle$$

$$= \int |\varphi^l\rangle c(\omega)^* d\omega + |\varphi\rangle c(\Omega)^*$$

which with (C-1) gives

$$|\chi^l\rangle = \int |\varphi^l\rangle \langle \varphi^l | c(k,\omega) c(\ell,\omega)^* d\kappa d\omega + |\varphi\rangle \int c(\omega) c(\ell,\omega)^* d\omega$$

$$+ \int |\varphi^l\rangle \langle \varphi^l | c(k,\Omega) c(\ell,\Omega)^* d\kappa + |\varphi\rangle \int c(\Omega) c(\ell,\Omega)^*$$

$$|\chi\rangle = \int |\varphi^l\rangle \langle \varphi^l | c(k,\omega) c(\omega)^* d\kappa d\omega + |\varphi\rangle \int |c(\omega)|^2 d\omega$$

$$+ \int |\varphi^l\rangle \langle \varphi^l | c(k,\Omega) c(\Omega)^* d\kappa + |\varphi\rangle \int |c(\Omega)|^2.$$

From this result we see that a necessary and sufficient condition for the $\varphi$'s to be complete is that

$$|\chi^l\rangle = |\varphi^l\rangle$$

$$|\chi\rangle = |\varphi\rangle$$
or

(a) \[ \int c(k, \omega) c(\ell, \omega)^* d\omega + c(k, \Omega) c(\ell, \Omega)^* = \delta(k-\ell) \]

(b) \[ \int c(\omega) c(\ell, \omega)^* d\omega + c(\Omega) c(\ell, \Omega)^* = 0 \]

(c) \[ \int |c(\omega)|^2 d\omega + |c(\Omega)|^2 = 1. \quad (C-7) \]

In order to verify this result we use the dispersion relation (D-5)

\[ R(\ell) \equiv D(\ell)^{-1} = (\ell-\Omega)^{-1} |c(\Omega)|^2 + \int (\ell-\omega)^{-1} |c(\omega)|^2 d\omega \]

obtained in the following appendix.

Equation (C-7c) follows from

\[ \lim_{\ell \to \infty} \ell R(\ell) = |c(\Omega)|^2 + \int |c(\omega)|^2 d\omega = \lim_{\ell \to \infty} \ell D(\ell)^{-1} = 1 \]

since \( D(\ell) \to \ell \) as \( \ell \to \infty \). From (2-14a) we may write (b) as

\[ c(\ell) + V(\ell)^* \int (\omega - \ell)^{-1} |c(\omega)|^2 d\omega + |c(\Omega)|^2 V(\ell)^*(\Omega - \ell)^{-1} \]

\[ = c(\ell) - V(\ell)^* R(\ell) = 0 \]

and similarly (a) becomes
\[
\int [\delta(k-w)+(w-e^{-k})^{-1}V(k)c(w)] [\delta(\ell-w)+(w_{e^{-\ell}})^{-1}V(\ell)c(\omega)] d\omega \\
+ (\Omega-k)^{-1}(\Omega-\ell)^{-1}V(k)V(\ell)*|c(\Omega)|^2 \\
= \delta(k-\ell)V(\ell)* (k-\ell)^{-1} \int \left[ \frac{1}{\omega-e^{-k}} - \frac{1}{\omega_{e^{-\ell}}} \right] |c(\omega)|^2 d\omega \\
+ (k-\ell)^{-1}[-V(k)c(\ell)+V(\ell)c(k)*] \\
+ (k-\ell)^{-1}V(k)V(\ell)*|c(\Omega)|^2 \left[ \frac{1}{\Omega-k} - \frac{1}{\Omega-\ell} \right] \\
= \delta(k-\ell)+(k-\ell)^{-1}V(k)V(\ell)*[R(\ell)-R(k)*-R(\ell)+R(k)*] \\
= \delta(k-\ell)
\]

where we have again made use of the dispersion relation (C-8). Thus we see that the states \( \Psi^w, \Psi \) are complete.

C-2 Normalization of the States

We calculate

\[
(\Psi^w, \Psi^G) = \left[ \int \phi^k c(k,\omega)dk + \phi c(\omega), \int \phi^\ell c(\ell,\sigma)d\ell + \phi c(\sigma) \right] \\
= \int c(\ell,\omega)*c(\ell,\sigma)d\ell + c(\omega)*c(\sigma)
\]

which with (2-14) gives
Decomposing the integrand of the last term into partial fractions gives

\[ (w-\epsilon)^{-1}(\epsilon-\ell)^{-1} = (\sigma_2-\omega)^{-1}(w_2-\ell)^{-1} \]

which with the fact that \( \sigma_2 \) gives equivalent results as \( \sigma_\epsilon \) implies

\[ (\psi^w, \psi^\sigma) - \eta^w c(\omega) c(\sigma) = \int [\eta^w \eta^\sigma (\ell-\omega) \delta(\epsilon-\ell)] \frac{1}{V(\ell)} c(\sigma) \]

\[ + \eta^\sigma (\ell-\omega) (\epsilon-\ell)^{-1} V(\ell) c(\sigma) \]

\[ + \eta^\sigma (\ell-\omega) (w-\epsilon)^{-1} V(\ell) c(\omega) * \]

\[ + (w-\epsilon)^{-1}(\epsilon-\ell)^{-1} |V(\ell)|^2 c(\omega) c(\sigma) \]

\[ = |\eta^w|^2 \delta(\omega-\sigma) + \eta^w (\sigma_\epsilon-\omega)^{-1} V(\omega) c(\sigma) + \eta^\sigma (\omega-\sigma)^{-1} V(\sigma) c(\omega) * \]

\[ + c(\omega) c(\sigma) \int (w-\epsilon)^{-1}(\epsilon-\ell)^{-1} |V(\ell)|^2 d\ell. \]

