SCATTERING AND TIME DELAY
IN A
PERIODIC MEDIUM

A Thesis

Submitted in Partial Fulfillment of

the Requirements for the Degree of

Doctor of Philosophy

At

The University of Manitoba

By

Lionel Walter MacMillan

July, 1978

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LIONEL WALTER MACMILLAN

A dissertation submitted to the Faculty of Graduate Studies of the University of Manitoba in partial fulfillment of the requirements of the degree of

DOCTOR OF PHILOSOPHY

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ACKNOWLEDGEMENTS

The author wishes to express his gratitude to his supervisor, Dr. T.A. Osborn, for his guidance during the preparation of this thesis. The kindly encouragement of Dr. J.S.C. McKee is also gratefully acknowledged. The hospitality offered by the Cyclotron Laboratory, Department of Physics, University of Manitoba, during sabattical leave from Brandon University, Brandon, Manitoba, was much appreciated.

ABSTRACT

The quantum-mechanical motion of a particle in a periodic potential is discussed, and the absolute continuity of the spectrum demonstrated. The time-dependent theory of scattering from an impurity in a periodic potential is discussed, and the existence and asymptotic completeness of the Möller wave operators is demonstrated, together with their isometry and intertwining properties. Global time delay for a particle scattering from an impurity in a periodic potential is defined, and the existence and uniqueness of the time delay operator is shown. The spectral property of the time delay is obtained. The shift in the spectrum due to the impurity is related to the time delay, and to a general form of Levinson's theorem. The general time delay form of Levinson's theorem is studied by using the Born expansion and several mathematical theorems derived for this purpose.

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Chapter 1

Introduction

1.1 Goals of the Thesis

The goal of this thesis is to give the definition of time delay in the case of scattering from an impurity in a periodic medium, and to analyze the consequences of this definition. To achieve this goal we must first develop the necessary background in scattering theory, and review the properties of the unperturbed system (particle in a periodic potential).

1.2 Time Delay

The time delay of a scattering process refers to the difference between the time spent by the colliding particles in a certain region of space during the collision, and the time that would have been spent in the same region had the particles not interacted. To obtain a time delay independent of the size and shape of a certain region of space we take the limit as the region approaches all of space. This limit should exist for potentials which go to zero at infinity sufficiently rapidly. Physically, if the wave functions and interaction energies involved are such that the particles attract one another strongly, one will expect a pronounced time retardation, while a strong repulsion should lead to a large time advancement. These effects are energy-dependent, so that the time delay is closely connected to the structure of the spectrum of the interacting system. By considering a single particle impinging on a one-dimensional potential, or the radial motion of a single particle in three dimensions, one will readily admit an intimate relation between the time delay and the phase shift caused by the interaction.

The foregoing concept of time delay does not refer to specific incident or outgoing directions, but is an integrated or global time delay. There is also a concept of time delay which refers to specific incident and outgoing directions, which is called angular time delay. The angular time delay is the more natural concept for experimental work of course; the global time delay appears as the weighted sum of the angular time delay over all angles. However the global time delay has considerable fundamental importance, and we shall be concerned almost entirely with this concept; thus when we use the term time delay without qualification we shall mean the global time delay.

The time delay was first defined by Smith [1960], from the point of view of time-independent (or stationary) scattering theory. Later, Goldberger and Watson [1964] gave a time-dependent wave-packet definition of time delay. Then Jauch and Marchand [1967] gave a rigourous analysis based only on the simplest abstract properties of the time-dependent approach to scattering theory. All of these authors analyzed the consequences of their definitions to a greater or lesser extent. In particular, Jauch and Marchand associated with the time delay an operator Q, whose diagonal matrix elements (f,Qf) give the value of the time delay for an incident state f. Bollé and Osborn [1975 a] showed the equivalence of the time-independent definition of Smith and the time-dependent method of Jauch and Marchand. The paper of Bollé and Osborn also introduced an important improvement in connection with the limit of the time delay as the size of the region becomes infinitely large. The foregoing work is concerned with two-body collisions. Osborn and Bollé [1975 b], [1976 a] have extended the time-dependent method to define time delay for the three-body system. One very important conclusion of this work is that the

time delay which is essentially equivalent to the phase shift for the two-body situation, naturally takes the place of the phase shift in multi-particle problems.

The connection between the spectral properties of the scattering system and the time delay are embodied in the spectral property of the time delay. According to this property the change in state density at energy E, when the unperturbed and perturbed scattering systems are compared, is proportional to the trace of the time delay operator at that energy. This type of relation is first found in the work of Jauch, Sinha, and Misra [1972], and was simplified and extended by Osborn and Tsang [1975 c], [1976 b]. Since the state density occurs in a fundamental way in statistical mechanics, it is natural to expect that the time delay can be used in this field. This has been done by Smith [1963 a], [1963 b], [1972], and by Osborn and Tsang [1976 b].

Even though we shall not be concerned with angular time delay, we mention a few points here for completeness. This concept was first approached using simple wave-packet arguments by Wigner [1955] and Bohm [1951], and has since been studied by Brenig and Haag [1959], Froissart, Goldberger, and Watson [1963], and Goldrich and Wigner [1972] (the general nature of the concept of time delay is shown by the fact that these ideas have been applied to Maxwell's equations in connection with the Goos-Hänchen Effect (see Agudin [1968], Chiu and Quinn [1972])). The connection between angular and global time delay, already mentioned, has been dealt with by Nussenzweig [1972], and by Bollé Osborn [1976 a].

1.3 Outline of the Thesis

In Chaper 2 we present some necessary background material on the motion of a particle in a periodic potential (band theory). In particular,

the absolute continuity of the spectrum is demonstrated.

In Chapter 3 we discuss scattering theory for an impurity in a periodic potential, with particular reference to time-dependent scattering theory. The projection and intertwining properties, as well as the existence and asymptotic completeness, of the Möller wave operators is demonstrated.

In Chapter 4 we give the definition of the time delay. The usual definition given for two-body scattering in free space is applicable. The existence and uniqueness of the time delay operator are demonstrated. An extensive examination of the connection between the time delay and the spectrum yields the spectral property of the time delay for scattering in a periodic medium.

In Chapter 5 we pursue the connection between the time delay and the spectra of the unperturbed and perturbed Hamiltonians characterizing the scattering system. We obtain a time delay form of Levinson's theorem, and connect this with the Born expansion.

In Chapter 6 we develop mathematical methods to be used in extending the work of Chapter 5.

In Chapter 7 we use the methods developed in Chapter 6 to study the time delay form of Levinson's theorem for a particle in a localized potential in free space. The results are of use in Chapter 8.

In Chapter 8 we use the methods of Chapter 6, and the results of Chapter 7, to study the time delay form of Levinson's theorem for a particle in a localized potential in a periodic medium.

Chapter 2

PARTICLE IN A PERIODIC POTENTIAL

2.1 *Introduction*

Before we can discuss the scattering of a particle by an impurity potential embedded in a periodic potential we must consider the pure periodic potential. The main aim is to establish some of the features associated with a periodic potential, and, in particular, to establish the absolute continuity of the spectrum.

2.2 The Free Particle

A non-relativistic spinless quantum-mechanical particle of mass m is described by assigning to each real number t, $-\infty < t < \infty$, an element ψ_t of the Hilbert space $\mathcal{H} = L^2(R^3)$, such that $||\psi_t|| = 1$. ψ_t is the wave function, or state, of the particle at time t. $|\psi_t(x)|^2$ is the position probability density for the particle at time t, i.e., the probability that the particle is in any (measurable) subset S of R^3 at time t is $\int_S |\psi_t(x)|^2 dx$. We have $\int_{R^3} |\psi_t(x)|^2 dx = ||\psi_t||^2 = 1$.

The equation of motion for ψ_t is the Schrödinger equation

$$\psi_t = e^{-iht}\psi_o \quad ,$$

where h is the Hamiltonian, a self-adjoint linear transformation of $L^2(R^3)$ into itself, and ψ_o is any state ($||\psi_o|| = 1$). ψ_t is a trajectory or orbit in $\mathcal{H} = L^2(R^3)$. h characterizes the physical nature of the particle, and the environment of the particle. h will in general be an unbounded operator, that is, the energy will have no upper bound (although it will be expected to have a lower bound). The unboundedness of h implies that the domain of h, D(h), is a proper subset of $\mathcal{H}$. If ψ_o belongs to D(h),

then ψ_t is strongly differentiable (and conversely), so that in this case

$$i \frac{d\psi_t}{dt} = h\psi_t \ .$$

This equation is usually called the Schrödinger equation also.

The quantum-mechanical spinless free particle of mass m is assigned the Hamiltonian

$$h_o = - \frac{\Delta}{2m} \ , \quad \Delta = \nabla^2 = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2} \ .$$

h_o given in this form can act only on suitably differentiable functions, and is not self-adjoint (Simon [1971], Kato [1976]). We must find a unique self-adjoint extension of h_o to use as the Hamiltonian for the free particle. The symbol h_o will also be used for the self-adjoint extension. This is done by performing a Fourier transformation (Kato [1976])

$$\tilde{\psi}_t(k) = \text{l.i.m.} \ \frac{1}{(2\pi)^{3/2}} \int_{R^3} e^{-ikx} \psi_t(x) dx \ .$$

The Fourier transformation is a unitary transformation of $L^2(R^3)$ into itself, with inverse

$$\psi_t(x) = \text{l.i.m.} \ \frac{1}{(2\pi)^{3/2}} \int_{R^3} e^{ikx} \tilde{\psi}_t(k) dk \ .$$

We have $||\tilde{\psi}_t|| = || = ||\psi_t|| = 1$. Physically $|\tilde{\psi}_t(k)|^2$ is the momentum probability density for the particle at time t. We now define $h_o\psi$ by specifying the Fourier transform of $h_o\psi$ to be

$$(\tilde{h_o\psi})(k) = \frac{k^2}{2m} \tilde{\psi}(k) \ ,$$

and by requiring ψ to satisfy the condition

$$\int_{R^3} \left| \frac{k^2}{2m} \tilde{\psi}(k) \right|^2 dk < \infty \quad .$$

The second relation defines the domain of h_o, $D(h_o)$, while the first relation now defines a self-adjoint operator. This means, roughly, that we define h_o as $\frac{k^2}{2m}$ in momentum space. This gives the required unique self-adjoint extension.

2.3 The Particle in a Periodic Potential

The quantum-mechanical particle moving in a three-dimensional periodic potential $w(x)$ is assigned the Hamiltonian

$$h = -\frac{\Delta}{2m} + w = h_o + w \quad ,$$

where W is the operation of multiplication by the real function $w(x)$. We are again faced with the question of the existence of a unique self-adjoint extension. This question has been dealt with by Kato (Kato [1951], [1976]), where the existence of a unique self-adjoint extension of h for $w(x)$ bounded is established. The symbol h will be used for this extension also. We have

$$D(W) \supseteq D(h_o) = D(h) \quad ,$$

$D(W)$, $D(h_o)$, $D(h)$ being the domains of W, h_o, h respectively. A periodic potential need not be bounded; however we will deal only with bounded periodic potentials.

One may enquire whether it is possible to exhibit the self-adjoint extension of h in an explicit form, as was done in the case of a free particle, where the extension was obtained by defining h_o to be multiplication by $\frac{k^2}{2m}$ in momentum space. Another way of phrasing this question is to ask whether there is an analogue of the Fourier transform for the present case

of a particle in a periodic potential. That this is plausible can be seen from the following considerations. The existence and properties of the Fourier transform are derived ultimately from the translation group of R^3, and the usefulness of the Fourier transform in the free-particle case derives from the invariance of $-\frac{\Delta}{2m}$ under the translation group of R^3. For a periodic potential there is also a translation group, namely the discrete translation group of the three-dimensional lattice under consideration, and $-\frac{\Delta}{2m} + W$ is invariant under this group. We can thus expect the existence of functions, analogous to the exponentials e^{-ikx}, which will act as the kernels of unitary transformations of $L^2(R^3)$ into itself. The properties of this transformation should allow the explicit definition of the self-adjoint extension of h as, conjecturally, multiplication by a function of k. Such a transformation should be of practical use in facilitating conceptualization and computation. Before discussing this in more detail we examine the nature of the spectrum of $h = h_o + W$.

2.4 The Spectrum of a Particle in a Periodic Potential

The energy spectrum of a Schrödinger particle in a three-dimensional periodic potential has been studied by Avron, Grossmann and Rodriguez [1974]. These authors work in momentum space, and it is worthwhile summarizing their results because of the clarity with which the band structure emerges in their method.

The Hamiltonian is $h = p^2 + W$, where we have written p^2 instead of $\frac{k^2}{2m}$, and W is the operator of multiplication by the function w(x); w(x) is periodic in three dimensions, $w(x + a) = w(x)$. Denote the reciprocal lattice corresponding to the periodic potential by Γ. Then w(x) can be expanded in terms of reciprocal lattic vectors K as follows (Kittel [1963])

$$w(x) = \sum_{K \in \Gamma} a(K)\, e^{iKx} \quad .$$

This is just the Fourier integral expansion of a periodic function, i.e., a function with only delta-functions of various weights at the points $p = K$ in momentum space. Thus the Fourier transform of $w(x)$ is

$$\tilde{w}(p) = \sum_{K \in \Gamma} a(K)\delta(K - p) \quad .$$

We then have

$$w(x) = \int \tilde{w}(p)\, e^{ipx} dp$$

$$= \int \sum_{K \in \Gamma} a(K)\delta(K - p)\, e^{ipx} dp$$

$$= \sum_{K \in \Gamma} a(K)\, e^{iKx} \quad ,$$

as required. We will assume that

$$\sum_{K \in \Gamma} |a(K)|^2 = \int_{\Lambda} |w(x)|^2 dx = a^2$$

is finite, the integral being taken over a unit cell Λ in the direct lattice.

The matrix element of W in momentum space is (Messiah [1961])

$$< p|W|p' > = \tilde{w}(p - p') = \sum_{K \in \Gamma} a(K)\delta(K - p + p') \quad .$$

Thus for a state $|\psi>$ we have

$$< p|W|\psi > = \int < p|W|p' >< p'|\psi > dp'$$

$$= \int \sum_{K \in \Gamma} a(K)\delta(K - p + p')\psi(p')dp'$$

$$= \sum_{K \in \Gamma} a(K)\psi(p - K) \quad .$$

We also have $< p|p^2|\psi > = p^2\psi(p)$. Thus we have for the Hamiltonian $h = p^2 + W$ in momentum space

$$< p|h|\psi > = (h\psi)(p) = < p|(p^2 + W)|\psi >$$

$$= p^2\psi(p) + \sum_{K \in \Gamma} a(K)\psi(p - K) \quad .$$

In the absence of the periodic potential (all $a(K) \equiv 0$), h is just multiplication by p^2 in momentum space; the periodic potential gives the second term.

The quantity $(h\psi)(p)$ has contributions from points in momentum space of the form $p - K = -K + p$ only. K runs over all reciprocal lattice vectors, and hence so does -K. Thus the points in question are just the points of the reciprocal lattice, displaced rigidly by amount p. We will denote this set of points by Γ_p (or $\Gamma + p$), and refer to it as the Γ-coset of p. Note that two values of p which differ by a reciprocal lattice vector have the same Γ-coset, i.e. $\Gamma_{p+q} = \Gamma_p$ if $q \in \Gamma$. As far as the Hamiltonian h is concerned, different Γ-cosets are decoupled. This suggests that we can profitably study h by first looking at how h acts with respect to the individual cosets, and then assembling these separate pieces of information to obtain the overall behaviour of h.

We noted above that two values of p which differ by a reciprocal lattice vector have the same Γ-coset. This suggests that we seek a unique way of labelling Γ-cosets. To this end consider a set of points $p \in R^3$ (R^3 is momentum space here) such that each point is in a unique Γ-coset Γ_p, and the union of all these cosets is all of R^3. Such a set of points will uniquely label the Γ-cosets, and can be chosen in many ways. Such a set of points is called a quotient set of R^3 by Γ, symbolized by R^3/Γ. The most useful choice for R^3/Γ is as a proximity (Wigner - Seitz) cell (Fletcher [1971]) in Γ centered on the origin of Γ, that is, the conventional first Brillouin zone, denoted by B. Then each point $k \in B$ labels

a unique Γ-coset, Γ_k, and if q runs over Γ the points k+q run over this unique Γ-coset. Put p = k+q; then $\Gamma_k = \Gamma_{k+q} = \Gamma_p$. We can thus restrict ourselves to a single Γ-coset by choosing a fixed value for k, and considering points of the form p = k+q, q ε Γ. If we then let k run over B we reach all points in R^3 (momentum space).

We now consider a square-integrable function ϕ (complex-valued, in general) in momentum space,

$$\int_{R^3} |\phi(p)|^2 dp < \infty \quad .$$

The restriction of this function to the Γ-coset Γ_k is just ϕ evaluated at the points of Γ_k, i.e., a three-dimensional sequence, which we will denote by ϕ^k. The square-integrability of ϕ implies that the sequences ϕ^k are square-summable

$$\sum_{p \varepsilon \Gamma_k} |\phi^k(p)|^2 = \sum_{q \varepsilon \Gamma} |\phi^k(k+q)|^2 < \infty \quad .$$

If we consider the space $L^2(R^3)$ of all square-integrable (complex-valued) functions in momentum space, then the set of all corresponding three-dimensional sequences, for a fixed value of k, will be the sequence space ℓ^2 (or rather, ℓ^2_k). In each such ℓ^2_k space we can define a scalar product

$$(\phi^k,\psi^k) = \sum_{p \varepsilon \Gamma_k} \phi^{k*}(p)\psi^k(p) < \infty \quad ,$$

and this is related to the scalar product in $L^2(R^3)$ by

$$(\phi,\psi) = \int \phi^*(p)\psi(p)dp = \int_B dk \sum_{p \varepsilon \Gamma} \phi^{k*}(p)\psi^k(p) = \int_B dk(\phi^k,\psi^k) \quad .$$

In brief, we have a direct-integral (Naimark and Fomin [1957], Vilenkin [1968]) decomposition of $L^2(R^3)$ in terms of the spaces ℓ^2_k, symbolized

by

$$L^2(R^3) = \int_B^{\oplus} \ell_k^2 \, dk \quad ,$$

$$\phi = \int_B^{\oplus} \phi^k \, dk \quad .$$

Thus, in considering an individual coset Γ_k, we need only deal with sequences in ℓ_k^2, rather than with functions in $L^2(R^3)$. Similarly, operators in $L^2(R^3)$ are decomposed in terms of operators in ℓ_k^2; symbolically this is denoted by

$$A\phi = \int_B^{\oplus} A^k \phi^k \, dk \quad ,$$

$$A = \int_B^{\oplus} A^k \, dk \quad .$$

Returning now to the Hamiltonian k defined by

$$(h\psi)(p) = p^2\psi(p) + \sum_{K \in \Gamma} a(K)\psi(p - K) \quad ,$$

let us restrict p to lie in the Γ-coset Γ_k, i.e., $p = k + q$, with k fixed in B, and $q \in \Gamma$. Then $K \in \Gamma$ implies $p - K = \ell \in \Gamma_k$, so that $K = p - \ell$, and

$$\sum_{K \in \Gamma} = \sum_{\ell \in \Gamma_k} \quad .$$

h acts entirely in ℓ_k^2, so we denote h by h^k, and ψ by ψ^k. We then have

$$(h^k \psi^k)(p) = p^2\psi^k(p) + \sum_{\ell \in \Gamma_k} a(p - \ell)\psi^k(\ell)$$

$$(h^k \psi^k)(p) = T^k \psi^k(p) + V^k \psi^k(p)$$

$$= (T^k + V^k)\psi^k(p) \quad .$$

The operator T^k is diagonal in the momentum representation,

$$< p|T^k|p' > \; = \; p'^2 \, \delta_{pp'} \quad ,$$

for p,p' both in Γ_k. The spectrum of T^k is just the discrete set of positive values $\{p^2 | p \varepsilon \Gamma_k\}$. The resolvent of T^k is $(z - T^k)^{-1} = G_T^k$, with matrix elements

$$< p|G_T^k|p' > \; = \; (z - p'^2)^{-1} \, \delta_{pp'} \quad .$$

The Schmidt norm (Schatten [1970] of G_T^k is given by

$$|| \, G_T^k \, ||_2^2 \; = \; \text{Trace} \, [\, G_T^{k\dagger} G_T^k \,]$$

$$= \sum_p \sum_{p'} | < p|G_T^k|p' > |^2$$

$$= \sum_p |(z - p^2)^{-1}|^2$$

$$= \sum_p |z - p^2|^{-2} \quad .$$

The points p run over the denumerable set Γ_k, and z is not in the spectrum of T^k, so the series converges. Hence G_T^k is in the Schmidt class of operators on ℓ_k^2. A Schmidt class operator is necessarily compact. Thus T^k has compact resolvent.

The operator V^k has been defined by

$$V^k \psi^k(p) \; = \sum_{\ell \, \varepsilon \, \Gamma_k} a(p - \ell)\psi^k(\ell) \quad .$$

The matrix elements of V^k are, for p,p' both in Γ_k,

$$< p|V^k|p' > \;=\; \sum_{\ell \,\varepsilon\, \Gamma_k} a(p - \ell)\delta_{p'\ell}$$

$$= a(p - p') \quad .$$

The Schmidt norm of $V^k\, G_T^k$ is given by

$$|| \; V^k \, G_T^k \; ||_2^2 \;=\; \sum_p \sum_{p'} | < p|V^k \, G_T^k|p' > |^2$$

$$= \sum_p \sum_{p'} | < p|V^k|p' > (z - p'^2)^{-1}|^2$$

$$= \sum_{p'} |z - p'^2|^{-2} \sum_p | < p|V^k|p' > |^2$$

$$= \sum_{p'} |z - p'^2|^{-2} \; a^2 \quad ,$$

with

$$a^2 \;=\; \sum_p | < p|V^k|p' > |^2 \;=\; \sum_{p \,\varepsilon\, \Gamma_k} |a(p - p')|^2 \;=\; \sum_{K \,\varepsilon\, \Gamma} |a(K)|^2 = a^2 \quad .$$

We have assumed $a^2 < \infty$, so that

$$|| \; V^k \, G_T^k \; ||_2^2 \;=\; a^2 \; || \; G_T^k \; ||_2^2 < \infty \quad .$$

Thus $V^k \, G_T^k$ is in the Schmidt class, hence compact. The uniform norm of any operator is never larger than the Schmidt norm, so that from the foregoing result

$$|| \; V^k \, G_T^k \; || \;\leq\; || \; V^k \, G_T^k \; ||_2 \;\leq\; a \; || \; G_T^k \; ||_2 = a \left[\sum_p |z - p^2|^{-2} \right]^{1/2} \quad .$$

Let us define $E_o < 0$, E_o real, by $\sum_p |E_o - p^2|^{-2} = 1/a^2$. Then for all $z < E_o$ on the real axis we have $|| \; V^k \, G_T^k \; || < 1$. Thus for z in this range $1 - V^k \, G_T^k$ is non-singular (Kato [1976]), and so $(1 - V^k \, G_T^k)^{-1}$ exists

and is bounded. For z in this range G_T^k is in the Schmidt class, and hence so is $G_T^k(1 - V^k G_T^k)^{-1}$, being the product of a Schmidt class operator and a bounded operator. However if we consider the resolvent of $h^k = T^k + V^k$,

$$G^k = (z - h^k)^{-1}$$

$$= G_T^k + G^k V^k G_T^k \quad ,$$

so that $G^k(1 - V^k G_T^k) = G_T^k$, or $G^k = G_T^k(1 - V^k G_T^k)^{-1}$. Thus G^k is in the Schmidt class for all real $z < E_o$. Hence the spectrum of h^k is bounded below by $E_o < 0$. Using the Hilbert identity

$$G^k(z_1) - G^k(z_2) = (z_2 - z_1)G^k(z_1)G^k(z_2) \quad ,$$

which is valid for z_1, z_2 such that the resolvents exist, we immediately conclude that $G^k(z)$ is in the Schmidt class for any z not in the spectrum h^k. Thus h^k has compact resolvent, and hence (Kato [1976]) the spectrum of h^k consists entirely of real isolated points of finite multiplicity, and the eigenvectors of h^k form a basis for ℓ^2_k. We denote the eigenvalues (possibly degenerate) of h^k by $E_n(k)$, counted from below.

If n is held fixed and k is varied over the first Brillouin zone B, we obtain the n^{th} energy band function $E_n(k)$. These functions have been the object of an enormous amount of study, both analytical and numerical, because of their fundamental importance for describing the properties of solids. We will refer to these results as we need them, merely noting that our understanding of the energy band functions is by no means complete. If we use k and the eigenvalues of h^k to label states, we obtain the crystal momentum representation (Adams [1952], Callaway [1976]), as opposed to the momentum representation which we have used above.

It is of importance for the scattering problem to determine whether or not $h = p^2 + W$, W a periodic potential, has any part of its' spectrum in the form of a point spectrum, i.e., has eigenvalues. We have just seen that h^k has a pure point spectrum. However, when one considers an energy band function $E_n(k)$ one sees that the variation with k in the first Brillouin zone B will in general be continuous. The pure point spectrum of h^k is responsible for producing the different energy bands. We can attempt to visualize the spectrum of h by considering surfaces of constant energy $E_n(k) = E$ in B for $n = 0, 1, 2, \ldots$. We know the spectrum is bounded below for each k, and $E_n(0)$ is a discrete sequence, possibly degenerate. Starting at $k = 0$, which need not be the lowest energy for $E_o(k)$, we allow the surface of constant energy to expand outwards until all $k \in B$ have been accounted for. In this way we can visualize picking up a spectral density ρ (density of states) which could look like that shown in Fig. 1. Going to the next band, repeat the procedure. If the lowest energy in $E_1(k)$ is above the highest energy in $E_o(k)$, we have a band gap; otherwise the bands overlap. And so on. (See Fig. 1). If h has a point spectrum (eigenvalues), these will appear as δ-functions in the spectral density (at these energies an entire subspace (eigenspace) of states is picked up). Before looking at this question in more detail we must review the abstract classification of the spectrum of a self-adjoint operator.

A general discussion of the classification of the spectrum of a self-adjoint operator is found in Kato [1976]. The spectrum is classified into the point spectrum and the continuous spectrum. The continuous spectrum is in turn classified into the absolutely continuous and the singularly continuous spectrum. It is the absolutely continuous part of

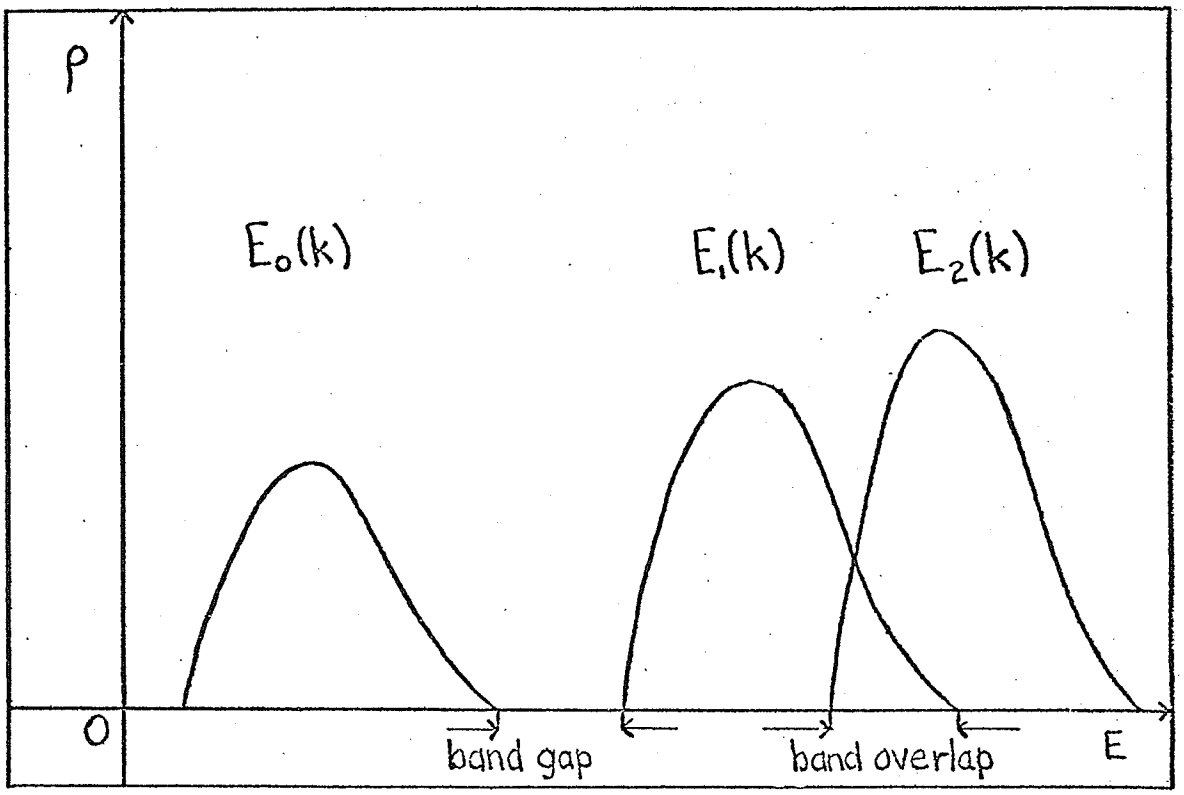


Fig. 1. Density of states for first few bands (illustrative only).

the spectrum which is called continuous in the physics literature. The Hilbert space $\mathcal{H}$ in which the self-adjoint operator acts is decomposed (reduced) into three corresponding subspaces

$$\mathcal{H} = \mathcal{H}_p \oplus \mathcal{H}_c = \mathcal{H}_p \oplus \mathcal{H}_{ac} \oplus \mathcal{H}_{sc} .$$

For a given particular self-adjoint operator it is usually a difficult problem to determine these subspaces. In physical problems one usually expects that $\mathcal{H}_{sc}$ is empty, i.e., there is no singularly continuous spectrum. In scattering problems, which we will look at later, the incoming state must be in $\mathcal{H}_{ac}$. It is essential in scattering problems that any state of the free Hamiltonian be a possible incoming state, i.e., that $\mathcal{H} = \mathcal{H}_{ac}$. In our situation the free Hamiltonian is $h = p^2 + W$, W a periodic potential. We must thus examine whether or not in this case we have $\mathcal{H} = \mathcal{H}_{ac}$, i.e., whether or not the spectrum of $h = p^2 + W$ is absolutely continuous. Before discussing this we return to a question raised earlier, whether there is an analogue, for a particle in a periodic potential, of the Fourier transform.

2.5 The Bloch Transform

The complex exponential function e^{ikx}, which appears as the kernel of the transformation from momentum to position space, arises as a solution to the eigenvalue equation $h_o\psi = E\psi$, with $h_o = -\Delta$, $E = k^2$. The eigenfunctions e^{ikx} are not square-integrable (not in $L^2(R^3)$), and so are referred to as improper (or generalized) eigenfunctions. However, square-integrable wave-functions can be constructed as superpositions of functions e^{ikx}, k varying, called wave-packets, i.e., by using Fourier transforms of momentum space wave-functions, and conversely, as already discussed (Taylor [1972]). A wave packet which is sharply peaked at a

wave vector k is approximately a plane wave e^{ikx}. We now try to adapt this view-point to the case of a particle in a periodic potential.

We thus consider the eigenvalue problem

$$h\psi = E\psi \quad ,$$

with $h = p^2 + W$, W a periodic potential. This equation has no solutions in $L^2(R^3)$, so we seek solutions in the space of bounded (complex-valued) continuous functions. Odeh and Keller [1964] (see also Troianiello [1973]) then establish that the functions (called Bloch waves)

$$\psi_n(x,k) = e^{ikx} U_n(k,x)$$

are (improper or generalized) eigenfunctions of h, with $U_n(k,x)$ being the eigenfunction belonging to $E_n(k)$; $E_n(k)$ is the band function for the n^{th} band. The function $U_n(k,x)$ has the same periodicity as the periodic direct lattice. For any $\phi \in L^2(R^3)$ the expansion formula

$$\phi(x) = \text{ℓ.i.m.} \sum_n \int_B dk\, \psi_n(x,k)\tilde{\phi}_n(k) \tag{2.1}$$

is valid, with $\tilde{\phi}_n(k)$ given by

$$\tilde{\phi}_n(k) = \text{ℓ.i.m.} \int \psi_n^*(x,k)\phi(x)dx \quad . \tag{2.2}$$

Equation (2.2) defines a bounded linear transformation from $L^2(R)$ to $L^2(B)$. This transformation is an isometry, i.e., Parsevals' formula holds

$$\int |\phi(x)|^2 dx = \sum_n \int_B |\tilde{\phi}_n(k)|^2 dk \quad ,$$

i.e.

$$|| \phi ||^2_{L^2(R^3)} = \sum_n || \tilde{\phi}(k) ||^2_{L^2(B)} \quad .$$

Equation (2.1) expresses any function in $L^2(R^3)$ in terms of Bloch waves; we say that the Bloch waves are complete in $L^2(R^3)$. The two formulas (2.1), (2.2) are analogous to the Fourier transformation, and define the Bloch transformation. $\phi(x)$ is the representative of a state vector in the position representation, while $\tilde{\phi}(k)$ represents the same state in the crystal momentum (or Bloch) representation (CMR).

For completeness we indicate how the Dirac notation can be used for a periodic potential. We consider a state $| \phi >$, whose representative in the position representation is $< r|\phi > = \phi(r)$, and whose representative in the CMR is $< nk|\phi > = \phi_n(k)$. We have denoted by $|nk >$ the state such that

$$< r|nk > = \psi_n(k,r)$$

$$= e^{ikr} U_n(k,r) \quad ,$$

with $h\psi_n(k,r) = E_n(k)\psi_n(k,r)$. The orthogonality relations hold

$$< nk|\ell q > = \delta_{n\ell}\delta(k - q) \quad ,$$

i.e.

$$\int_{R^3} dx < nk|x > < x|\ell q > = \delta_{n\ell}\delta(k - q) \quad ,$$

or

$$\int_{R^3} dx \, \psi^*_n(k,x)\psi_\ell(q,x) = \delta_{n\ell}\delta(k - q) \quad .$$

The completeness relations hold

$$\sum_n \int_B dk |nk\rangle\langle nk| = 1 \quad ,$$

i.e.

$$\sum_n \int_B dk \langle r|nk\rangle\langle nk|r'\rangle = \langle r|r'\rangle = \delta(r - r') \quad ,$$

or

$$\sum_n \int_B dk \, \psi_n^*(k,r')\psi_n(k,r) = \delta(r - r') \quad .$$

The expansion formula is

$$\langle r|\phi\rangle = \phi(r) = \sum_n \int_B \langle r|nk\rangle\langle nk|\phi\rangle$$

$$= \sum_n \int \psi_n(k,r)\phi_n(k) \quad ,$$

while the inverse is

$$\langle nk|\phi\rangle = \phi_n(k) = \int dr \langle nk|r\rangle\langle r|\phi\rangle .$$

$$= \int dr \, \psi_n^*(k,r)\phi(r) \quad .$$

Parseval's formula is obtained by writing $\langle \phi|\phi\rangle$ in alternative ways. Finally, the Schrödinger equation for a particle in a periodic potential, with an impurity potential V superimposed, is

$$i \frac{\partial}{\partial t} |\phi\rangle t = (h + V)|\phi\rangle_t \quad ,$$

with $h = p^2 + W$, W periodic. In the CMR we have

$$i \frac{\partial}{\partial t} < nk|\phi >_t = < nk|(h + V)|\phi >_t$$

$$= < nk|h|\phi >_t + < nk|V|\phi >_t \quad .$$

We have $< nk|\phi > = \phi_n(k)$, and since $h|nk > = E_n(k)|nk >$, we obtain

$$< nk|h|\phi > = \sum_m \int_B dq < nk|h|mq > < mq|\phi >$$

$$= \sum_m \int_B dq < nk|mq > E_m(q)\phi_m(q)$$

$$= E_n(k)\phi_n(k) \quad .$$

Also

$$< nk|V|\phi > = \sum_m \int_B dq < nk|V|mq > \phi_m(q) \quad ,$$

with

$$< nk|V|mq > = \int dr \, \psi_n^*(k,r)v(r)\psi_m(q,r) \quad ,$$

where $< r|V|r' > = v(r)\delta(r - r')$. Thus the Schrödinger equation is

$$i\hbar \frac{\partial}{\partial t} \phi_n(k,t) = E_n(k)\phi_n(k,t) + \sum_m \int_B dq < nk|V|mq > \phi_m(q,t) \quad .$$

For $V \equiv 0$, h is unitarily equivalent to multiplication by $E_n(k)$.

2.6 Absolute Continuity of the Spectrum

We now show that $h = p^2 + W$, W periodic, has an absolutely continuous spectrum with respect to $L^2(R^3)$, i.e., the subspaces $\mathcal{H}_p$ and $\mathcal{H}_{sc}$ are empty. We apply the method of Kato [1976], Chapter 10, Examples 1.9, 1.10. In the Hilbert space $\mathcal{H} = L^2(E)$, E being a region of R^3, consider the operator A of multiplication by a real-valued function f(x), i.e. we define A by $A\,u(x) = f(x)\,u(x)$, $u \in \mathcal{H}$. Kato shows that if f(x) is continuously differentiable and $\nabla f(x) \neq 0$ almost everywhere in E, then A is spectrally absolutely continuous. Kato applies this to the operator $h_o = -\Delta$ in $L^2(R^3)$ by noting that $-\Delta$ is unitarily equivalent, by the Fourier transform to multiplication by the function $f(k) = |k|^2$, $k \in R^3$, which is continuously differentiable, and for which $\nabla f(k) \neq 0$ almost everywhere in $E = R^3$. Thus $-\Delta$ is spectrally absolutely continuous. This is just the well known fact that a free particle has a continuous spectrum (the real axis segment $[o,\infty)$), and no eigenvalues. To apply this to a particle in a periodic potential we note that $h = -\Delta + W$, W periodic, is unitarily equivalent, by the Bloch transform, to multiplication by the function $f(k) = E_n(k)$, $k \in B$. $E_n(k)$ is holomorphic in each of the three components k_1, k_2, k_3 of k separately (but not in general single-valued as a function of k), and the set of points at which $\nabla_k E_n(k) = 0$ (the critical points) has measure zero. For these results see Thomas [1973]. We apply Kato's result to conclude that $h = p^2 + W$ is spectrally absolutely continuous. The particle in a periodic potential differs spectrally from a free particle only in that the spectrum of the former is concentrated in bands along the real (energy) axis, with a concomitant distortion of the density of states. Thomas [1973] has derived the absolute continuity of the spectrum of $h = p^2 + W$ by a more elaborate method, based on the work of Avron, Grossmann, and Rodiguez [1974].

Chapter 3

TIME-DEPENDENT SCATTERING THEORY

3.1 *Introduction*

We discuss the scattering of a particle by an impurity potential embedded in a periodic potential. The main aim is to establish some basic features of the so-called time-dependent scattering theory, with a view to applications in the study of time-delay.

3.2 Scattering Theory

The quantum-mechanical motion of a single particle in a potential is one of the most extensively studied problems in all mathematical physics. Mathematically, we seek solutions of the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \Psi(r,t) = \left(-\frac{\hbar^2}{2m} \nabla^2 + V(r)\right)\Psi(r,t) \quad .$$

This equation is usually attacked by putting $\Psi(r,t) = \psi(r)\, e^{-iEt/\hbar}$, yielding the following equation for $\psi(r)$

$$[\nabla^2 + k^2 - U(r)]\psi(r) = 0 \quad ,$$

with $E = \hbar^2 k^2/2m$, $U(r) = \frac{2m}{\hbar^2} V(r)$. This equation can be written in the form of an eigenvalue equation

$$H\psi = E\psi \quad ,$$

with $H = -\nabla^2 + U(r)$, $E = k^2$, i.e., as an operator equation in a function space. The probability interpretation of the wave function leads to the requirement that the functions $\Psi(r,t)$ and $\psi(r)$ be square-integrable, and normalized to unity. Thus the natural function space in which to seek solutions of the operator equation $H\psi = E\psi$ is the Hilbert space $L^2(R^3)$. This leads to a very successful treatment of eigenvalues and eigenfunctions (discrete spectrum), for example, the hydrogen atom.

In the treatment of scattering problems we want to deal with a situation in which an incoming or an outgoing particle can exist (continuous spectrum, scattering states). The particle is represented at any moment by a square-integrable wave-function, and its motion in time can be visualized as a trajectory in the Hilbert space $L^2(R^3)$. This approach, the so-called time-dependent (or wave packet) method does not lend itself readily to the computation of practical results, so that scattering theory has usually been approached by working in a larger function space than $L^2(R^3)$. In this alternative approach, the so-called time-independent (or stationary scattering) method, one seeks solutions of the operator equation $H\psi = E\psi$ in the space, for example, of bounded, continuous (complex-valued) functions. This space is no longer a Hilbert space, but becomes a Banach space with suitable choice of norm. Typical examples of such solutions are the plane waves e^{ikr}, and the radial waves $f(\theta,\phi)\, e^{ikr}/r$. The totality of solutions, namely the eigenfunctions as well as the generalized eigenfunctions corresponding to the continuous spectrum, are assumed to satisfy a completeness relation (Parseval's formula), which allows any function in $L^2(R^3)$ to be expanded in terms of the totality of eigenfunctions (generalized Fourier transform). The completeness relation can be proven rigourously for many systems of physical interest, and is, of course, a problem of interest and applicability whenever differential equations with boundary conditions are involved. The analogy between the discrete and continuous spectrum can be carried to considerable lengths. The representation of physical states by functions which are not square-integrable, as is done in the time-independent method, means that the probability interpretation of the wave function can no longer be strictly maintained. However, a physically

reasonable interpretation in terms of probability currents associated with a stationary beam of particles can be constructed. (It was, in fact, the search for, and formulation of, this interpretation which led Born [1926] to propose the probability interpretation of the wave function). This leads to a very successful and universally used practical treatment of scattering problems, especially in the case of spherically symmetric potentials, in which case the partial-wave analysis is available. Elaborate approximation schemes can be based on the differential equation $H\psi = E\psi$.

It is usually acknowledged that the physical constructions of the time-independent method require justification in terms of a time-dependent approach. This often takes the form of a wave-packet analysis, in which one uses superpositions of plane waves, sharply peaked near a given energy, to show that the scattered wave-packet can be described correctly by the quantities calculated by the time-independent method. A more thorough-going time-dependent approach would be to adopt the attitude that one should at all times work within the framework of the Hilbert space $L^2(R^3)$, and use only operations defined in this space. This approach yields insight into the scattering process which is clearly consistent with the principles of quantum mechanics, and can avail itself of the well-developed theory of operators in Hilbert space. The time-independent theory will then be deduced from the time-dependent theory (see, for example, Amrein, Georgescu, Jauch [1971]). The form which the time-independent theory now takes is much more complicated mathematically than the theory based on stationary scattering solutions of the time-independent Schrödinger equation. This is because in this program we do not allow ourselves the luxury of leaving Hilbert space when dealing with fundamental

issues. What is lost in simplicity and immediacy is more than made up for in precision and generality.