Thus, we see that if we take \( \eta^w \) as a phase factor, the \( \psi^w \) are orthonormal,

\[ (\psi^w, \psi^\sigma) = \delta(\omega-\sigma). \quad (C-9) \]

Since any basis vector is determined up to an arbitrary phase we are free to set \( \eta^w = 1 \). In order for the state \( \psi \)
to be normalized we must have

\[(\Psi, \Psi) = 1 = \int |c(\ell, \Omega)|^2 d\ell + |c(\Omega)|^2\]
\[= \left[ \int (\ell - \omega)^{-2} |V(\ell)|^2 d\ell + 1 \right] |c(\Omega)|^2 \quad \text{(C-10)}\]

which from (2-11) gives

\[|c(\Omega)|^2 = D'(\Omega)^{-1}. \quad \text{(C-11)}\]

Finally repeating (C-10) for \(\Psi, \Psi^w\) we find

\[(\Psi, \Psi^w) = \int c(\ell, \Omega) * c(\ell, \omega) d\ell + c(\omega) c(\Omega)\]
\[= \int (\Omega - \ell)^{-1} V(\ell) c(\Omega) [\delta(\ell - \omega) + (\omega - \ell)^{-1} V(\ell) c(\omega)] d\ell \]
\[+ c(\omega) c(\Omega)\]
\[= (\omega - \Omega)^{-1} c(\Omega) \{-V(\omega) + c(\omega) \int |V(\ell)|^2 [(\ell - \omega)^{-1}
- (\ell - \Omega)^{-1}] d\ell + c(\omega) c(\Omega)\}
\[= (\omega - \Omega)^{-1} c(\Omega) \{-V(\omega) + c(\omega) [\Omega - \omega + D(\omega) + \omega - \Omega] \}
\]

or

\[(\Psi, \Psi^w) = 0. \quad \text{(C-12)}\]

Thus the states \(\Psi, \Psi^w\) are orthonormal.
APPENDIX D

DISPERSION RELATION

D-1 General Dispersion Relations

A dispersion relation expresses an analytic function of a complex variable $z$ as an integral of its imaginary part along a contour approaching the real axis in the upper half of the complex plane. If $F(z)$ is analytic except for a finite number, $n$, of poles, has a branch cut along the positive real axis, and goes to zero as $z$ tends to infinity, one can apply Cauchy's integral formula with the contour of Figure D-1 to obtain

$$F(z) = \frac{1}{2\pi i} \oint \frac{F(\zeta)}{\zeta - z} \, d\zeta$$

$$= - \sum_{j=1}^{n} \frac{\text{residues of } F}{z_j - z} + \frac{1}{2\pi i} \oint \frac{F(\xi+i\epsilon) - F(\xi-i\epsilon)}{\xi - z} \, d\xi.$$

If we also assume $F^*(z) = F(z)$ for $z$ in some real interval, Schwarz's principle $F(z) = F^*(z^*)$ holds and hence

$$F(\xi+i\epsilon) - F(\xi-i\epsilon) = F(\xi+i\epsilon) - F(\xi+i\epsilon)^* = 2\pi i \text{ Im} \, F(\xi+i\epsilon).$$

Thus we obtain the general dispersion relation

$$F(z) = - \sum_{j} \frac{\text{residues of } F}{z_j - z} + \frac{1}{\pi} \int \frac{\text{Im} \, F(\xi+i\epsilon)}{\xi - z} \, d\xi. \quad (D-1)$$

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D-2 The Dispersion Relation for $R(w)$

Since $\omega D(\omega)^{-1} \gg 1$ as $|\omega| \gg \infty$, we get $R(\omega) \gg 0$ as $\omega \gg \infty$. We also know that $D(\omega) \neq 0$ for $\omega$ complex in the first Riemann sheet so that poles of $R(\omega)$ can only occur for real $\omega$, corresponding to the zeros of $D(\omega)$. Arguing as in the equation below (4-13) with (2-14b) we see that the residues of $R(\omega)$ are given by

$$|c(\Omega)|^2 = D'(\Omega)^{-1}.$$  \hfill (D-2)

$R(\omega)$ has a branch cut with

$$2i \text{Im} R(\omega) = D(\omega_\epsilon)^{-1} - D(\omega_\epsilon)^{-1} = \frac{D(\omega_\epsilon)^* - D(\omega_\epsilon)}{|D(\omega)|^2} = -2i |R(\omega)|^2 \text{Im} D(\omega),$$ \hfill (D-3)
which with (2-9) gives

\[ \text{Imag } R(\omega) = -\pi |V(\omega)|^2. \quad (D-4) \]

Thus by (D-1)

\[ R(\omega) = (\omega - \Omega)^{-1} |c(\Omega)|^2 + \int (\omega - \xi_e)^{-1} |V(\xi)R(\xi)|^2 d\xi \quad (D-5) \]

which is the desired dispersion relation.
REFERENCES