Naturally, the results of the time-independent theory based on solutions of the differential equation $H\psi = E\psi$ do not lose their validity. The quantities of physical interest (such as phase-shifts) depend essentially on the nature of the spectrum of the operator H in the Hilbert space $L^2(R^3)$. It is clear that we can obtain information concerning this spectrum by a variety of means. In particular, we need not restrict ourselves entirely to the Hilbert space $L^2(R^3)$ once the basic principles of interpretation have been laid down. The use of larger spaces of functions than $L^2(R^3)$ (in which $L^2(R^3)$ is embedded), and of smaller spaces of functions (contained in $L^2(R^3)$) is a common and important method in scattering theory. In the hands of Faddeev [1965], for example, such techniques have provided rigourous proofs and new insight for the scattering of a particle by a potential (or, equivalently, for the two-body problem), and for the far more difficult three-body problem.

3.3 Time-Dependent Scattering Theory

Scatterity theory deals with particles that are not free, but which interact in some way with an obstacle, with the interest centering on the asymptotic behaviour in time. The entire history of the particle is governed by a wave-function of the form

$$\psi_t = e^{-iht}\psi_o \quad ,$$

where h characterizes the system composed of the particle and the obstacle. We want to consider a particle in a periodic potential which encounters a localized impurity. We assume h has the form

$$h = h_o + W + V \quad ,$$

where $h_o = -\Delta/2m$, W is multiplication by the real function w(x) which is periodic in space, and V is multiplication by the real function v(x) which is localized in space in some way. The existence of a unique self-adjoint extension of h has been established by Kato [1951], for w(x) bounded, and v(x) square-integrable. The domains of definition satisfy

$$D(V + W) \supseteq D(h_o) = D(h) \quad .$$

Consider for a moment a particle in free space, scattering from an obstacle, for which $h = h_o + V$. A scattering event can be visualized as taking place in three stages. During the first stage the particle is far from the obstacle, and moves freely, i.e., its motion is governed by h_o. This is the incident state, or the prepared state (i.e., the incoming particle). During the second stage the interaction with the obstacle occurs, and the motion is governed by h. During the third stage the scattered particle is far from the obstacle, and again moves freely, i.e., its motion is governed by h_o. This discussion assumes that the potential is sufficiently localized that initially and finally the particle is not appreciably affected by the potential. During the third stage we speak of the scattered state, or the detected state (i.e., the outgoing particle).

For a particle moving in a periodic potential the foregoing description will also apply, but with the free motion governed by $h_o + W$. In the general discussion which follows we will use the notation h_o for the Hamiltonian which governs the free motion, on the understanding that h_o can equally well refer to $h_o + W$. We will use the notation h for the Hamiltonian which governs the interacting motion, and $h = h_o + V$ (so that h can be $h_o + W + V$ equally well).

We now attach a mathematical meaning to the descriptions of the scattering process given above. Consider a particle moving freely at all times according to

$$f_t = e^{-ih_o t} f_o \quad .$$

f_o is the value of f_t at $t = o$. Now, suppose that this particle, instead of moving freely for all times, only moves freely during the first stage of a scattering process, i.e., for times $t << o$. As the particle begins to encounter the (sufficiently localized) obstacle, the motion will diverge from that described by f_t, being described now by a different wave-function, say ψ_t. ψ_t will be governed by h

$$\psi_t = e^{iht} \psi_o \quad .$$

ψ_o is the value of ψ_t at $t = o$. f_t and ψ_t are different orbits in $L^2(R^3)$; however, for $t << o$ we expect that f_t and ψ_t should be close together (in some sense), since for $t << o$ the effect of the obstacle is still negligible. The question now is what criterion to use for closeness. This involves choosing a topology in $L^2(R^3)$. A theory applicable to many situations can be constructed by using the usual L^2 norm

$$|| \psi || = \sqrt{\int_{R^3} |\psi(x)|^2 dx} \quad ,$$

which gives the metric (distance between two vectors in $L^2(R^3)$)

$$|| \psi - f || = \sqrt{\int_{R^3} |\psi - f|^2 dx} \quad .$$

Thus, the statement that ψ_t and f_t are close together is taken to mean that $|| \psi_t - f_t ||$ is small. We thus require that

$$\lim_{t \to -\infty} || \psi_t - f_t || = 0 \quad ,$$

or

$$\lim_{t \to -\infty} || e^{-iht}\psi_o - e^{-ih_o t} f_o || = 0$$

f_t is often symbolized by ψ_t^{in}, and f_o by ψ_o^{in}. The type of convergence involved here is referred to as strong vector convergence.

A similar discussion applied to the second and third stages of the scattering process leads us to expect the existence of a freely propagating state

$$\psi_t^{out} = e^{-ih_o t} \psi_o^{out}$$

which is close to the scattering state ψ_t at $t >> 0$. This is expressed as

$$\lim_{t \to +\infty} || \psi_t - \psi_t^{out} || = 0 \quad ,$$

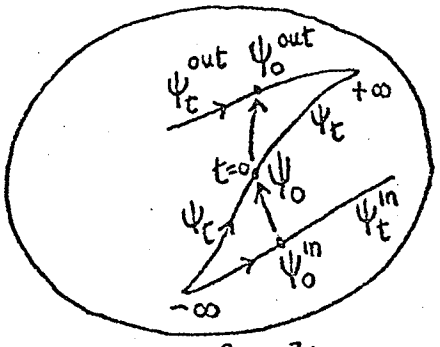
or

$$\lim_{t \to +\infty} || e^{-iht}\psi_o - e^{-ih_o t} \psi_o^{out} || = 0 \quad .$$

We give a pictorial summary of this discussion in Fig. 2(a). The eventual aim of the theory is to be able to predict (calculate) a unique ψ_t^{out}, given ψ_t^{in} (and given $\mathcal{H}$, h_o, h).

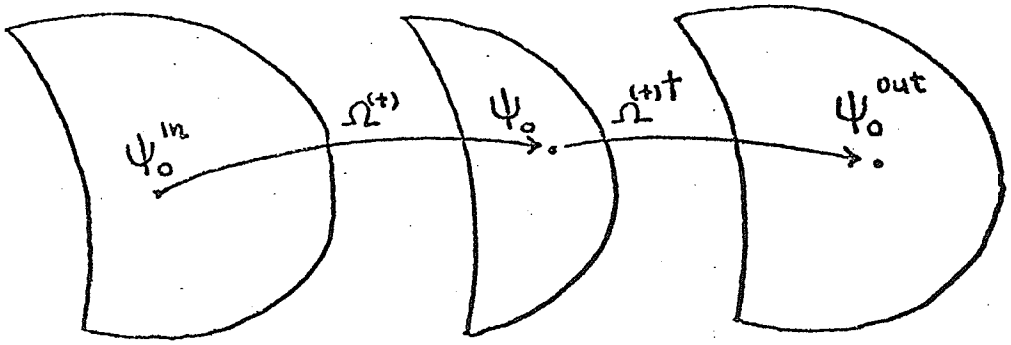
We now adopt the following point of view. We regard the Hilbert space $\mathcal{H}$ and the Hamiltonians h_o and h as given. We require that there exist wave functions ψ_o^{in}, ψ_o^{out} in $\mathcal{H}$ such that

$$\lim_{t \to -\infty} || e^{-iht}\psi_o - e^{-ih_o t} \psi_o^{in} || = 0$$



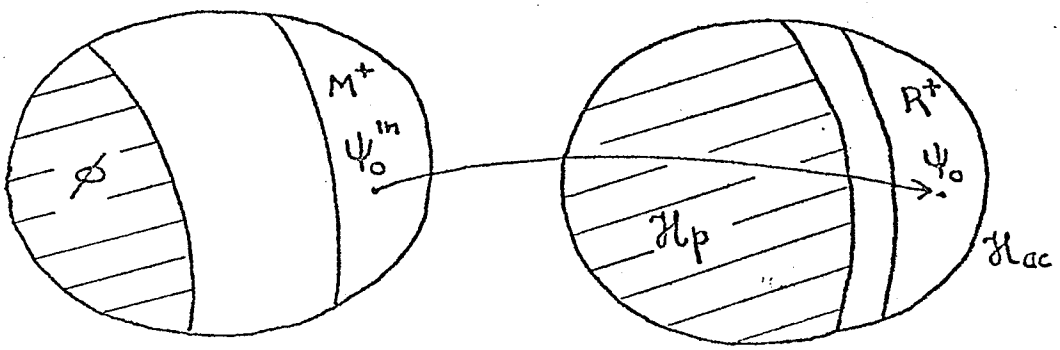
$\mathcal{H} = L^2(R^3)$

Fig. 2(a)



$\mathcal{H}_{0,ac}$ $\mathcal{H}_{ac}$ $\mathcal{H}_{0,ac}$

Fig. 2(b)



$\mathcal{H} = \mathcal{H}_{0,ac}$ $\mathcal{H} = \mathcal{H}_p \oplus \mathcal{H}_{ac}$

Fig. 2(c)

Fig. 2 Pictorial summary of spaces involved in the description of the scattering process.

and

$$\lim_{t \to +\infty} || e^{-iht}\psi_o - e^{-ih_o t}\psi_o^{out} || = 0 \quad .$$

We visualize ψ_o^{in} at $t = -\infty$ evolving into ψ_o at $t = 0$, under h, and then ψ_o evolving into ψ_o^{out} at $t = +\infty$, under h. As we have already noted this scheme may not be adequate to completely describe scattering processes involving long-range (e.g., Coulomb) potentials. Physically, for such potentials we can never get far enough back or forward in time, i.e., far enough from the scattering center, to be able to compare ψ_t with free states ψ_o^{in}, ψ_o^{out}. In general, given $\mathcal{H}$, h_o, h, to have a useful theory it is necessary to establish that the limits in question exist for a wide enough class of in and out states. We now turn to a discussion of what we expect physically in this regard.

Physically the Hilbert space $\mathcal{H} = L^2(R^3)$ is divided into two subspaces with respect to any Hamiltonian h, namely the subspace of eigenstates (bound states) and the subspace of continuum states. $\mathcal{H}$ will be the direct sum of these subspaces. Both h and h_o will, in general, have a subspace of eigenstates in $\mathcal{H}$, the subspace for h_o not coinciding in general with the subspace for h. Eigenstates are localized in space, i.e., the probability of finding the particle in a region at a great distance from the obstacle is negligible. If ψ_o^{in} is an eigenstate of h_o, then so is $e^{-ih_o t}\psi_o^{in} = \psi_t^{in}$. Thus ψ_t^{in}, being localized in space, is not a reasonable representation for an incident particle. Similarly, if ψ^{out} is an eigenstate of h_o, $e^{-ih_o t}\psi_o^{out} = \psi_t^{out}$ is not a reasonable representation for an outgoing particle. Hence we exclude the possibility that ψ_o^{in} and ψ_o^{out} are eigenstates of h_o. In an actual scattering experiment one deals with Hamiltonians h_o which have no bound states in $\mathcal{H}$. Mathematically,

given an operator h_o, it can be a difficult question to decide whether h_o has any bound states or not. We denote the subspace of eigenstates of h_o by $\mathcal{H}_{o,p}$, and that of h by $\mathcal{H}_p$.

Turning to the complete Hamiltonian h, suppose that ψ_o is an eigenstate of h. Then $e^{-iht}\psi_o = \psi_t$ is an eigenstate of h, and so cannot evolve into a freely propagating state at $t = +\infty$, nor from a freely propagating state at $t = -\infty$. Hence we exclude the possibility that ψ_o is an eigenstate of h. We thus arrive at the following physical picture. At $t = -\infty$ a continuum state of h_o evolves freely during the first stage of a scattering process. During the second stage of the scattering process the state evolves as a continuum state of h. At $t = +\infty$, the state evolves again as a continuum state of h_o. It is convenient to deal with the time-independent states ψ_o^{in}, ψ_o, and ψ_o^{out}, which are the values at $t = 0$ of ψ_t^{in}, ψ_t, and ψ_t^{out}. ψ_o^{in} is a continuum state of h_o, and is mapped into ψ_o, a continuum state of h, by the interaction. In turn, ψ_o is mapped into ψ_o^{out}, a continuum state of h_o. We give a pictorial summary of this discussion in Fig. 2(b). We denote the subspace of continuum states of h_o by $\mathcal{H}_{o,ac}$, and that of h by $\mathcal{H}_{ac}$.

The foregoing discussion merely defines our expectations regarding reasonable scattering processes. In general it is necessary to establish mathematically that these expectations are met in a particular case (i.e., given $\mathcal{H}$, h_o, h).

We have already pointed out that, mathematically, $\mathcal{H}$, is decomposed into three subspaces with respect to a self-adjoint operator:

$$\mathcal{H} = \mathcal{H}_p \oplus \mathcal{H}_{ac} \oplus \mathcal{H}_{sc} .$$

This applies to both h_o and h, in $\mathcal{H} = L^2(R^3)$. In the cases we will

consider h_o has only an absolutely continuous spectrum (free particle, particle in a periodic potential). We indicate this by writing

$$\mathcal{H} = L^2(R^3) = \mathcal{H}_{o,ac} \quad .$$

h can have a point spectrum as well as an absolutely continuous spectrum, but we will assume that $\mathcal{H}_{sc}$ is empty for h. We have then, for h,

$$\mathcal{H} = L^2(R^3) = \mathcal{H}_p \oplus \mathcal{H}_{ac} \quad .$$

The mathematical formulation of the discussion of the previous paragraph is then that $\psi_o^{in} \in \mathcal{H}_{o,ac}$ is mapped into $\psi_o \in \mathcal{H}_{ac}$, which in turn is mapped into $\psi_o^{out} \in \mathcal{H}_{o,ac}$. It would be useful to have operators which effect these mappings.

Consider the condition

$$\lim_{t \to -\infty} || e^{-iht}\psi_o - e^{-ih_o t}\psi_o^{in} || = 0 \quad ,$$

or, since e^{iht} is a unitary operator,

$$\lim_{t \to -\infty} || \psi_o - e^{iht} e^{-ih_o t}\psi_o^{in} || = 0$$

Put

$$\Omega(t) = e^{iht} e^{-ih_o t} \quad ,$$

so that the required condition reads now:

$$\lim_{t \to -\infty} || \psi_o - \Omega(t)\psi_o^{in} || = 0 \quad .$$

We may also express this in terms of strong limits of vectors in $\mathcal{H}$ as

$$s - \lim_{t \to -\infty} \Omega(t)\psi_o^{in} = \psi_o \quad .$$

(s - ℓim denotes the strong limit, which is defined by the equation preceding). For given $\psi_o^{in} \in \mathcal{H} = \mathcal{H}_{o,ac}$ the limit above may not exist. Denote by M^+ the set of vectors ψ_o^{in} in $\mathcal{H}$ for which the limit does exist. If the limit exists it is unique. Denote by R^+ the set of vectors ψ_o in $\mathcal{H}$ which are the limits, ψ_o^{in} in M^+. We summarize this discussion pictorially in Fig. 2(c). In Fig. 2(c) we have indicated that $R^+ \subseteq \mathcal{H}_{ac}$, since we expect this on physical grounds: of course this must be proven. M^+ and R^+ are closed linear subspaces of $\mathcal{H}$. We can define the operator $\Omega^{(+)}$ (Möller wave operator) by

$$\Omega^{(+)}: \quad M^+ \to R^+$$

$$\Omega^{(+)}: \quad \psi_o^{in} \to \psi_o = \Omega^{(+)}\psi_o^{in} = \underset{t \to -\infty}{s - \ell\text{im}}\ \Omega(t)\psi_o^{in} \quad .$$

Using the strong operator limit (on M^+) we can write

$$\Omega^{(+)} = \underset{t \to -\infty}{\ell\text{im}}\ \Omega(t) \quad .$$

As the strong operator limit of a sequence of unitary operators, $\Omega^{(+)}$ is isometric on M^+ to R^+, i.e.,

$$|| \psi_o || = || \Omega^{(+)}\psi_o^{in} || = || \psi_o^{in} || \quad .$$

If we define $\Omega^{(+)}g \equiv 0$ for $g \in (M^+)^{\perp}$, then $\Omega^{(+)}$ is partially isometric on $\mathcal{H}$ with domain M^+ and range R^+. This is in accordance with the following definition: A bounded linear operator U defined on $\mathcal{H}$ is partially isometric with domain M and range R if $|| Uf || = || f ||$ for every $f \in M$, and $|| Ug || = 0$ for every $g \in M^{\perp}$. The following properties then follow:

1. $< Uf | Ug > = < f | g >$, for all $f,g \in M$

2. $U^\dagger U$ = projector on $M = P_M$.

3. $U^\dagger$ is partially isometric with domain R and range M.

We conclude that $\Omega^{(+)\dagger}$ is isometric on R^+ to M^+, and that $\Omega^{(+)\dagger}\Omega^{(+)}$ = projector on $M^+ = P_{M^+}$. Also then $\Omega^{(+)}\Omega^{(+)\dagger}$ = projector on $R^+ = P_{R^+}$. The isometry of $\Omega^{(+)}$, $\Omega^{(+)\dagger}$ implies that M^+, R^+ are closed subspaces of $\mathcal{H}$. This describes the transition from stage one to stage two of the scattering process.

The transition from stage two to stage three of the scattering process is described by the condition.

$$\lim_{t \to +\infty} || e^{-iht}\psi_o - e^{-ih_o t}\psi_o^{out} || = 0 \quad .$$

We can carry out the same discussion for this limit as for the limit at $t = -\infty$. We arrive at an operator $\Omega^{(-)}$ defined by

$$\Omega^{(-)}: \quad M^- \to R^-$$

$$\Omega^{(-)}: \quad \psi_o^{out} \to \psi_o = \Omega^{(-)}\psi_o^{out} = \operatorname*{s-lim}_{t \to +\infty} \Omega(t)\psi_o^{out} \quad ,$$

or

$$\Omega^{(-)} = \lim_{t \to +\infty} \Omega(t) \quad .$$

We have $\Omega^{(-)\dagger}\Omega^{(-)} = P_{M^-}$, $\Omega^{(-)}\Omega^{(-)\dagger} = P_{R^-}$.

We can now demonstrate the so-called intertwining property:

$$e^{iht}\Omega^{(\pm)} = \Omega^{(\pm)} e^{ih_o t}$$

We have

$$e^{iht}\Omega^{(\pm)} = e^{iht}\left(\lim_{s \to \mp\infty} e^{ihs} e^{-ih_o s} \right)$$

$$= \lim_{s \to \mp\infty} e^{ih(t+s)} e^{-ih_o s}$$

$$e^{iht}\Omega^{(\pm)} = \left(\lim_{s \to \mp \infty} e^{ih(t+s)} e^{-ih_o(t+s)} \right) e^{ih_o t}$$

$$= \Omega^{(\pm)} e^{ih_o t}$$

The continuity (boundedness) of e^{iht} has been used to move it through the limit operation. From the intertwining property it follows that $f(h)\Omega^{(\pm)} = \Omega^{(\pm)} f(h_o)$, and in particular that $h\Omega^{(\pm)} = \Omega^{(\pm)} h_o$. Multiplying by $\Omega^{(\pm)\dagger}$ we have

$$\Omega^{(\pm)\dagger} h \Omega^{(\pm)} = \Omega^{(\pm)\dagger}\Omega^{(\pm)\dagger} h_o = P_{M^\pm} h_o \ .$$

Since

$$P_{R^\pm}\Omega^{(\pm)} = \Omega^{(\pm)}\Omega^{(\pm)\dagger}\Omega^{(\pm)} = \Omega^{(\pm)} P_{M^\pm} \ ,$$

we obtain

$$P_{R^\pm}\Omega^{(\pm)} P_{M^\pm} = \Omega^{(\pm)} P_{M^\pm} P_{M^\pm} = \Omega^{(\pm)} \ .$$

Hence, substituting into the original relation

$$\Omega^{(\pm)\dagger} h \, P_{R^\pm}\Omega^{(\pm)} P_{M^\pm} = P_{M^\pm} h_o \ ,$$

or multiplying into $P_{M^\pm}$,

$$\Omega^{(\pm)\dagger} (h \, P_{R^\pm}) \Omega^{(\pm)} = P_{M^\pm} h_o P_{M^\pm} \ .$$

We now suppose that $M^\pm$ is all of $\mathcal{H}$, i.e.,

$$M^\pm = \mathcal{H} = \mathcal{H}_{o,ac} \ .$$

If this is the case then $P_{M^\pm} = 1$. This implies that the limits $s - \lim_{t \to \mp \infty} \Omega(t) f$ exist for all $f \in \mathcal{H}$. Further, from the relation at the end of the

preceding paragraph we have

$$\Omega^{(\pm)\dagger}(h\, P_{R^{\pm}})\Omega^{(\pm)} = h_o \ .$$

This tells us that the space $\mathcal{H} = \mathcal{H}_{o,ac}$ is unitarily equivalent to the space $R^{\pm}$, so that the spectrum of h in $R^{\pm}$ is the same as that of h_o in $\mathcal{H} = \mathcal{H}_{o,ac} = L^2(R^3)$, i.e., the spectrum of h in $R^{\pm}$ is absolutely continuous. The property that $M^{\pm}$ is all of $\mathcal{H}$ is not trivial (as might be surmised from its consequences). This property must be demonstrated to be true, and if it does hold we will say that the wave operators exist, meaning that the strong limits $\underset{t \to \mp \infty}{s - \ell im}\, \Omega(t)f$ exist for all $f \in \mathcal{H}$.

We now consider the entire scattering process from the physical point of view again. ψ_o^{in} and ψ_o^{out} are the objects which are experimentally accessible, and we define the S-operator by

$$\psi_o^{out} = S\, \psi_o^{in}$$

Now we have $\psi_o^{out} = \Omega^{(-)\dagger}\psi_o$ and $\psi_o = \Omega^{(+)}\psi_o^{in}$, so that $\psi_o^{out} = \Omega^{(-)\dagger}\Omega^{(+)}\psi_o^{in}$, that is,

$$S = \Omega^{(-)\dagger}\Omega^{(+)} \ .$$

Physically, we require S to be unitary, i.e., S is to be a one-one invertible isometry on $\mathcal{H} = \mathcal{H}_{o,ac} = L^2(R^3)$. An examination of the preceding discussions shows immediately that S is unitary if and only if $R^+ = R^- = R$, say. We have so far not dealt with the singularly continuous spectrum, nor with those states which may be in $\mathcal{H}_{ac}$ but not in R. Physically it is reasonable to require that

$$R = \mathcal{H}_{ac} \ ,$$

and that no singularly continuous spectrum exist. This is equivalent to setting

$$\mathcal{H} = \mathcal{H}_{o,ac} = \mathcal{H}_p \oplus \mathcal{H}_{ac} ,$$

or, with $B = \mathcal{H}_p$, the subspace of bound states of h,

$$L^2(R^3) = B \oplus R .$$

We have thus required that any state in the continuum of h, namely in $\mathcal{H}_{ac} = R$, be accessible as an intermediate state in the scattering process. We have also that any state in the continuum of h_o, namely in $\mathcal{H} = \mathcal{H}_{o,ac} = L^2(R^3)$ is possible as an initial or final state. The property in question, namely that $L^2(R^3) = B \oplus R$, is called asymptotic completeness (of $\Omega^{(\pm)}$) and must be proven in a given case.

3.4 Existence and Asymptotic Completeness of Wave Operators

The methods by which existence and asymptotic completeness (which includes the unitarity of S) are demonstrated for given $\mathcal{H}$, h, h_o, are technically complex, and the subject of considerable current research. One of the principal, and most useful, results of the theory is the following theorem of Kato [1976]:

> Let h_o and $h = h_o + V$ be self-adjoint and bounded from below. Let $V = V_1 V_2$, where
>
> $$V_1^{\dagger}(h_o - E)^{-1} \quad \text{and} \quad V_2(h_o - E)^{-1}$$
>
> both belong to the Schmidt class for some E smaller than the lower bound of h_o. Then $\Omega^{(\pm)}$ exist and are (asymptotically) complete.

As an application of this result Kato shows that with $\mathcal{H} = L^2(R^3)$, $h_o = -\Delta$, $h = h_o + V$, $V \in L^1 \cap L^2$, $\Omega^{(\pm)}$ exist and are complete.

We want to apply this theorem to the case of a particle in a periodic potential, $h = h_o + V$, $h_o = p^2 + W$, W periodic. We know that h_o is self-adjoint and bounded from below. h is self-adjoint with the same domain as h_o, and will be bounded from below for V a localized potential. We will put $V = V_1 V_2$, with V the operation of multiplication by v(x), V_2 the operation of multiplication by $|v(x)|^{1/2}$, and V_1 the operation of multiplication by $|v(x)|^{1/2}$ sign (v(x)). We will denote V_1 by $V^{1/2}$, and V_2 by $|V|^{1/2}$. Thus

$$V = V^{1/2}|V|^{1/2} \quad .$$

We must thus consider the operators $V^{1/2}(h_o - z)^{-1} = V^{1/2}r_o(z)$, $|V|^{1/2}(h_o - z)^{-1} = |V|^{1/2}r_o(z)$, where z is on the real axis and sufficiently negative. We will at first let z be any complex number not in the spectrum of h_o.

First consider $r_o(z) = (h_o - z)^{-1}$, the resolvent of $h_o = p^2 + W$. The resolvent for a free particle is $(p^2 - z)^{-1}$, which we denote by $r_{oo}(z)$. Then $r_o(z)$ and $r_{oo}(z)$ are related by

$$r_o(z) = r_{oo}(z) - r_{oo}(z)Wr_o(z) \quad ,$$

for values of z such that the resolvents exist. Multiplying by $V^{1/2}$ we have

$$V^{1/2}r_o(z) = V^{1/2}r_{oo}(z) - V^{1/2}r_{oo}(z)Wr_o(z) \quad .$$

It is known that $V^{1/2}r_{oo}(z)$ is in the Schmidt class for z not on the positive real axis, and for $v(x) \in L^1 \cap L^2$ (see Appendix 1). The spectrum of h_o is bounded below, say by E_o, so that for z not on the real axis at or greater than E_o, $r_o(E)$ exists (is bounded). Then $Wr_o(z)$ is a bounded

operator for such z. Thus $V^{1/2}r_{oo}(z)Wr_o(z)$ is in the Schmidt class for z not on the real axis at or greater than E_o, being the product of a Schmidt class and a bounded operator for such z. $V^{1/2}r_o(z)$ then, as the sum of two Schmidt class operators for z not on the real axis at or greater than E_o, is Schmidt class for such values of z. The same argument applies for $|V|^{1/2}r_o(z)$. We can thus apply Kato's theorem to conclude that $\Omega^{(\pm)}$ exist and are asymptotically complete for a particle in a periodic potential and subject to an impurity potential $v(x)\epsilon L^1 \cap L^2$.

This conclusion has also been reached by different (and more elaborate) methods by Thomas [1973], Troianiello [1973], Bentosela [1976], and Kuroda [1969]. These authors are capable of refining somewhat the conditions on the potential which must be imposed in order that the wave operators exist and be asymptotically complete. Since we are interested in a broad view of our subject at this stage, it does not seem desirable to embark on studies in this direction at this point.

We have laid the foundations for scattering theory in a periodic potential. The actual computation of the scattering operator, and related experimentally accessible quantities, is carried out by methods usually involving the time-independent approach to scattering theory. The transition to the time-independent theory is discussed by Amrein, Georgescu, Jauch [1971], and Chandler and Gibson [1973]. For actual computations of impurity scattering see Callaway [1976].

Chapter 4

TIME DELAY

4.1 *Introduction*

We define the time delay of a scattering process, and examine the meaning of the definition, in particular in what sense a time delay operator exists and is unique. We derive properties of the time delay, in particular the so-called spectral property.

4.2 Definition of Time Delay

We consider scattering of a particle by a fixed impurity in a crystalline lattice. The impurity will be represented by a potential added to the lattice potential. The time delay of the scattering process is defined by considering a region Σ_R which includes the fixed impurity, and whose boundary is never more than a distance R from the fixed impurity. Let ψ_t be a scattering state of the particle which behaves as a freely evolving state ϕ_t as $t \to -\infty$. That is, $\phi_t = e^{-ih_o t}\phi$, and $\phi = \psi_o^{in}$, in a notation already established. Let P(R) be the projection operator for the region Σ_R, i.e.,

$$P(R)g(x) = \begin{cases} g(x), & x \text{ in } \Sigma_R \text{ or on boundary,} \\ 0, & x \text{ not in } \Sigma_R. \end{cases}$$

Denote the inner product of states α,β by (α,β) (this is an integral over configuration space). The probability density for finding the particle in Σ_R at time t is

$$(P(R)\psi_t, P(R)\psi_t) = (\psi_t, P(R)\psi_t) ,$$

since $P^2(R) = P(R)$, and $P^+(R) = P(R)$. The average amount of time the particle

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spends in Σ_R during the time interval t to t + dt is $(\psi_t, P(R)\psi_t)dt$, so that the average total time the particle spends in Σ_R is

$$\int_{-\infty}^{\infty} (\psi_t, P(R)\psi_t)dt \quad .$$

In a precisely similar manner, the average total time the particle spends in Σ_R in the absence of an impurity, but with the same incoming state, is

$$\int_{-\infty}^{\infty} (\phi_t, P(R)\phi_t)dt \quad .$$

We define the time delay for the region Σ_R to be the difference between the two total times given above

$$T_R(\phi) = \int_{-\infty}^{\infty} \{(\psi_t, P(R)\psi_t) - (\phi_t, P(R)\phi_t)\}dt \quad .$$

In summary, the time delay for the region Σ_R is the difference between the time spent by the particle in the region Σ_R during the scattering process, and the time that would have been spent in the same region had the particle moved freely. It is physically reasonable that $T_R(\phi)$ exists for a wide class of potentials. We will consider this, as well as uniqueness, subsequently. To obtain a time delay independent of the size of a particular region, we will want to consider the limit $R \to \infty$. Physically it seems reasonable that $\lim_{R \to \infty} T_R(\phi)$ should exist for a wide class of potentials, and particularly for short-range potentials. The problem of defining conditions under which the limit $R \to \infty$ exists will be discussed later.

Using the intertwining property, $e^{iht}\Omega^{(\pm)} = \Omega^{(\pm)} e^{ih_o t}$, a useful alternative form of the time delay can be obtained. We have $\psi_t = e^{-iht}\psi_o$, and $\psi_o = \Omega^{(+)}\psi_o^{in}$. We have used the notation $\psi_o^{in} = \phi$. Then $\psi_t = e^{-iht}\Omega^{(+)}\phi$. Thus

$$\begin{aligned}(\psi_t, P(R)\psi_t) &= (e^{-iht}\Omega^{(+)}\phi, P(R)\, e^{-iht}\Omega^{(+)}\phi) \\ &= (\Omega^{(+)} e^{-ih_o t}\phi, P(R)\Omega^{(+)} e^{-ih_o t}\phi) \\ &= (\phi, e^{ih_o t}\Omega^{(+)\dagger}P(R)\Omega^{(+)} e^{-ih_o t}\phi) \quad .\end{aligned}$$

Also, similarly,

$$(\phi_t, P(R)\phi_t) = (\phi, e^{ih_o t} P(R)\, e^{-ih_o t}\phi) \quad .$$

We can thus write the time delay as

$$\begin{aligned}T_R(\phi) &= \int_{-\infty}^{\infty} (\phi, e^{ih_o t}\left[\Omega^{(+)\dagger}P(R)\Omega^{(+)} - P(R)\right] e^{-ih_o t}\phi)dt \\ &= \int_{-\infty}^{\infty} (\phi, e^{ih_o t}\Gamma(R)\, e^{-ih_o t}\phi)dt \quad ,\end{aligned}$$

with $\Gamma(R) = \Omega^{(+)\dagger}P(R)\Omega^{(+)} - P(R)$.

4.3 Existence and Uniqueness of the Time Delay Operator

Let us put $T_R(\phi)$ equal to the diagonal matrix elements of an operator $Q(R)$

$$(\phi, Q(R)\phi) = \int_{-\infty}^{\infty} (\phi, e^{ih_o t}\Gamma(R)\, e^{-ih_o t}\phi)dt \quad .$$

The existence and uniqueness of the time delay operator Q(R) can be studied by examining the symmetric sesquilinear form

$$Q(R)(\psi,\phi) = \int_{-\infty}^{\infty} (\psi, e^{ih_o t} \Gamma(R) e^{-ih_o t} \phi)dt \quad .$$

If the integral defining $Q(R)(\psi,\phi)$ is finite for all ψ,ϕ in a dense set of $\mathcal{H}$, then $Q(R)(\psi,\phi)$ will be a bounded sesquilinear form on $\mathcal{H}$, and will define a unique bounded operator Q(R) on $\mathcal{H}$ such that

$$Q(R)(\psi,\phi) = (\psi, Q(R)\phi) \quad .$$

Converseley, Q(R) will uniquely define the sesquilinear form. This problem was first studied by Jauch and Marchand [1967], and in much more detail by Jauch, Sinha, and Misra [1972]. The work of Jauch, Sinha, and Misra has been given in a very general form by Martin and Misra [1973], [1973]. We follow the latter authors here.

The main result of Martin and Misra is stated as follows:

> Let $g \to U_g$ denote an absolutely continuous representation (in the Hilbert space $\mathcal{H}$) of the locally compact Abelian group G, and let the correspondence $\psi \to \psi_\varepsilon$ yield the direct integral representation of $\mathcal{H}$ ($\hat{G}$ is the dual group of G)
>
> $$\mathcal{H} = \int_{\hat{G}}^{\oplus} H_\varepsilon d\varepsilon \quad ,$$
>
> which diagonalizes the representation $g \to U_g$. Let D denote the (dense) set of all ψ in $\mathcal{H}$ for which ess. $\sup_{\varepsilon \in \hat{G}} ||\psi_\varepsilon||_\varepsilon < \infty$
> Then:
> (a) For every trace-class operator T in $\mathcal{H}$

$$B(\psi,\phi) = \int_G (\psi, U_g^\dagger T U_g \phi) dg$$

is finite for all ψ,ϕ in D, and for almost all $\varepsilon \in \hat{G}$ there exist trace-class operators $b(\varepsilon)$ acting in H_ε such that

$$B(\psi,\phi) = \int_{\hat{G}} (\psi_\varepsilon, b(\varepsilon)\phi_\varepsilon) d\varepsilon$$

for all ψ,ϕ in D. The family $b(\varepsilon)$ is essentially unique in the sense that if $b^1(\varepsilon)$ is another family of operators satisfying the preceding relation, then $b^1(\varepsilon) = b(\varepsilon)$ for almost all $\varepsilon \in \hat{G}$.

(b) The following hold:

$$\mathrm{Tr}\ T = \int_{\hat{G}} \mathrm{tr}\ b(\varepsilon) d\varepsilon \quad ,$$

$$\int_{\hat{G}} || b(\varepsilon) ||, d\varepsilon \leq || T ||_1 \quad ,$$

where Tr, tr are trace in $\mathcal{H}$, H_ε respectively, and $|| \ ||_1$ is the trace-norm.

This (rather long) statement of the theorem uses concepts and results from abstract harmonic analysis; these ideas are summarized by Martin and Misra. The proof the theorem proceeds by direct verification for rank one operators, by immediate extension to finite-rank operators, and finally to arbitrary trace-class operators represented as limits of finite-rank operators. The application of this theorem to time delay is indicated by Martin-Misra, for a particle in free space scattering from a localized

potential. We indicate here the application to a particle in a periodic potential scattering from an impurity.

We give a discussion of the concepts involved in the theorem of Martin-Misra, in order to clarify the applications we make. Since we intend to identify the locally compact Abelian group of the theorem with the time-translation group, and choose the unitary representation $t \to U_t = e^{-ih_o t}$, $h_o = -\Delta + W$, we will deal specifically with this case in this discussion.

Stone's theorem (Riesz-Nagy [1956], Maurin [1967]) gives us the spectral representation of the operator U_t as

$$U_t = \int e^{-i\lambda t} dE(\lambda) \quad ,$$

or

$$(\psi, U_t \phi) = \int e^{-i\lambda t} (\psi, dE(\lambda)\phi) \quad .$$

The integral is over the real line R, but in fact $dE(\lambda)$ gives no contribution unless λ is in the spectrum of h_o, so the integral is in reality over the spectrum of h_o. The spectrum of h_o is absolutely continuous, and hence the measure $(\psi, dE(\lambda)\phi)$ is absolutely continuous (with respect to Lebesque measure on R). (Stone's theorem has been generalized to the so-called SNAG theorem (Stone-Naimark-Ambrose-Godement) according to which every unitary representation of a locally compact Abelian group G in a Hilbert space $\mathcal{H}$ has a projection-valued measure $dE(\lambda)$ on the dual group $\hat{G}$ such that

$$U_g = \int_{\hat{G}} \overline{< g, \lambda >} \, dE(\lambda) \quad .$$

$< g,\lambda >$ is the character λ of G at g; the set of all characters is the dual group $\hat{G}$ (see Loomis [1953]). In our case the group G is the real line, and $\hat{G}$ is also the real line. The character is $< g,\lambda > = e^{i\lambda t}$.

The direct integral of Hilbert spaces is a generalization of the direct sum of Hilbert spaces. The direct sum of Hilbert spaces $H_1, H_2, \ldots, H_n, \ldots$ is the space of all possible sequences

$$h = (h_1, h_2, \ldots, h_n, \ldots)$$

with $h_n \in H_n$ and $||h||^2 = \sum_n ||h_n||_n^2 < \infty$. $||h_n||_n$ is the norm of $h_n \in H_n$. It is convenient sometimes to denote h by $\overset{\oplus}{\sum_n} h_n$. Addition and multiplication by a scalar are defined point wise, as is the scalar product. If $\psi = (\psi_1, \psi_2, \ldots, \psi_n, \ldots) = \overset{\oplus}{\sum_n} \psi_n$, and $\phi = (\phi_1, \phi_2, \ldots, \phi_n, \ldots) = \overset{\oplus}{\sum_n} \phi_n$, then the scalar product in the direct sum space is

$$(\psi,\phi) = \sum_n (\psi_n, \phi_n)_n ,$$

with $(\psi_n, \phi_n)_n$ the scalar product in H_n. The direct sum space is denoted by $\overset{\oplus}{\sum_n} H_n$. The direct integral is a generalization of the direct sum to a continuum of Hilbert spaces H_ε, ε being a continuous parameter in a measure space Λ. We replace $\overset{\oplus}{\sum_n}$ by $\overset{\oplus}{\int_\Lambda}$, so that if $\psi = \{\psi_\varepsilon\}$, we write $\psi = \overset{\oplus}{\int_\Lambda} \psi_\varepsilon d\varepsilon$. For details consult Naimark-Fomin [1957], Vilenkin [1968], or Maurin [1967]. The direct integral bears the same relation to the direct sum as a function of a real variable does to a sequence. The scalar product is, for $\psi = \overset{\oplus}{\int_\Lambda} \psi_\varepsilon d\varepsilon$, $\phi = \overset{\oplus}{\int_\Lambda} \phi_\varepsilon d\varepsilon$

$$(\psi,\phi) = \int_\Lambda (\psi_\varepsilon,\phi_\varepsilon)_\varepsilon d\varepsilon ,$$

with $(\psi_\varepsilon,\phi_\varepsilon)_\varepsilon$ being the scalar product in H_ε. In particular

$$|| \psi ||^2 = \int_\Lambda || \psi_\varepsilon ||^2_\varepsilon \, d\varepsilon \quad ,$$

which is required to be finite. The direct integral space is denoted by $\oplus \int_\Lambda H_\varepsilon d\varepsilon$.

The spectral theorem, in the form given by von Neumann (Maurin [1967]) gives us the representation of the operator $U_t = e^{-ih_o t}$ in diagonal form, after a unitary transformation V:

$$U_t \phi \overset{V}{\to} e^{-i\varepsilon t}\phi_\varepsilon \quad ;$$

the unitary transformation V maps the Hilbert space $\mathcal{H}$ into a direct integral, $\phi \overset{V}{\to} \phi_\varepsilon$,

$$\mathcal{H} \overset{V}{\to} \int_\Lambda H_\varepsilon d\varepsilon \quad .$$

We can identify $\mathcal{H}$ with this direct product. In the case $U_t = e^{-ih_o t}$ the measure space Λ is the real line, $d\varepsilon$ being Lebesgue measure. We have for the scalar product (invariant under V)

$$(\psi, U_t\phi) = \int_\varepsilon (\psi_\varepsilon, e^{-i\varepsilon t}\phi_\varepsilon)_\varepsilon d\varepsilon$$

$$= \int_\varepsilon e^{-i\varepsilon t}(\psi_\varepsilon,\phi_\varepsilon)_\varepsilon d\varepsilon \quad .$$

Also, from the spectral representation

$$(\psi, U_t\phi) = \int_\lambda e^{-i\lambda t}(\psi, dE(\lambda)\phi) \quad .$$

The parameters ε and λ can be identified, so that

$$(\psi_\varepsilon,\phi_\varepsilon)_\varepsilon d\varepsilon \sim (\psi,dE(\lambda)\phi) \quad ;$$

i.e., the measure $(\psi,dE(\lambda)\phi)$, which is non-zero only in the spectrum of h_o, and which is governed by the spectral density of h_o, is equivalent to $(\psi_\varepsilon,\phi_\varepsilon)_\varepsilon d\varepsilon$, $d\varepsilon$ being Lebesgue measure. Heuristically, we can say that the direct integral incorporates the spectral measure of h_o into the distribution of the spaces H_ε over ε, or the spaces H_ε have "density" in ε equivalent to the spectral density of h_o. Direct integrals are thus integrals over the spectrum of h_o, "weighted" by the spectral density of h_o. (The relation of the spectral theorem to direct integrals can also be generalized to unitary representations of locally compact Abelian (in fact, locally compact) groups. Λ becomes $\hat{G}$, and $e^{i\varepsilon t}$ becomes the character $< t,\varepsilon >$ (Naimark-Fomin [1957])).

We now consider a rank one operator

$$T = \lambda(u, \ )v \quad ,$$

$\lambda > 0$, u,v normalized. T acts on vectors f in $\mathcal{H}$ according to $Tf = \lambda(u,f)v$. We consider the scalar product $(\psi, U_t^\dagger T U_t \phi)$ integrated over t:

$$\begin{aligned} B(\psi,\phi) &= \int_t (\psi, U_t^\dagger T U_t \phi)dt \\ &= \int_t (U_t\psi, TU_t\phi)dt \\ &= \int_t (U_t\psi, \lambda(u,U_t\phi)v)dt \\ &= \int_t \lambda(u,U_t\phi)(U_t\psi,v)dt \end{aligned}$$

$$B(\psi,\phi) = \lambda \int_t (u,\phi_t)(\psi_t,v)dt \quad .$$

We have put $\phi_t = U_t\phi$, $\psi_t = U_t\psi$. Using the direct integral we have

$$(u,\phi_t) = (u,U_t\phi) = \int_\varepsilon e^{-i\varepsilon t}(u_\varepsilon,\phi_\varepsilon)_\varepsilon d\varepsilon \quad ,$$

and similarly for (v,ψ_t). Now $(u_\varepsilon,\phi_\varepsilon)_\varepsilon$ is square-integrable for ϕ in a set to be specified in a moment. (Jauch, Sinha, Misra [1972]). Schwartz's inequality in H_ε gives

$$|(u_\varepsilon,\phi_\varepsilon)_\varepsilon|^2 \leq || u_\varepsilon ||_\varepsilon^2 \; || \phi_\varepsilon ||_\varepsilon^2 \quad ,$$

so that

$$\int_\varepsilon |(u_\varepsilon,\phi_\varepsilon)_\varepsilon|^2 \, d\varepsilon \leq \int_\varepsilon || u_\varepsilon ||_\varepsilon^2 \; || \phi_\varepsilon ||_\varepsilon^2 \, d\varepsilon \quad .$$

For $|| \phi_\varepsilon ||_\varepsilon$ bounded in ε (essentially bounded is enough) we have

$$\int_\varepsilon |(u_\varepsilon,\phi_\varepsilon)_\varepsilon|^2 \, d\varepsilon \leq \underset{\varepsilon \in R}{\text{ess. sup}} || \phi_\varepsilon ||_\varepsilon^2 \int_\varepsilon || u_\varepsilon ||_\varepsilon^2 \, d\varepsilon$$

or

$$\int_\varepsilon |(u_\varepsilon,\phi_\varepsilon)_\varepsilon|^2 \, d\varepsilon \leq \underset{\varepsilon \in R}{\text{ess. sup}} || \phi_\varepsilon ||_\varepsilon^2 \; || u || < \infty \quad ,$$

so that $(u_\varepsilon,\phi_\varepsilon)_\varepsilon$ is square-integrable for $\phi \in D$, D being the set of $\phi \in \mathcal{H}$ such that $\underset{\varepsilon \in R}{\text{ess. sup}} || \phi_\varepsilon ||_\varepsilon < \infty$. D is a dense linear subset of $\mathcal{H}$. Since (u,ϕ_t) is the Fourier transform of $(u_\varepsilon,\phi_\varepsilon)_\varepsilon$, then (u,ϕ_t) is square-integrable also, for $\phi \in D$. The same applies to (v,ψ_t) for $\psi \in D$. Thus for $\phi,\psi \in D$ the integral $B(\psi,\phi)$, explicitly

$$\lambda \int_t (u,\phi_t)(\psi_t,v)dt \quad ,$$

is finite. Parseval's formula gives

$$\lambda \int_t (u,\phi_t)(\psi_t,v)dt = \lambda \int_\varepsilon (u,\hat{\phi}_t)(\hat{\psi}_t,v)d\varepsilon$$

$$= \lambda \int_\varepsilon (u_\varepsilon,\phi_\varepsilon)_\varepsilon(\psi_\varepsilon,v_\varepsilon)_\varepsilon d\varepsilon \quad ,$$

$\hat{}$ denoting the Fourier transform. Now consider the rank one operator

$$b(\varepsilon) = \lambda(u_\varepsilon, \ )_\varepsilon v_\varepsilon \quad .$$

We have

$$d \int_\varepsilon (\psi_\varepsilon,b(\varepsilon)\phi_\varepsilon)_\varepsilon d\varepsilon = \int_\varepsilon (\psi_\varepsilon,\lambda(u_\varepsilon,\phi_\varepsilon)_\varepsilon v_\varepsilon)d\varepsilon$$

$$= \lambda \int_\varepsilon (u_\varepsilon,\phi_\varepsilon)_\varepsilon(\psi_\varepsilon,v_\varepsilon)_\varepsilon d\varepsilon$$

$$= B(\psi,\phi) \quad .$$

Thus

$$B(\psi,\phi) = \int_t (\psi, U_t^\dagger T U_t \phi)dt$$

$$= \int_\varepsilon (\psi_\varepsilon,b(\varepsilon)\phi_\varepsilon)_\varepsilon d\varepsilon \quad .$$

It is simple to prove that $b(\varepsilon)$ is essentially unique. T can be symbolically written as

$$T = \int_\varepsilon^\oplus b(\varepsilon)d\varepsilon \quad .$$

For the trace of T in $\mathcal{H}$ we have, with $\{w_n\}$ a complete orthonominal set in $\mathcal{H}$,

$$\begin{aligned} \mathrm{Tr}\ T &= \sum_n (w_n, Tw_n) \\ &= \sum_n (w_n, \lambda(u, w_n)v) \\ &= \sum_n \lambda(u, w_n)(w_n, v) \\ &= \lambda(u,v) \\ &= \int_\varepsilon \lambda(u_\varepsilon, v_\varepsilon)_\varepsilon d\varepsilon \\ &= \int_\varepsilon \mathrm{tr}\ b(\varepsilon) d\varepsilon \quad . \end{aligned}$$

tr $b(\varepsilon)$ is the trace in H_ε; choosing a basis in H_ε and proceeding as above we have

$$\mathrm{tr}\ b(\varepsilon) = \lambda(u_\varepsilon, v_\varepsilon)_\varepsilon \quad .$$

We have demonstrated the validity of the theorem of Martin-Misra for rank one operators in the case of the time translation group with unitary representation $t \to U_t = e^{-ih_o t}$. The extension to finite rank operators is immediate. The extension to arbitrary trace-class operators utilizes the canonical representation of an arbitrary trace-class operator as the limit of operators of finite rank. The case of an arbitrary locally compact Abelian group differs only in interpretation, because of the complete analogy between harmonic analysis on such a group and Fourier analysis on the real line.

Returning now to the proposed application of the theorem of Martin-Misra,

we identify the locally compact Abelian group G with the time-translation group, with representation $U_t = e^{-ih_o t}$. The parameter ε then becomes the energy E, taking values in the spectrum of h_o. We put

$$T = A^\dagger \Gamma(R) A \quad ,$$

with $\Gamma(R) = \Omega^{(+)\dagger} P(R) \Omega^{(+)} - P(R)$, as before, and A an as yet unspecified operator. We first require that A be such as to make $T = A^\dagger \Gamma(R) A$ trace-class. Assuming for the moment that such an A exists, the theorem of Martin-Misra asserts the finiteness of the following integral for $\psi, \phi \in D$

$$B(\psi,\phi) = \int_t (\psi, e^{ih_o t} A^\dagger \Gamma(R) A e^{-ih_o t} \phi) dt \quad ,$$

and the existence of unique b(E) such that

$$B(\psi,\phi) = \int_E (\psi_E, b(E)\phi_E) dE \quad ,$$

for all ψ, ϕ in D. Furthermore we have, according to the theorem,

$$Tr(A^\dagger \Gamma(R) A) = \int_E tr\ b(E)\ dE \quad ,$$

and

$$\int_E || b(E) ||_1 dE \leq || A^\dagger \Gamma(R) A ||_1 \quad .$$

We now compare $B(\psi,\phi)$ with the time delay sesquilinear form

$$Q(R)(\psi,\phi) = \int_{-\infty}^{\infty} (\psi, e^{ih_o t} \Gamma(R) e^{-ih_o t} \phi) dt \quad .$$

$Q(R)(\psi,\phi)$ and $B(\psi,\phi)$ differ only in that the former has $\Gamma(R)$ under the integral, while the latter has $A^\dagger\Gamma(R)A$. It would seem attractive to put $A = 1$, and to work with $\Gamma(R)$ rather than $A^\dagger\Gamma(R)A$. However $\Gamma(R)$ is not in general in the trace-class, so the general theorem will not apply. We can still make deductions concerning $Q(R)(\psi,\phi)$ from properties of $B(\psi,\phi)$ if $\Gamma(R)$ and $T = A^\dagger\Gamma(R)A$ are related in a simple enough way on a dense set of functions in $\mathcal{H}$. We try to achieve this by choosing A suitably.

The operator A is so far unspecified except for the requirement that $T = A^\dagger\Gamma(R)A$ be trace-class. Let us also require that $[A,h_o] = 0$. Then, for ψ,ϕ in D we have

$$
\begin{aligned}
B(\psi,\phi) &= \int_{-\infty}^{\infty} (\psi,\, U_t^\dagger T U_t \phi)dt \\
&= \int_{-\infty}^{\infty} (\psi,\, e^{ih_o t} A^\dagger \Gamma(R) A\, e^{-ih_o t}\phi)dt \\
&= \int_{-\infty}^{\infty} (\psi,\, A^\dagger U_t^\dagger \Gamma(R) U_t A\phi)dt \\
&= \int_{-\infty}^{\infty} (A\psi, U_t^\dagger \Gamma(R) U_t (A\phi))dt \\
&= \int_{-\infty}^{\infty} (\alpha,\, U_t^\dagger \Gamma(R) U_t \beta)dt \quad , \\
&= Q(R)(\alpha,\beta) \quad ,
\end{aligned}
$$

with $\alpha = A\psi$, $\beta = A\phi$. Let us examine the set of vectors from which α,β can be chosen. Let D_o be the set of all vectors $A\theta$, for $\theta \in D$: $D_o = \{A\theta \mid \theta \in D\}$. Then α,β are in D_o. Let us now require that A be

bounded with domain $\mathcal{H}$ and range dense in $\mathcal{H}$. Then Cauchy sequences are mapped by A into Cauchy sequences, and since the closure of D is $\mathcal{H}$, the closure of D_o will also be $\mathcal{H}$. That is, D_o is dense in $\mathcal{H}$. Then the finiteness of $B(\psi,\phi)$ for ψ,ϕ in D implies the finiteness of $Q(R)(\alpha,\beta)$ for $\alpha,\beta \in$ the dense set D_o. According to the remarks at the beginning of this section, this demonstrates the existence and uniqueness of the time delay operator Q(R), if we can find an operator A with the following properties

(i) $A^\dagger\Gamma(R)A$ is trace-class;

(ii) $[A,h_o] = 0$;

(iii) A is bounded with domain $\mathcal{H}$ and range dense in $\mathcal{H}$.

A convenient choice for A is $A = r_o(z) = (h_o - z)^{-1}$, the resolvent of z, z not in the spectrum of h_o. Properties (ii) and (iii) are immediate. Property (i) requires more effort to verify. We have

$$\begin{aligned} A^\dagger\Gamma(R)A &= r_o^\dagger(z)[\Omega^{(+)\dagger}P(R)\Omega^{(+)} - P(R)]r_o(z) \\ &= r_o^\dagger(z)\Omega^{(+)\dagger}P(R)\Omega^{(+)}r_o(z) - r_o^\dagger(z)P(R)r_o(z) \\ &= [P(R)\Omega^{(+)}r_o(z)]^\dagger[P(R)\Omega^{(+)}r_o(z)] - [P(R)r_o(z)]^\dagger[P(R)r_o(z)] \end{aligned}$$

The operator $P(R)r_o(z)$ is in the Schmidt-class. This can be seen by noting that $r_o(z) = r_{oo}(z) - r_{oo}(z)Wr_o(z)$, where $r_{oo}(z)$ is the resolvent of a free particle, $r_{oo}(z) = (p^2 - z)^{-1}$, so that

$$P(R)r_o(z) = P(R)r_{oo}(z) - P(R)r_{oo}(z)Wr_o(z) .$$

Now $P(R)r_{oo}(z)$ is in the Schmidt class for z not in the spectrum of p^2, i.e., not 0 or on the positive real axis (see Appendix 1). Also $Wr_o(z)$ is bounded for z not in the spectrum of $h_o = p^2 + W$. Hence $P(R)r_{oo}(z)Wr_o(z)$

is in the Schmidt class for the same values of z. Finally $P(R)r_o(z)$ is the sum of two Schmidt class operators, hence is itself in the Schmidt class. Also, the operator $P(R)\Omega^{(+)}r_o(z)$ is in the Schmidt class. This can be seen by using the intertwining relation in the form $r(z)\Omega^{(+)} = \Omega^{(+)}r_o(z)$, with $r(z) = (h - z)^{-1}$, $h = p^2 + W + V$, and $r_o(z)$ as above. Then

$$P(R)\Omega^{(+)}r_o(z) = P(R)r(z)\Omega^{(+)} \quad ,$$

and $r(z) = r_o(z) - r_o(z)Vr(z)$, so that $P(R)r(z) = P(R)r_o(z) - P(R)r_o(z)Vr(z)$. We have seen that $P(R)r_o(z)$ is in the Schmidt class for z not in the spectrum of h_o, so that by the same argument as above, $P(R)r(z)\Omega^{(+)}$ is the Schmidt class for z not in the spectrum of h. Finally $A^\dagger\Gamma(R)A$ is the sum of two operators, each of which is the product of Schmidt-class operators, and so $A^\dagger\Gamma(R)A$ is a trace-class operator, for z not in the spectrum of h, and $A = r_o(z)$. This completes the demonstration of property (i).

4.4 The Spectral Property of the Time-Delay Operator

We make a further application of the general theorem of the last section. The subspaces entering into the direct-integral representation of $\mathcal{H}$

$$\mathcal{H} = \int_{\hat{G}}^{\oplus} H_\varepsilon d\varepsilon$$

are labelled by energy $E = \varepsilon$. In any such subspace A is a multiplication operator, since $[A,h_o] = 0$. That is, A is a function of E, A(E). In the subspace labelled by E the relations $\alpha = A\psi$ and $\beta = A\phi$ become $\alpha_E = A(E)\psi_E$ and $\beta_E = A(E)\phi_E$, respectively. We have

$$Q(R)(\alpha,\beta) = B(\psi,\phi) = \int_E (\psi_E, b(E)\phi_E)dE$$

$$= \int_E \left(\frac{\alpha_E}{A(E)} , b(E) \frac{\beta_E}{A(E)} \right)dE$$

$$= \int_E (\alpha_E, \frac{b(E)}{|A(E)|^2} \beta_E)dE$$

$$= \int_E (\alpha_E, \frac{q(E,R)}{2\pi} \beta_E)dE \quad .$$

We have put

$$\frac{q(E,R)}{2\pi} = \frac{b(E)}{|A(E)|^2} \quad .$$

The factor 2π is introduced for later convenience. We will refer to $q(E,R)$ as the reduced time-delay. The word "reduced" is intended to convey that this is the time-delay in a subspace labelled by E, the total time-delay being given by an integral over the reduced time-delay.

Further, the general theorem gives the result

$$Tr(A^\dagger \Gamma(R) A) = \int_E tr\ b(E)\ dE \quad ,$$

or using the cyclic property of the trace,

$$Tr(|A|^2 \Gamma(R)) = \int_E |A(E)|^2 tr \frac{q(E,R)}{2\pi}\ dE \quad ,$$

with $|A|^2 = A^\dagger A$. We have put $A = r_o(z)$, so that we have

$$Tr(|r_o(z)|^2 \Gamma(R)) = \int_E |r_o(E,z)|^2 tr \frac{q(E,R)}{2\pi}\ dE \quad .$$

With $r_o(z) = (h_o - z)^{-1}$, we have used the notation $r_o(E,z)$ for $(E - z)^{-1}$.

We now utilize a formula of Osborn and Tsang [1976]. This formula was originally derived for the case of a particle in free space subject to a localized potential; we review the derivation here to show that it also applies to the case of a particle in a periodic medium, scattering from an impurity. We begin by considering the quantity

$$2i \text{ Im Tr}[r(z) - r_o(z)] \quad .$$

We must first establish that $r(z) - r_o(z)$ is in the trace class. We have $r(z) = r_o(z) - r_o(z)Vr(z)$, so that $r(z) - r_o(z) = -r_o(z)Vr_o(z)$ $[1 - Vr(z)]$. The operator in the square bracket is bounded for Im $z \neq 0$. The operator $r_o(z)Vr_o(z)$ is in the trace-class. This can be seen by writing $V = V^{1/2}|V|^{1/2}$, as previously, and noting that $V^{1/2}r_o(z)$ and $|V|^{1/2}r_o(z)$ have been previously shown to be in the Schmidt class. Hence $r_o(z)V^{1/2}$ is in the Schmidt class. Finally then, $r(z) - r_o(z)$ is in the trace class, being the product of a trace class and a bounded operator. Then also $[r(z) - r_o(z)]^\dagger = r^\dagger(z) - r_o^\dagger(z)$ is in the trace class, so that we may write

$$2i \text{ Im Tr}[r(z) - r_o(z)] = \text{Tr}[r(z) - r_o(z) - r^\dagger(z) + r_o^\dagger(z)] = \text{Tr } C \quad ,$$

with $C = r(z) - r_o(z) - r^\dagger(z) + r_o^\dagger(z)$. C is in the trace class, being the sum of two trace class operators.

We evaluate Tr C by using the fact that

$$\text{Tr } C = \text{Tr } \lim_{R \to \infty} P(R)C = \lim_{R \to \infty} \text{Tr } P(R)C \quad ,$$

for any trace class operator C, where P(R) is the projector on the region

R, used in the discussion of time delay. This result is established by Osborn and Tsang [1976]. We have then that

$$P(R)C = P(R)[r(z) - r_o(z) - r_o(z) - r^\dagger(z) + r_o^\dagger(z)]$$

$$= P(R)[r(z) - r^\dagger(z)] - P(R)[r_o(z) - r_o^\dagger(z)]$$

We can show that $P(R)[r(z) - r^\dagger(z)]$ and $P(R)[r_o(z) - r_o^\dagger(z)]$ are both trace class. By the Hilbert identity

$$r_o(z) - r_o^\dagger(z) = (z - z^*)r_o(z)r_o^\dagger(z) \quad ,$$

since $r_o^\dagger(z) = r_o(z^*)$. Then

$$P(R)[r_o(z) - r_o^\dagger(z)]P(R) = (z - z^*)P(R)r_o(z)r_o^\dagger(z)P(R)$$

$$= (z - z^*)P(R)r_o(z)[P(R)r_o(z)]^\dagger \quad .$$

A precisely similar expression holds for $P(R)[r(z) - r^\dagger(z)]P(R)$, with $r_o(z)$ replaced by $r(z)$. Now we have already seen that $P(R)r_o(z)$ and $P(R)r(z)$ are in the Schmidt class for $\mathrm{Im}\, z \neq 0$. Hence $P(R)[r_o(z) - r_o^\dagger(z)]P(R)$ and $P(R)[r(z) - r^\dagger(z)]P(R)$ are in the trace-class, and since

$$\mathrm{Tr}[P(R)[r_o(z) - r_o^\dagger(z)]P(R)] = \mathrm{Tr}[P(R)[r_o(z) - r_o^\dagger(z)]]$$

by the cyclic property of the trace, and the fact that $P_R^2 = 1$, with a precisely similar expression for $\mathrm{Tr}[P(R)[r(z) - r^\dagger(z)]]$, we have our result. Thus we have

$$\mathrm{Tr}\, P(R)C = \mathrm{Tr}\, P(R)[r(z) - r^\dagger(z)] - \mathrm{Tr}\, P(R)[r_o(z) - r_o^\dagger(z)]$$

$$= \mathrm{Tr}\, P(R)(z - z^*)r(z)r^\dagger(z) - \mathrm{Tr}\, P(R)(z - z^*)r_o(z)r_o^\dagger(z)$$

$$\mathrm{Tr}\ P(R)C = (z - z^*)\mathrm{Tr}\ r^\dagger(z)P(R)r(z) - (z - z^*)\mathrm{Tr}\ r_o^\dagger(z)P(R)r_o(z)$$

We now utilize the asymptotic completeness property, according to which

$$L^2(R^3) = B + \mathcal{H}_{ac} \ ,$$

as previously discussed. This may also be formulated as

$$1 = P(B) + P(\mathcal{H}_{ac}) \ ,$$

where $P(B)$ is the projector on $\mathcal{H}_p$, the subspace of bound states, and $P(\mathcal{H}_{ac}) = \Omega^{(+)}\Omega^{(+)\dagger}$ is the projector on $\mathcal{H}_{ac}$, the absolutely continuous subspace of $\mathcal{H}$. We will also use the intertwining property in the form $r(z)\Omega^{(+)} = \Omega^{(+)}r_o(z)$. Then we have

$$\begin{aligned}
\mathrm{Tr}\ r^\dagger(z)P(R)r(z) &= \mathrm{Tr}\,1r^\dagger(z)P(R)r(z) \\
&= \mathrm{Tr}[P(B) + \Omega^{(+)}\Omega^{(+)\dagger}]r^\dagger(z)P(R)r(z) \\
&= \mathrm{Tr}\ P(B)r^\dagger(z)P(R)r(z) \\
&\qquad + \mathrm{Tr}\ \Omega^{(+)}\Omega^{(+)\dagger}r^\dagger(z)P(R)r(z)
\end{aligned}$$

The first term can be written as $\sum_i \dfrac{(\phi_i, P(R)\phi_i)}{|E_i - z|^2}$, where ϕ_i is an orthonormal basis for $\mathcal{H}_p$, and $h\phi_i = E_i\phi_i$. The second term can be written as

$$\begin{aligned}
\mathrm{Tr}[[r(z)\Omega^{(+)}]^\dagger P(R)r(z)\Omega^{(+)}] &= \mathrm{Tr}[[\Omega^{(+)}r_o(z)]^\dagger P(R)\Omega^{(+)}r_o(z)] \\
&= \mathrm{Tr}\ r_o^\dagger(z)\Omega^{(+)\dagger}P(R)\Omega^{(+)}r_o(z) \ .
\end{aligned}$$

Thus

$$\mathrm{Tr}\ P(R)C = (z - z^*) \sum_i \frac{(\phi_i, P(R)\phi_i)}{|E_i - z|^2} + (z - z^*)\mathrm{Tr}\ r_o^\dagger(z)\Omega^{(+)\dagger}P(R)\Omega^{(+)}r_o(z)$$

$$- (z - z^*)\mathrm{Tr}\ r_o^\dagger(z)P(R)r_o(z)$$

$$= (z - z^*) \sum_i \frac{(\phi_i, P(R)\phi_i)}{|E_i - z|^2} + (z - z^*)\mathrm{Tr}\ r_o^\dagger(z)\Gamma(R)r_o(z)$$

with $\Gamma(R) = \Omega^{(+)\dagger}P(R)\Omega^{(+)} - P(R)$. Finally, using $\mathrm{Tr}\ C = \lim_{R \to \infty} \mathrm{Tr}\ P(R)C$, we have $(z - z^* = 2i\ \mathrm{Im}\ z)$

$$\mathrm{Tr}\ C = 2i\ \mathrm{Im}\ \mathrm{Tr}[r(z) - r_o(z)]$$

$$= (2i\ \mathrm{Im}\ z) \sum_i \frac{1}{|E_i - z|^2} + \lim_{R \to \infty} (2i\ \mathrm{Im}\ z)\mathrm{Tr}[|r_o(z)|^2\Gamma(R)] \ .$$

This is the formula of Osborn and Tsang.

We now use the result, already discussed,

$$\mathrm{Tr}(|r_o(z)|^2\Gamma(R)) = \int_E |r_o(E,z)|^2 \mathrm{tr}\ \frac{q(E,R)}{2\pi}\, dE \ ,$$

with $r_o(E,z) = (E - z)^{-1}$. The second term on the right-hand side of the formula of Osborn and Tsang can now be written

$$\lim_{R \to \infty} (2i\ \mathrm{Im}\ z)\mathrm{Tr}(|r_o(z)|^2\Gamma(R)) = \lim_{R \to \infty} 2i \int \mathrm{Im}\ z|r_o(E,z)|^2 \mathrm{tr}\ \frac{q(E,R)}{2\pi}\, dE \ .$$

The limit as $R \to \infty$ exists, as a function of E, from the formula of Osborn and Tsang. We would like to be able to write the limit in the form of an

integral, as follows

$$\lim_{R \to \infty} 2i \int \mathrm{Im}\, z |r_o(E,z)|^2 \mathrm{tr}\, \frac{q(E,R)}{2\pi}\, dE = 2i \int \mathrm{Im}\, z |r_o(E,z)|^2 \frac{f(E)}{2\pi}\, dE \ .$$

We discuss this question in Appendix 2, where we show that this is indeed possible. $f(E)$ will be written as $\mathrm{tr}\, q(E)$, since the existence of the limit in the above sense implies the existence in the same sense of a limiting value of $\mathrm{tr}\, q(E,R)$. Again in the same sense there is implied a limiting value for $q(E,R)$ as $R \to \infty$, which we denote by $q(E)$, consistent with the notation introduced above. $q(E)$ is referred to as the reduced time delay for all of space. We can thus write

$$\lim_{R \to \infty} (2i\ \mathrm{Im}\, z)\mathrm{Tr}[r_o(z)|^2 r(R)] = 2i \int \mathrm{Im}\, z |r_o(E,z)|^2 \mathrm{tr}\, \frac{q(E)}{2\pi}\, dE \ ,$$

where $q(E)$ is the reduced time-delay for all of space. We thus have

$$2i\ \mathrm{Im}\, \mathrm{Tr}[r(z) - r_o(z)] = (2i\ \mathrm{Im}\, z) \sum_i \frac{1}{|E_i - z|^2} + 2i \int \frac{\mathrm{Im}\, z}{|E - z|^2} \mathrm{tr}\, \frac{q(E)}{2\pi}\, dE \ .$$

Put $z = \xi + i\eta$, so that $|E - z|^2 = (E - \xi)^2 + \eta^2$, $\mathrm{Im}\, z = \eta$, and allow $\mathrm{Im}\, z = \eta$ to approach zero onto the continuous spectrum of h. Then $E_i - z$ is never zero, so the first term on the right-hand side goes to zero. Also the representation for the δ-function $\pi\delta(x) = \lim_{\eta \to \infty} \frac{\eta}{x^2 + \eta^2}$ yields

$$2i\ \mathrm{Im}\, \mathrm{Tr}[r(\xi + io) - r_o(\xi + io)] = 2i \int \pi\delta(E - \xi)\mathrm{tr}\, \frac{q(E)}{2\pi}\, dE$$

$$= i\mathrm{tr}\, q(\xi) \ .$$

We finally have the spectral property of the time delay

$$2\ \mathrm{Im}\ \mathrm{Tr}[r(E + io) - r_o(E + io)] \;=\; \mathrm{tr}\ q(E) \quad ,$$

E in the absolutely continuous spectrum of h.

4.5 Time Delay in the Crystal Momentum Representation

We have had the formula for the time-delay in a region Σ_R

$$T_R(\phi) \;=\; (\phi, Q(R)\phi) \;=\; \int_{-\infty}^{\infty} (\phi,\ e^{ih_o t}\, \Gamma(R)\, e^{-ih_o t}\, \phi)dt \quad ,$$

with $\Gamma(R) = \Omega^{(+)\dagger} P(R)\Omega^{(+)} - P(R)$. Introducing the crystal-momentum representation we have (B is the Brillouin zone)

$$T_R(\phi) \;=\; \int_{-\infty}^{\infty} dt \int_B \sum_n \int_{B',n'} \sum (\phi|k,n><k,n|\, e^{ih_o t}\, \Gamma(R)\, e^{-ih_o t}\, |k',n'><k',n'|\phi)$$

$$= \int_{-\infty}^{\infty} dt \int_B \sum_n \int_{B',n'} \sum \phi_n^*(k)\, e^{iE_n(k)t} <k,n|\Gamma(R)|k',n'> e^{-iE_{n'}(k')t}\, \phi_{n'}(k')$$

$$= \int_B \sum_n \int_{B',n'} \sum \phi_n^*(k) \left\{ \int_{-\infty}^{\infty} dt\, e^{i(E - E')t} \right\} <k,n|\Gamma(R)|k',n'> \phi_{n'}(k')$$

$$= \int_B \sum_n \int_{B',n'} \sum \phi_n^*(k) 2\pi\delta(E - E') <k,n|\Gamma(R)|k',n'> \phi_{n'}(k') \quad .$$

Let us write this expression as

$$T_R(\phi) \;=\; (\phi,Q(R)\phi) \;=\; \int_B \sum_n \int_{B',n'} \sum \phi_n^*(k) <k,n|Q(R)|k',n'> \phi_{n'}(k') \quad ,$$

thereby introducing the crystal-momentum kernel

$$< k,n|Q(R)|k',n' > \;=\; 2\pi\delta(E - E') < k,n|\Gamma(R)|k',n') \quad .$$

Q(R) conserves energy. It is useful to make use of this to rewrite $< k,n|Q(R)|k',n' >$ as a matrix element on the energy shell. To this end, consider a surface $E_n(k)$ = constant. Denote states with this energy by $|\hat{k},n >$. We will consider an integral over k to be an integral first over the constant energy surface, then over energy. We thus put

$$< k,n|Q(R)|k',n' > \;=\; \delta(E - E') < \hat{k},n|q(E,R)|\hat{k}',n' > \frac{1}{k^2} \frac{dE}{dk} \quad ,$$

where $\frac{dE}{dk} = |\nabla_k E(k)|$. This defines the reduced time delay q(E,R), which operates in the Hilbert space of states $|\hat{k},n >$. (We will show later that this is the same as the reduced time delay already introduced). We have

$$2\pi < k,n|\Gamma(R)|k',n' > \;=\; < \hat{k},n|q(E,R)|\hat{k}',n' > \frac{1}{k^2} \frac{dE}{dk} \quad ,$$

or

$$< \hat{k},n|q(E,R)|\hat{k}',n' > \;=\; 2\pi < k,n|\Gamma(R)|k',n' > k^2 / \frac{dE}{dk} \quad .$$

We thus have

$$(\phi,Q(R)\phi) \;=\; \int_B \sum_n \int_B \sum_{n'} \phi_n^*(k)\delta(E - E') < \hat{k},n|q(E,R)|\hat{k}',n > k^2 / \frac{dE}{dk} \quad .$$

Let us now look at $\mathrm{Tr}(|r_o(z)|^2\Gamma(R))$ in the crystal-momentum representation. We have seen the importance of this quantity already. We obtain

$$\mathrm{Tr}(|r_o(z)|^2\Gamma(R)) \;=\; \int_B \sum_n < k,n| \; |r_o(z)|^2\Gamma(R)|k,n > \quad .$$

The matrix element under the integral can be written as

$$< k,n|\ |r_o(z)|^2\Gamma(R)|k,n > \ = \ \int_{B'} \sum_{n'} < k,n|\ |r_o(z)|^2|k',n' < k',n'|\Gamma(R)|k,n >$$

$$= \int_{B'} \sum_{n'} \frac{1}{|E_n(k) - z|^2}\ \delta(k - k')\delta_{nn'} < k',n'|\Gamma(R)|k,n >$$

$$= \frac{1}{|E_n(k) - z|^2} < k,n|\Gamma(R)|k,n >$$

$$= \frac{1}{|E_n(k) - z|^2} < \hat{k},n|q(E,R)|\hat{k},n > \frac{1}{k^2}\frac{dE}{dk}\ \frac{1}{2\pi}\ .$$

Thus

$$\mathrm{Tr}(|r_o(z)|^2\Gamma(R)) \ = \ \int_B \sum_n \frac{1}{|E_n(k) - z|^2} < \hat{k},n|q(E,R)|\hat{k}\ ,n > \frac{1}{k^2}\frac{dE}{dk}\ \frac{1}{2\pi}$$

$$= \int k^2 \left(\frac{dE}{dk}\right)^{-1} dE\ \frac{1}{|E - z|^2}\ \frac{1}{2\pi}\ \frac{1}{k^2}\ \frac{dE}{dk} \int d\hat{k} < \hat{k},n|q(E,R)|\hat{k},n >$$

$$= \int \frac{1}{|E - z|^2}\ \frac{1}{2\pi}\ \mathrm{tr}\ q(E,R)dE\ .$$

The integration over dE is over the continuous spectrum of h; we have transformed $\int_B \sum_n$ into an angular integral, $\int d\hat{k}$, integrated in turn over energy, $\int dE$. We have re-derived our former expression for $\mathrm{Tr}(|r_o(z)|^2\Gamma(R))$ showing that the reduced time delay introduced in this section is the same as that originally introduced. We could also use this point to enter the proof of the spectral property.

Chapter 5

SPECTRAL SHIFT AND LEVINSON'S THEOREM

5.1 *Introduction*

We define the spectral shift function, and relate this to the time delay. Both these quantities are then related to a general form of Levinson's theorem. It is shown how the Born expansion can be used to obtain information about the spectral shift function, and hence about the time delay and Levinson's theorem.

5.2 The Spectral Function

Consider a spectral family $\{e(\lambda)\}$ of projection operators, corresponding to a self-adjoint operator h, in terms of which h has the spectral decomposition

$$h = \int_{-\infty}^{\infty} \lambda de(\lambda)$$

(Riesz-Nagy [1956]). We put $\sigma(\lambda) = \mathrm{Tr}\, e(\lambda)$ and call this function the spectral function. We assume the existence of the trace. $\sigma(\lambda)$ is a non-decreasing function of λ, with jumps at the positions of the eigenvalues of h, and is constant outside the spectrum of h. The rate of change of $\sigma(\lambda)$ with λ measures the rate at which states are picked up as the projectors $e(\lambda)$ run through values of λ. In the terminology customarily used in physics, $\rho(\lambda) = d\sigma(\lambda)/d\lambda$ is the density of states for h. $\rho(\lambda)$ exists almost everywhere, but with δ-functions at the eigenvalue positions.

The resolvent of h is $r(z) = (h - z)^{-1}$, and according to the spectral theorem has the representation

$$r(z) = \int_{-\infty}^{\infty} \frac{1}{\lambda - z}\, de(\lambda) \quad .$$

Assuming that $\mathrm{Tr}(r(z))$ exists, we have

$$\mathrm{Tr}(r(z)) = \int_{-\infty}^{\infty} \frac{1}{\lambda - z} \mathrm{Tr}(de(\lambda))$$

$$= \int_{-\infty}^{\infty} \frac{1}{\lambda - z} d\sigma(\lambda) \quad .$$

This has meaning as a Stieltjes integral. The Stieltjes-Perron inversion formula (Akhiezer [1965]) states the following:

Let $f(z) = \int_{-\infty}^{\infty} \frac{1}{\lambda - z} d\sigma(\lambda)$, $\mathrm{Im}\ z > 0$, $\sigma(\lambda)$ real and of bounded variation in every finite interval, and $\int_{-\infty}^{\infty} \frac{|d\sigma(\lambda)|}{1 + |\lambda|} < \infty$.

Then $\mathrm{Im}\ f(z) = \int_{-\infty}^{\infty} \frac{y}{(x-\lambda)^2 + y^2} d\sigma(\lambda)$, $z = x + iy$, and

$$\lim_{y \to o} \frac{1}{\pi} \int_{c}^{E} \mathrm{Im}\ f(z)dx = \frac{1}{2}[\sigma(E+o) + \sigma(E-o)] - \frac{1}{2}[\sigma(c+o) + \sigma(c-o)],$$

for any real c.

At points of continuity of $\sigma(\lambda)$, $\lim_{y \to o} \frac{1}{\pi} \int_{c}^{E} \mathrm{Im}\ f(z)dx = \sigma(E) - \sigma(c)$, and we shall use this form, on the understanding that at points of discontinuity the complete expression is to be inserted. We thus have, assuming the conditions of the inversion formula are met,

$$\lim_{y \to o} \frac{1}{\pi} \int_{c}^{E} \mathrm{Im}\ \mathrm{Tr}[r(x + iy)]dx = \sigma(E) - \sigma(c) \quad ,$$

which we shall write as

$$\frac{1}{\pi} \int_{c}^{E} \mathrm{Im}\ \mathrm{Tr}[r(x + io)]dx = \sigma(E) - \sigma(c) \quad .$$

This corresponds to a formula very often met with in the physics literature, namely

$$\rho(E) = \frac{d\sigma(E)}{dE} = \frac{1}{\pi} \operatorname{Im} \operatorname{Tr}[r(E + i0)] ,$$

$\rho(E)$ being the density of states. Since $r^{\dagger}(z) = r(z^{*})$, we have $2i \operatorname{Im} r(z) = r(z) - r(z^{*})$, so that we can also write

$$\frac{1}{2\pi i} \int_{c}^{E} \operatorname{Tr}[r(x + i0) - r(x - i0)]dx = \sigma(E) - \sigma(c) .$$

$r(x + i0) - r(x - i0)$ is the discontinuity of $r(z)$ across the real axis. In the physics literature it is a common practise to put

$$\delta(h - E) = \frac{1}{2\pi i} [r(E + i0) - r(E - i0)] ,$$

so that

$$\rho(E) = \operatorname{Tr} \delta(h - E) .$$

Suppose now that $\operatorname{Tr} r(z) = f(z)$ is analytic in the z-plane cut along the spectrum of h. Assume the spectrum of h is bounded below by b. Referring to Fig. 3 we have

$$\int_{C_R} f(z)dz = 0 .$$

Deforming the contour as shown in Fig. 3, we have

$$0 = \int_{C_R} f(z)dz = \int_{2}^{C} f(z-)dz + \int_{C}^{1} f(z+)dz + \lim_{\operatorname{Im} 1,2 \to 0} \int_{C_E} f(z)dz ,$$

where $f(z-)$, $f(z+)$ indicate values just below and just above the real axis,

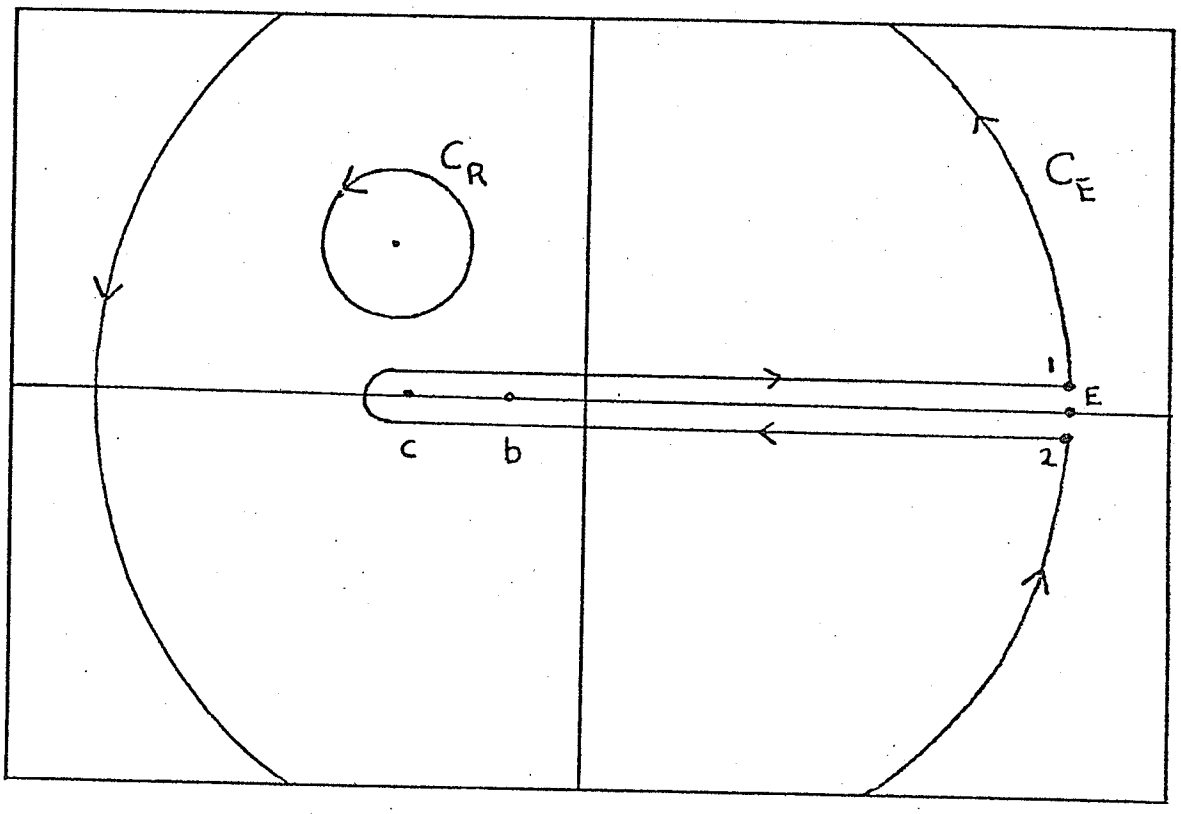


Fig. 3 Contours for integration of f(z) = Tr r(z).

respectively, and correspondingly, the points 1, 2 are to approach zero in imaginary part. We have then

$$\int_C^E [f(z+) - f(z-)]dz = - \lim_{\text{Im } 1,2 \to 0} \int_{C_E} f(z)dz \quad .$$

Then with $f(z) = \text{Tr } r(z)$, $f(z+) - f(z-) = \text{Tr}[r(x + io) - r(x - io)]$, so that

$$\int_C^E \text{Tr}[r(x + io) - r(x - io)]dx = - \lim_{\text{Im } 1,2 \to 0} \int_{C_E} \text{Tr}[r(z)]dz$$

$$= [\sigma(E) - \sigma(c)]2\pi i$$

We can take $\sigma(c) = 0$, since h has no spectrum below b.

5.3 The Spectral Shift Function

We now consider two self-adjoint operators, h_o and $h = h_o + V$. The spectral families corresponding to h_o and h will be denoted by $\{e_o(\lambda)\}$ and $\{e(\lambda)\}$ respectively, so that we have the spectral representations

$$h_o = \int_{-\infty}^{\infty} \lambda de_o(\lambda) \quad , \quad h = \int_{-\infty}^{\infty} \lambda de(\lambda) \quad .$$

The spectral shift function $\xi(\lambda)$ is defined by

$$\xi(\lambda) = \sigma(\lambda) - \sigma_o(\lambda)$$

$$= \text{Tr } e(\lambda) - \text{Tr } e_o(\lambda)$$

$$= \text{Tr}[e(\lambda) - e_o(\lambda)] \quad .$$

The spectral shift function gives the change in the spectral function due to the perturbation V.

Introducing the resolvents corresponding to h_o and h, respectively,

$$r_o(z) = (h_o - z)^{-1} = \int_{-\infty}^{\infty} \frac{de_o(\lambda)}{\lambda - z} \quad , \quad r(z) = (h - z)^{-1} = \int_{-\infty}^{\infty} \frac{de(\lambda)}{\lambda - z} \quad ,$$

we obtain

$$r(z) - r_o(z) = \int_{-\infty}^{\infty} \frac{de(\lambda) - de_o(\lambda)}{\lambda - z} \quad .$$

Then

$$\mathrm{Tr}[r(z) - r_o(z)] = \int_{-\infty}^{\infty} \frac{\mathrm{Tr}[de(\lambda) - de_o(\lambda)]}{\lambda - z}$$

$$= \int_{-\infty}^{\infty} \frac{d\xi(\lambda)}{\lambda - z} \quad .$$

Proceeding precisely as in the case of the spectral function, we obtain from the Stieltjes-Perron inversion formula

$$\frac{1}{\pi} \int_C^E \mathrm{Im}\ \mathrm{Tr}[r(x + io) - r_o(x + io)]dx = \xi(E) - \xi(C) \quad .$$

This can be written, at points of differentiability of $\xi(E)$, as

$$\frac{d\xi(E)}{dE} = \frac{1}{\pi} \mathrm{Im}\ \mathrm{Tr}[r(E + io) - r_o(E + io)]$$

$$= \frac{1}{2\pi} \mathrm{tr}\ q(E) \quad ,$$

by the spectral property of the time delay (i.e., for E in the continuous spectrum). Also $\xi(E) - \xi(C) = \frac{1}{2\pi} \int_C^E \mathrm{tr}\ q(E)dE$.

Assuming that $\mathrm{Tr}[r(z) - r_o(z)]$ is analytic in the z-plane cut along the spectrum of h, we obtain precisely as in the case of the spectral function

$$-\frac{1}{2\pi i} \lim_{\mathrm{Im}\, 1,2 \to 0} \int_{C_E} \mathrm{Tr}[r(z) - r_o(z)]dz = \xi(E) - \xi(c) \quad .$$

If we assume that the spectra of h and of h_o are both bounded below by b, and $c \leq b$, then $\xi(c) = 0$.

The foregoing relations, even though we have proceeded formally, and also have introduced notations which had to be properly interpreted, are quite general. Let us now introduce assumptions concerning the spectrum of h, consistent with its' being the Hamiltonian of a particle in a periodic potential, subject to an impurity potential, $h = p^2 + W + V$. Thus, we assume the continuous spectrum occurs in bands, with eigenvalues in the band gaps. It is possible for an eigenvalue to coincide with a point inside a band, but we will exclude this possibility for now. We also assume the spectrum of h_o is absolutely continuous, and unitarily equivalent to the absolutely continuous part of the spectrum of h. The contour integral expression for $\xi(E)$ can now be modified, by using the contours shown in Fig. 4. We put b = infimum of absolutely continuous spectrum. Assuming $\mathrm{Tr}[r(z) - r_o(z)] = F(z)$ is analytic in the z-plane cut along the absolutely continuous spectrum of h, except for poles at the eigenvalues, we have

$$\int_{C_R} F(z)dz = 0 = \int F(z)dz + \int_b^E [F(z+) - F(z-)]dz + \lim_{\mathrm{Im}\, 1,2 \to 0} \int_{C_E} F(z)dz \quad .$$

eigenvalues continuous spectrum

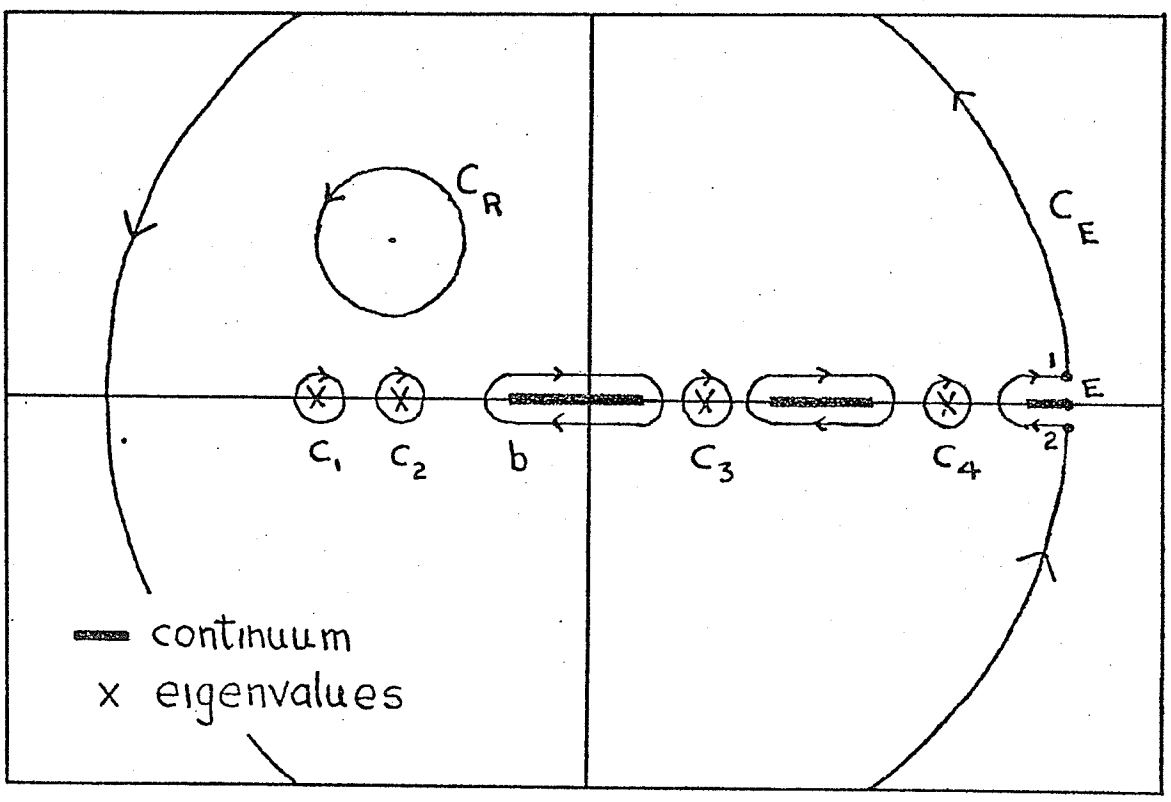


Fig. 4 Contours for integration of $F(z) = \mathrm{Tr}[r(z) - r_o(z)]$.

The integral over the eigenvalues can be evaluated as follows. Let the eigenvalues be E_i, $h\phi_i = E_i\phi_i$, and let the degeneracy of E_i be N_i, so ϕ_i has a label α running from 1 to N_i. Then

$$\int_{\text{eigenvalues}} F(z)dz = \sum_{\substack{i \\ E_i < E}} \int_{C_i} \mathrm{Tr}[r(z) - r_o(z)]dz$$

$$= \sum_{\substack{i \\ E_i < E}} \int_{C_i} \sum_{\alpha=1}^{N_i} \langle \phi_{i\alpha}|r(z) - r_o(z)|\phi_{i\alpha}\rangle dz$$

$$= \sum_{\substack{i \\ E_i < E}} \sum_{\alpha=1}^{N_i} \int_{C_i} \frac{\langle \phi_{i\alpha}|\phi_{i\alpha}\rangle}{E_i - z}$$

$$= \sum_{\substack{i \\ E_i < E}} \sum_{\alpha=1}^{N_i} (+ 2\pi i) = + \sum_{\substack{i \\ E_i < E}} 2\pi i\, N_i$$

$$= + 2\pi i\, N(E) \quad .$$

We have put $\sum_{\substack{i \\ E_i < E}} N_i = N(E)$, the total number of eigenvalues of energy less than E, counting multiplicity. We have used the fact that $r_o(z)$ is analytic outside the continuous spectrum. The integral over the continuous spectrum can be written as

$$\int_b^E \{\mathrm{Tr}[r(x + io) - r_o(x + io)] - \mathrm{Tr}[r(x - io) - r_o(x - io)]\}dx$$

$$\text{continuous spectrum} = \int_b^E 2i\ \mathrm{Im}\ \mathrm{Tr}[r(x + io) - r_o(x - io)]dx$$

$$= i\int_b^E \mathrm{tr}\, q(x)dx$$

We have, as before, $\lim_{\text{Im } 1,2 \to 0} \int_{C_E} F(z)dz = -2\pi i\, \xi(E)$. Thus

$$0 = 2\pi i\, N(E) + i \int_b^E \text{tr } q(x)dx - 2\pi i\, \xi(E) \quad ,$$

continuous spectrum

or

$$\xi(E) - N(E) = \frac{1}{2\pi} \int_b^E \text{tr } q(x)dx \quad .$$

This is a prototype of Levinson's theorem (Osborn [1978]). We have decomposed the spectral shift into a part due to the eigenvalues, giving the N term, and a term due to the spectral shift in the continuous spectrum, which we have expressed in terms of the time delay.

We have excluded eigenvalues whose energies lie in the continuous spectrum. A moments' consideration shows that this is not necessary. What we have done is to decompose $\xi(E)$ into a step function (with jumps at the eigenvalues) and an absolutely continuous function (the shift in the continous spectrum). The step function gives the N(E) term above regardless of whether the jump is in or not in the continuous spectrum. The absolutely continuous part gives the time delay term.

5.4 The Born Expansion

We have had the relation

$$\xi(E) = \lim_{\text{Im } 1,2 \to 0} \frac{1}{2\pi i} \int_{C_E} \text{Tr}[r(x) - r_o(z)]dz \quad .$$

We can obtain $r(z) - r_o(z)$ by iterating the relation $r(z) = r_o(z) - r_o(z)Vr(z)$. We have (Born expansion)

$$r(z) - r_o(z) = -r_o(z)Vr(z)$$

$$= \sum_{n=1}^{\infty} r_o(z)[-Vr_o(z)]^n \quad ,$$

assuming this expansion converges (at least for $|z|$ large enough). Then, assuming $r(z) - r_o(z)$ is in the trace class

$$\mathrm{Tr}[r(z) - r_o(z)] = \mathrm{Tr} \sum_{n=1}^{\infty} r_o(z)[-Vr_o(z)]^n$$

$$= \sum_{n=1}^{\infty} \mathrm{Tr}\{r_o(z)[-Vr_o(z)]^n\} \quad ,$$

assuming the interchange of the trace and the summation is allowable, and $r_o(z)[-Vr_o(z)]^n$ is trace class. Then (omitting $\lim_{\mathrm{Im}\, 1,2 \to 0}$ for convenience in writing)

$$\xi(E) = -\frac{1}{2\pi i} \int_{C_E} \mathrm{Tr}[r(z) - r_o(z)]$$

$$= -\frac{1}{2\pi i} \int_{C_E} \sum_{n=1}^{\infty} \mathrm{Tr}\{r_o(z)[-Vr_o(z)]^n\}$$

$$= \sum_{n=1}^{\infty} \{-\frac{1}{2\pi i} \int_{C_E} \mathrm{Tr}\{r_o(z)[-Vr_o(z)]^n\}\}$$

$$= \sum_{n=1}^{\infty} \xi_n(E) \quad .$$

We have assumed that the interchange of integration and summation is permissible, and that $\mathrm{Tr}\{r_o(z)[-Vr_o(z)]^n\}$ is analytic inside C_E. We have put

$$\xi_n(E) = -\frac{1}{2\pi i}\int_{C_E} \mathrm{Tr}\{r_o(z)[-Vr_o(z)]^n\}dz \quad .$$

We have, now, for $n \geq 2$

$$\frac{d}{dz}[Vr_o(z)]^n = n[Vr_o(z)]^{n-1}V\frac{dr_o(z)}{dz}$$

$$= n[Vr_o(z)]^{n-1}Vr_o^2(z)$$

$$= n[Vr_o(z)]^n r_o(z) \quad .$$

Thus

$$\mathrm{Tr}\frac{d}{dz}[Vr_o(z)]^n = n\,\mathrm{Tr}\{r_o(z)[Vr_o(z)]^n\} \quad ,$$

using the cyclic property of the trace. Assuming that the trace and the derivative can be commuted, we have

$$\mathrm{Tr}\{r_o(z)[-Vr_o(z)]^n\} = \frac{(-1)^n}{n}\frac{d}{dz}\mathrm{Tr}[Vr_o(z)]^n \quad .$$

Thus we can write, for $n \geq 2$

$$\xi_n(E) = -\frac{1}{2\pi i}\int_{C_E}\frac{(-1)^n}{n}\frac{d}{dz}\mathrm{Tr}[Vr_o(z)]^n$$

$$= -\frac{1}{2\pi i}\frac{(-1)^n}{n}\{\mathrm{Tr}[Vr_o(E - i\delta)]^n - \mathrm{Tr}[Vr_o(E + i\delta)]^n\}$$

$$\xi_n(E) = -\frac{1}{2\pi i}\,\frac{(-1)^n}{n}\,\{\mathrm{Tr}[Vr_o(E + i0)]^n - \mathrm{Tr}[Vr_o(E - i0)]^n\} \quad .$$

We have denoted the z values at points 1, 2 respectively by $E + i\delta$, $E - i\delta$. The δ is to be allowed to go to zero, i.e., we need $\mathrm{Tr}[Vr_oE \pm i\delta]^n$ in the limit as $\delta \to 0$.

The foregoing discussion has been formal, and we must now turn to the problem of justifying the various assumptions made. In so far as this can be done we can obtain information concerning $\xi(E)$, hence time-delay and Levinson's theorem.

Chapter 6

TRACE CLASS OPERATORS AND THE BORN EXPANSION

6.1 *Introduction*

We give mathematical results which are useful in the study of the spectral shift and Levinson's theorem.

6.2 Interchange of Trace and Summation

Let us first very briefly summarize some Hilbert space concepts and notations (Kato [1976]). We deal with a Hilbert space $\mathcal{H}$, with inner product $< f,g >$ and norm $||f|| = \sqrt{< f,f >}$, $f \in \mathcal{H}$. A sequence of vectors $\{f_n\}$ converges strongly to a vector f if $||f - f_n|| < \epsilon$ for n large enough. We write $f_n \to f$ or $\lim f_n = f$. A sequence of vectors f_n converges weakly to a vector f if $< f_n,g > \to < f,g >$ for every $g \in \mathcal{H}$. Series are treated by dealing with the partial sums $f_n = \sum_{k=1}^{n} g_k$. Strong convergence implies weak convergence, but not conversely. A linear functional ϕ is bounded if and only if it is continuous. If $f_n \to f$ (strong convergence) then $\phi f_n \to \phi f$, i.e., $\lim(\phi f_n) = \phi(\lim f_n) = \phi f$, with ϕ continuous. Given ϕ, ϕ continuous, there exists a unique $g \in \mathcal{H}$ such that $\phi f = < f,g >$. Hence $\phi f = \lim(\phi f_n) = \lim < f_n,g > = \phi(\lim f_n) = < \lim f_n, g > = < f,g >$. A linear operator T is bounded if and only if it is continuous. If $f_n \to f$ (strong convergence) then $Tf_n \to Tf$, T continuous. The norm of T is $||T|| = \sup_{||f||=1} ||Tf||$. A sequence of operators $\{T_n\}$ converges uniformly to an operator T if $||T - T_n|| < \epsilon$ for n large enough. We write $T_n \to T$, or $\lim T_n = T$. A sequence of operators converges strongly if $T_n f \to Tf$ for all $f \in \mathcal{H}$ (strong vector convergence). A sequence of operators converges weakly if $< T_n f,g > \to < Tf,g >$ for all $f,g \in \mathcal{H}$ (weak vector convergence). Uniform convergence implies strong convergence, which

in turn implies weak convergence. The converses do not hold. Series are treated by dealing with partial sums, $T_n = \sum_{k=1}^{n} A_k$. Absolute convergence implies convergence. For a convergent series $\sum_{k=1}^{\infty} A_k = T$ (uniform convergence) we have $\sum_{k=1}^{n} A_k = T_n \to T$, by definition. Then $T_n f \to Tf$ for every $f \in \mathcal{H}$ (strong convergence), and $< T_n f,g > \to < Tf,g >$ for every $f,g \in \mathcal{H}$ (weak convergence). By the continuity of the scalar product, viewed as a linear functional, we have $<(\sum_{k=1}^{\infty} A_k)f,g > = < Tf,g > = \lim < T_n f,g > = < \lim T_n f,g > = \lim <(\sum_{k=1}^{n} A_k)f,g > = \lim \sum_{k=1}^{n} < A_k f,g >$, i.e.

$$\sum_{k=1}^{\infty} < A_k f,g > \; = \; <(\sum_{k=1}^{\infty} A_k)f,g > \; = \; < Tf,g > \quad ,$$

for every $f,g \in \mathcal{H}$.

We are now in a position to consider the interchange of the trace and summation operations. If T belongs to the trace class, then the trace is

$$\text{Trace } (T) \; = \; \text{Tr } T \; = \; \sum_{j} \; < T\phi_j,\phi_j > \quad ,$$

where ϕ_j is an orthonormal basis for $\mathcal{H}$ (assume $\mathcal{H}$ separable). Let us suppose that T is given as a convergent series $T = \sum_{k=1}^{\infty} A_k$, so that $\sum_{k=1}^{\infty} < A_k f,g > = < Tf,g >$, for all $f,g \in \mathcal{H}$, and thus $\sum_{k=1}^{\infty} < A_k \phi_j,\phi_j > = < T\phi_j,\phi_j >$. We have then

$$\text{Tr } T \; = \; \sum_{j} \sum_{k=1}^{\infty} \; < A_k \phi_j,\phi_j > \quad .$$

If the summations could be interchanged we could conclude that Tr T = Tr $\sum_{k=1}^{\infty} A_k = \sum_{k=1}^{\infty} \text{Tr } A_k$, given that the A_k, $k = 1,2,\ldots,\infty$, were in the

trace class. This is the result we wish to establish. We have the following theorem:

Theorem 1. If $T = \sum_{k=1}^{\infty} A_k$ is given as a convergent series, if T and each A_k is in the trace class, and if the series of trace norms $\sum_{k=1}^{\infty} ||A_k||_1$ converges, then

$$\operatorname{Tr} T = \sum_{k=1}^{\infty} \operatorname{Tr} A_k \quad .$$

Further, the series $\sum_{k=1}^{\infty} \operatorname{Tr} A_k$ converges absolutely.

Proof. We utilize the standard theorem on repeated series (Apostol [1957]), i.e., series of the form $\sum_{m=1}^{\infty} (\sum_{n=1}^{\infty} a_{mn})$.

> Let a_{mn} be a complex-valued double sequence; assume that $\sum_{n=1}^{\infty} a_{mn}$ converges absolutely for each m, and that $\sum_{m=1}^{\infty} \sum_{n=1}^{\infty} |a_{mn}|$ converges; then $\sum_{m=1}^{\infty} a_{mn}$ converges absolutely for each n, and $\sum_{n=1}^{\infty} (\sum_{m=1}^{\infty} a_{mn})$ converges absolutely and equals $\sum_{m=1}^{\infty} (\sum_{n=1}^{\infty} a_{mn})$.

Rather than considering the repeated series $\operatorname{Tr} T = \sum_{j} \sum_{k=1}^{\infty} < A_k \phi_j, \phi_j >$, let us try to apply the theorem to $\sum_{k=1}^{\infty} \sum_{j} < A_k \phi_j, \phi_j > = \sum_{k=1}^{\infty} \operatorname{Tr} A_k$. Denote $< A_k \phi_j, \phi_j >$ by a_{kj}. We examine the absolute convergence of $\sum_{j=1}^{\infty} a_{kj}$, for each k. We have $\sum_{j=1}^{\infty} a_{kj} = \sum_{j=1}^{\infty} < A_k \phi_j, \phi_j > = \operatorname{Tr} A_k$. Also $|\operatorname{Tr}(A_k)| \leq \sum_{j=1}^{\infty} | < A_k \phi_j, \phi_j > | < ||A_k||_1$. $||A_k||_1$ is to be finite by assumption, so that $\sum_{j=1}^{\infty} |a_{kj}| = \sum_{j=1}^{\infty} | < A_k \phi_j, \phi_j > |$ is finite, i.e., $\sum_{j=1}^{\infty} a_{kj}$ converges for each k. Then, as a series in k, $\sum_{k=1}^{\infty} \sum_{j} |a_{kj}| = \sum_{k=1}^{\infty} \sum_{j} | < A_k \phi_j, \phi_j > |$ has

each term dominated by $||A_k||_1$. $\sum_{k=1}^{\infty} ||A_k||_1$ is to converge by assumption. Hence $\sum_{k=1}^{\infty} \sum_j |a_{kj}|$ converges. We now apply the standard theorem on repeated series to conclude that $\sum_{k=1}^{\infty} a_{kj} = \sum_{k=1}^{\infty} < A_k\phi_j,\phi_j >$ converges absolutely for each j, and Tr T $= \sum_j \sum_{k=1}^{\infty} < A_k\phi_j,\phi_j >$ converges absolutely and equals $\sum_{k=1}^{\infty} \sum_j < A_k\phi_j,\phi_j > = \sum_{k=1}^{\infty}$ Tr A_k. This concludes the proof.

6.3 Interchange of Trace and Derivative

Since we are going to deal with derivatives of operator functions of a complex variable, we review briefly the analyticity of such operator functions. An operator T(z) is analytic in a region D of the complex plane if it can be expanded in a convergent power series at every point of the region; convergence is taken in the sense of uniform convergence. This is equivalent to differentiability in the region, and many of the usual theorems of complex analysis remain valid (Kato [1976]). For example, if S,T are analytic, so is the composition ST, and also T^{-1} is analytic if it exists. The same definitions can be used with convergence taken in the strong sense, and also in the weak sense. All three types of analyticity are equivalent. That is, if T(z) is analytic, then T(z)f is an analytic vector function of z for all $f \in \mathcal{H}$, and conversely $< T(z)f,g >$ is an analytic scalar function of z for all $f,g \in \mathcal{H}$, and conversely.

Suppose now that T(z) is analytic in D, and is also in the trace class for each $z \in D$. Then Tr $T(z) = \sum_j < T(z)\phi_j,\phi_j >$ is a point-wise convergent series of analytic functions for each $z \in D$. That is, putting $f_n(z) = \sum_{j=1}^{n} < T(z)\phi_j,\phi_j >$ the sequence $\{f_n(z)\}$ is a sequence of analytic functions for which $f_n(z) \to f(z) =$ Tr $T(z)$ for each $z \in D$. We now show

that the convergence is in fact uniform on compact subsets of D. To see this note that

$$|\mathrm{Tr}\ T(z)| \leq \sum_{j=1}^{\infty} | < T(z)\phi_j, \phi_j > | \leq ||T(z)||_1 \leq M \ ,$$

where M is an upper bound for the trace norm $||T(z)||_1$, $z \in D$. Then

$$|f_n(z)| = | \sum_{j=1}^{n} < T(z)\phi_j, \phi_j > | \leq \sum_{j=1}^{n} | < T(z)\phi_j, \phi_j > |$$

$$\leq \sum_{j=1}^{\infty} | < T(z)\phi_j, \phi_j > |$$

$$\leq ||T(z)||_1 \leq M \ .$$

Thus $f_n(z)$ is uniformly bounded for $z \in D$. By Vital's theorem (Rudin [1974]) the convergence of $f_n(z)$ to $f(z) = \mathrm{Tr}\ T(z)$ is uniform on every compact subset of D, and Tr T(z) is analytic in D. The same theorem yields the further result that the sequence of derivatives $\{\frac{d^m}{dz^m} f_n(z)\}$ converges uniformly to $\frac{d^m}{dz^m} f(z) = \frac{d^m}{dz^m} \mathrm{Tr}\ T(z)$, on every compact subset of D, m = 1,2,3, ...

We now have the following theorem:

Theorem 2. If T(z) is analytic in D, and is in the trace class for each $z \in D$, and if dT(z)/dz is in the trace class for each $z \in D$, then

$$\frac{d}{dz} \mathrm{Tr}\ T(z) = \mathrm{Tr}\ \frac{dT(z)}{dz}$$

Proof. Since T(z) is analytic in D, dT(z)/dz exists, and since T(z) is in the trace class in D, dTr T(z)/dt exists and is analytic in D. Since

$dT(z)/dz$ is in the trace class in D, $Tr[dT(z)/dz]$ exists and is analytic in D. Putting $f_n(z) = \sum_{j=1}^{n} < T(z)\phi_j,\phi_j >$, we have that $f_n(z) \to f(z) = Tr\ T(z)$, and $\frac{df_n(z)}{dz} \to \frac{df(z)}{dz}$, the convergence being uniform on compact subsets of D. Thus

$$\frac{d}{dz}\ Tr\ T(z) = \frac{df(z)}{dz} = \frac{d}{dz} \sum_{j=1}^{\infty} < T(z)\phi_j,\phi_j >$$

$$= \sum_{j=1}^{\infty} \frac{d}{dz} < T(z)\phi_j,\phi_j > ,$$

by uniform convergence. By the equivalence of the various types of analyticity, we have

$$\frac{d}{dz} < T(z)\phi_j,\phi_j > = < \frac{dT(z)}{dz}\ \phi_j,\phi_j > .$$

Thus

$$\frac{d}{dz}\ Tr\ T(z) = \sum_{j=1}^{\infty} < \frac{dT(z)}{dz}\ \phi_j,\phi_j > = Tr\ \frac{dT(z)}{dz} .$$

This concludes the proof.

If now $T(z)$ is given by a series $T(z) = \sum_{k=1}^{\infty} A_k(z)$, convergent for each $z \in D$, with $T(z)$ and all $A_k(z)$ analytic in D, and if $T(z)$ and all the $A_k(z)$ are in the trace class for each $z \in D$, then on the assumption that the series of trace norms, $\sum_{k=1}^{\infty} ||A_k(z)||_1$ converges, we have

$$Tr\ T(z) = Tr \sum_{k=1}^{\infty} A_k(z) = \sum_{k=1}^{\infty} Tr\ A_k(z) ,$$

for each $z \in D$. The series for $Tr\ T(z)$, $\sum_{k=1}^{\infty} Tr\ A_k(z)$, converges uniformly.

To see this note that

$$|\mathrm{Tr}\ A_k(z)| \ < \ ||A_k(z)||_1 \ = \ M_k \ ,$$

and

$$\sum_{k=1}^{\infty} M_k \ = \ \sum_{k=1}^{\infty} ||A_k(z)||_1$$

converges for each $z \in D$ by assumption. By Weierstrass' M-test the series $\sum_{k=1}^{\infty} \mathrm{Tr}\ A_k(z)$ converges uniformly in D. We have seen previously that this series converges absolutely. If now $\frac{dT(z)}{dz}$ is in the trace class for all $z \in D$, then from the previous theorem $\frac{d}{dz}\ \mathrm{Tr}\ T(z) = \frac{dT(z)}{dz}$, and by uniform convergence $\frac{dT(z)}{dz} = \frac{d}{dz} \sum_{k=1}^{\infty} A_k(z) = \sum_{k=1}^{\infty} \frac{d}{dz}\ A_k(z)$, so that we have

$$\frac{d}{dz}\ \mathrm{Tr}\ T(z) \ = \ \frac{d}{dz}\ \mathrm{Tr}\Big(\sum_{k=1}^{\infty} A_k(z)\Big) \ = \ \mathrm{Tr}\Big(\sum_{k=1}^{\infty} \frac{d}{dz} A_k(z)\Big) \ .$$

6.4 The Born Expansion

We consider Hamiltonians h_o and $h = h_o + V$, with corresponding resolvents $r_o(z) = (h_o - z)^{-1}$ and $r(z) = (h - z)^{-1}$, respectively. h_o is assumed to have an absolutely continuous spectrum, while h has a spectrum with an absolutely continuous part unitarily equivalent to the spectrum of h_o, plus a point spectrum. $r_o(z)$ is analytic outside the spectrum of h_o, and $r(z)$ is analytic outside the spectrum of h. We consider the case in which the Hilbert space is $L^2(R^3) = \mathcal{H}$, and V is an operation of multiplication by the function $v(x)$. We have already introduced the decomposition of V into $V = V^{1/2}|V|^{1/2}$, with $V^{1/2}$ being multiplication by $|v(x)|^{1/2}$ sign $(v(x))$, and $|V|^{1/2}$ being multiplication by $|v(x)|^{1/2}$. By composition of analytic functions the following operators are analytic outside the spectrum

of h_o: $Vr_o(z)$, $V^{1/2}r_o(z)$, $|V|^{1/2}r_o(z)$, $r_o(z)(-Vr_o(z))^n$, $n \geq 1$.

We now prove the following theorem.

Theorem 3. If $r(z) - r_o(z)$, and $r_o(z)[-Vr_o(z)]^n$, $n \geq 1$, are in the trace class for $z \in D$, and if the series of the trace norms $\sum_{n=1}^{\infty} ||r_o(z)[-Vr_o(z)]^n||_1$ converges for $z \in D$, then the Born expansion

$$r(z) - r_o(z) = \sum_{n=1}^{\infty} r_o(z)[-Vr_o(z)]^n$$

is valid for $z \in D$, and

$$Tr[r(z) - r_o(z)] = \sum_{n=1}^{\infty} Tr[r_o(z)[-Vr_o(z)]^n] \quad .$$

The latter series converges uniformly and absolutely.

Proof. Since $|Tr[r_o(z)[-Vr_o(z)]^n]| < ||r_o(z)[-Vr_o(z)]^n||_1$, the convergence of the series of trace norms implies the absolute convergence, and hence the convergence, of the series of traces $\sum_{n=1}^{\infty} Tr[r_o(z)[-Vr_o(z)]^n]$. By results already established the convergence is uniform as well as absolute. The uniform norm is never greater than the trace norm, so that $||r_o(z)[-Vr_o(z)]^n|| \leq ||r_o(z)[-Vr_o(z)]^n||_1$. Thus the convergence of the series of trace norms implies the absolute convergence, and hence the convergence, of the series $\sum_{n=1}^{\infty} r_o(z)[-Vr_o(z)]^n$. This latter series is precisely the limit of the iterated expression $r(z)-r_o(z) = -r_o(z)Vr_o(z) + r_o(z)Vr_o(z)Vr_o(z) - \ldots$ obtained from $r(z) = r_o(z)-r_o(z)Vr(z)$. We thus have $r(z)-r_o(z) = \sum_{n=1}^{\infty} r_o(z)[-Vr_o(z)]^n$ and thus $Tr[r(z)-r_o(z)] = Tr[\sum_{n=1}^{\infty} r_o(z)[-V(r_o(z)]^n]$. By results already established we can interchange the trace and the summation to obtain $Tr[r(z)-r_o(z)] = \sum_{n=1}^{\infty} Tr[r_o(z)[-Vr_o(z)]^n]$. This concludes the proof.

In order to apply the foregoing theorem in a particular situation, we must show that the series of trace norms $\sum_{n=1}^{\infty} ||r_o(z)[-Vr_o(z)]^n||_1$ converges for $z \in D$. We give a useful sufficient condition.

Theorem 4. If $K = V^{1/2} r_o(z) |V|^{1/2}$ is in the Schmidt class for $z \in D$, and if $r_o(z)$ is bounded for $z \in D$, then whenever $||K^2||_2 < 1$, the series $\sum_{n=2}^{\infty} ||K^n||_1$ and $\sum_{n=2}^{\infty} ||r_o(z)[-Vr_o(z)]^n||_1$ converge.

Proof. Since K is in the Schmidt class for $z \in D$, K^n is in the trace class for $n \geq 2$. For $n \geq 4$ we have

$$||K^n||_1 \leq ||K^2K^{n-2}||_1 \leq ||K^2||\,||K^{n-2}||_1 \leq ||K^2||_2\,||K^{n-2}||_1 .$$

We have used the fact that the uniform norm is never greater than the Schmidt norm. Thus if $n \geq 4$, and even,

$$||K^n||_1 \leq ||K^2||_2^{\frac{n-2}{2}}\,||K^2||_1 = c_1||K^2||_2^{\frac{n-2}{2}} ,$$

while if $n \geq 5$, and odd,

$$||K^n||_1 \leq ||K^2||_2^{\frac{n-3}{2}}\,||K^3||_1 = c_2||K^2||_2^{\frac{n-3}{2}} .$$

We have put $c_1 = ||K^2||_1$, and $c_2 = ||K^3||_1$. Now put $a = ||K^2||_2$. The series $\sum_{n=4}^{\infty} ||K^n||_1$ is dominated by the geometric series $c_1(a+a^2+a^3+ \ldots) + c_2(a+a^2+a^3+ \ldots) = (c_1+c_2)(a+a^2+a^3+ \ldots)$, which converges for $a = ||K^2||_2 < 1$. Hence, whenever $||K^2||_2 < 1$ the series

$$\sum_{n=2}^{\infty} ||K^n||_1 = ||K^2||_1 + ||K^3||_1 + \sum_{n=4}^{\infty} ||K^n||_1$$

converges.

Now, for $n \geq 2$, we have

$$||K^n||_1 = ||(V^{1/2} r_o(z) |V|^{1/2})^n||_1 = ||V^{1/2} r_o(z)[Vr_o(z)]^{n-1} |V|^{1/2}||_1$$

$$= ||Vr_o(z)[Vr_o(z)]^{n-1}||_1 = ||[Vr_o]^n||_1 = ||[-Vr_o]^n||_1 .$$

Hence, whenever $||K^2||_2 < 1$, the series $\sum_{n=2}^{\infty} ||[-Vr_o]^n||_1$ converges. For $r_o(z)$ bounded we have $||r_o(z)[-Vr_o(z)]^n||_1 \leq ||r_o(z)||\ ||[-Vr_o(z)]^n||_1$, so that the series $\sum_{n=2}^{\infty} ||r_o(z)[-Vr_o(z)]^n||_1$ is dominated by the convergent series $\sum_{n=2}^{\infty} ||r_o(z)||\ ||[-Vr_o(z)]^n||_1 = ||r_o(z)|| \sum_{n=2}^{\infty} ||[-Vr_o(z)]^n||_1$, for $||K^2||_2 < 1$. Hence, whenever $||K^2||_2 < 1$, the series $\sum_{n=2}^{\infty} ||r_o(z)[-Vr_o(z)]^n||_1$ converges. This concludes the proof.

If to the hypotheses of the foregoing theorem we add the hypothesis that $r_o(z)[-Vr_o(z)]$ is in the trace class, then we obtain the convergence of the series

$$||r_o(z)[-Vr_o(z)]||_1 + \sum_{n=2}^{\infty} ||r_o(z)[-Vr_o(z)]^n||_1 = \sum_{n=1}^{\infty} ||r_o(z)[-Vr_o(z)]^n||_1 .$$

The theorems of this chapter are based on the work of Osborn and Bollé [1976].

Chapter 7

PARTICLE IN A LOCALIZED POTENTIAL

7.1 *Introduction*

We apply the theorems derived in the previous chapter to the case of a particle in a localized potential, with Hamiltonian $h = p^2 + V$, $h_o = p^2$.

7.2 The Operator $K = V^{1/2} r_o(z) |V|^{1/2}$

We first show that K is in the Schmidt class for all z. We work in the position representation. The matrix elements of K are

$$\begin{aligned} \langle s|K|t\rangle &= \int\int dx\, dy \langle s|V^{1/2}|x\rangle \langle x|r_o(z)|y\rangle \langle y| \, |V|^{1/2}|t\rangle \\ &= \int\int dx\, dy |v(s)|^{1/2} \mathrm{sign}(v(s)) \delta(s-x) r_o(z,x,y) |r(t)|^{1/2} \delta(y-t) \\ &= |v(s)|^{1/2} \mathrm{sign}(v(s)) |v(t)|^{1/2} \, r_o(z,s,t) \ . \end{aligned}$$

The Schmidt norm, squared, of K is given by $||K||_2^2 = \mathrm{Tr}(K^\dagger K)$, or

$$\begin{aligned} ||K||_2^2 &= \int\int ds\, dt \, |\langle s|K|t\rangle|^2 \\ &= \int\int ds\, dt \, |v(s)| \, |v(t)| \, |r_o(z,s,t)|^2 \ . \end{aligned}$$

We have (Appendix 1) $\langle s|r_o(z)|t\rangle = r_o(z,s,t) = \frac{1}{4\pi} \frac{e^{ik|s-t|}}{|s-t|}$.
Thus

$$\begin{aligned} ||K||_2^2 &= \frac{1}{(4\pi)^2} \int\int ds\, dt \, \frac{|v(s)| \, |v(t)|}{|s-t|^2} \, e^{-2\mathrm{Im}\, k|s-t|} \\ &\leq \frac{1}{(4\pi)^2} \int\int ds\, dt \, \frac{|v(s)| \, |v(t)|}{|s-t|^2} = \frac{1}{(4\pi)^2} \, ||V||_R^2 \ . \end{aligned}$$

$||V||_R$ is the Rollnik norm of V. Potentials for which $||V||_R$ is finite are said to belong to the Rollnik class. Then, if V belongs to the Rollnik class, then K is in the Schmidt class, for all z. The Rollnik class has been extensively studied by Simon [1971]; in particular if $v(x) \in L^1 \cap L^2$, then V is in the Rollnik class.

We now consider K^2. Since K is in the Schmidt class for all z, K^2 is also. (In fact, K^2 and all higher powers of K are in the trace class). The matrix elements of K^2 in the position representation are

$$< s|K^2|t > = < s|V^{1/2} r_o(z) V r_o(z) |V|^{1/2}|t >$$

$$= \int\int dx\, dy < s|V^{1/2}|x > < x|r_o(z)Vr_o(z)|y > < y|\, |V|^{1/2}|t >$$

$$= |v(s)|^{1/2} \text{sign}(v(s)) |v(t)|^{1/2} < s|r_o(z)Vr_o(z)|t >$$

We have

$$< s|r_o(z)Vr_o(z)|t > = \int\int dx\, dy < s|r_o(z)|x > < x|V|y > < y|r_o(z)|t >$$

$$= \int dx < s|r_o(z)|x > v(x) < x|r_o(z)|t >$$

$$= \frac{1}{(4\pi)^2} \int dx\, v(x) \frac{e^{ik|s-x|}}{|s-x|} \frac{e^{ik|x-t|}}{|x-t|}$$

$$= \frac{1}{(4\pi)^2} I(s,t,z) \quad .$$

Thus

$$< s|K^2|t > = |v(s)|^{1/2} \text{sign}(v(s)) |v(t)|^{1/2} \frac{1}{(4\pi)^2} I(s,t,z) \quad .$$

We must examine I(s,t,z). Following Khuri [1957] and Jost and Pais [1951], put $I(s,t,z) = A(s,t,z)/|t|$. (We could also put $I(s,t,z) = B(s,t)/|s|$).

Then

$$A(s,t,z) = |t|\, I(s,t,z)$$

$$= \int dx\, v(x)\, \frac{e^{ik|s-x|}}{|s-x|} \cdot \frac{e^{ik|x-t|}}{|x-t|}\, |t| \quad .$$

For $\mathrm{Im}\, k \geq 0$ we have

$$|A(s,t,z)| \leq e^{-\mathrm{Im}\, k|s-t|} \int dx\, \frac{|v(x)|}{|s-x|\,|x-t|}\, |t|$$

Jost and Pais [1951] show that for $v(r)$ satisfying $|v(r)| < M^1/r^2$ (a smoothness condition) and $\int_0^\infty r|v(r)|dx \leq M < \infty$ (a falling-off at infinity condition), the integral on the right-hand side of the inequality for $|A(s,t,z)|$ is always less than a constant, say N. Thus for $\mathrm{Im}\, k \geq 0$ we have

$$|A(s,t,z)| \leq N\, e^{-\mathrm{Im}\, k|s-t|} \quad ,$$

and so

$$|I(s,t,z,)| \leq \frac{N}{|t|}\, e^{-\mathrm{Im}\, k|s-t|} \quad .$$

Khuri [1957] shows that for any $\epsilon > 0$, no matter how small, one can find k, $\mathrm{Im}\, k \geq 0$, with $|k|$ large enough, so that

$$|A(s,t,z)| \leq \epsilon\, e^{-\mathrm{Im}\, k|s-t|} \quad ,$$

i.e., $A(s,t,z)$ tends to zero uniformly in s and t as $k \to \infty$, $\mathrm{Im}\, k \geq 0$. This is in accordance with the observation that $|A(s,t,z)|$ will be small for large k, $\mathrm{Im}\, k \geq 0$, since it will be damped exponentially to zero for large imaginary k, or it will cancel to zero by oscillation for large

real k. The same then applies to I(s,t,z): I(s,t,z) tends to zero uniformly in s and t as $h \to \infty$, Im $k \geq 0$. (See also Newton [1966]).

We can now obtain the Schmidt norm of K. We have

$$||K^2||_2^2 = \int\int ds\, dt\, |\, <s|K^2|t>\, |^2$$

$$= \frac{1}{(4\pi)^4} \int\int ds\, dt\, |v(s)|\, |v(t)|\, |I(s,t,z)|^2 .$$

Since $I(s,t,z) \to 0$ uniformly in s and t as $k \to 0$, Im $k \geq 0$, we have (taking the limit under the integral)

$$\lim_{\substack{k \to \infty \\ \text{Im } k \geq 0}} ||K^2||_2^2 = 0 .$$

Thus certainly $||K^2||_2 < 1$ for $|k|$ large enough, Im $k \geq 0$.

7.3 The Trace of $r_o(z)Vr_o(z)$

We work in the momentum representation. The diagonal matrix elements of $r_o(z)Vr_o(z)$ are

$$<p|r_o(z)Vr_o(z)|p> = \int\int dq\, dr\, <p|r_o(z)|q><q|V|r><r|r_o(z)|p>$$

$$= \int\int dq\, dr\, \frac{\delta(p-q)}{p^2 - z} <q|V|r> \frac{\delta(r-p)}{p^2 - z}$$

$$= \frac{<p|V|p>}{(p^2 - z)^2} .$$

Also $<p|V|p> = \tilde{v}(p-p) = \tilde{v}(0)$, with $\tilde{v}(q)$ = Fourier transform of v(x), $\tilde{v}(q) = \frac{1}{(2\pi)^3} \int v(x)\, e^{-iqx} dx$. Thus $\tilde{v}(0) = \frac{1}{(2\pi)^3} \int v(x)dx$. We thus

have for the trace

$$\mathrm{Tr}[r_o(z)Vr_o(z)] = \int dp \frac{\langle p|V|p\rangle}{(p^2 - z)^2} = \tilde{v}(0) \int dp \frac{1}{(p^2 - z)^2}$$

$$= \tilde{v}(0) \frac{i\pi^2}{k}, \quad z = k^2 .$$

The integral $\int dp \frac{1}{(p^2 - z)^2}$ is easily done by the method of residues. At the risk of confusion, we will put $\tilde{v}(0) = \frac{\tilde{v}}{(2\pi)^3}$, i.e., $\tilde{v} = \int v(x)dx$. Then

$$\mathrm{Tr}[r_o(z)Vr_o(z)] = \frac{\tilde{v}}{(2\pi)^3} \frac{i\pi^2}{k} = \frac{i}{8\pi k} \tilde{v}$$

(Using $h_o = p^2/2\mu$ instead of $h_o = p^2$, we obtain $\mathrm{Tr}[r_o(z)Vr_o(z)] = (\frac{\mu}{2})^{3/2} \frac{i\tilde{v}}{\pi\sqrt{z}}$). This trace is finite for $\tilde{v} = \int v(x)dx$ finite. Since $r_o(z)V^{1/2}$ and $|V|^{1/2}r_o(z)$ are in the Schmidt class for z not in the spectrum of $h_o = p^2$, then $r_o(z)V^{1/2}|V|^{1/2}r_o(z) = r_o(z)Vr_o(z)$ is in the trace class for z not in the spectrum of h_o.

7.4 The Born Expansion and Levinson's Theorem

We now apply Theorem 4 of the previous chapter. $K = V^{1/2}r_o(z)|V|^{1/2}$ is in the Schmidt class for all z. $r_o(z)$ is bounded for z not in the spectrum of h_o. $||K^2||_2 < 1$ for $|z|$ large enough. Thus from theorem 4 we conclude that the series of trace norms $\sum_{n=2}^{\infty} ||r_o(z)[-Vr_o(z)]^n||_1$ converges for $|z|$ large enough, but z not in the spectrum of h_o. Since $r_o(z)[-Vr_o(z)]$ is in the trace class for z not in the spectrum of h_o, we obtain the convergence of the series of trace norms $\sum_{n=1}^{\infty} ||r_o(z)[-Vr_o(z)]^n||_1$.

We now apply Theorem 3 of the previous chapter. Since $||[-Vr_o(z)]^n||_1 =$

$||K^n||_1$, for $n \geq 2$, and since K^n is in the trace class for $n \geq 2$, $[-Vr_o(z)]^n$ is in the trace class for $n \geq 2$ (for all z). $r_o(z)$ is bounded for z not in the spectrum of h_o, so that $r_o(z)[-Vr_o(z)]^n$ is in the trace class for $n \geq 2$, and z not in the spectrum of h_o. We have already seen that $r_o(z)[-Vr_o(z)]$ is in the trace class for z not in the spectrum of h_o. Further $r(z) - r_o(z) = -r_o(z)Vr(z) = -r_o(z)Vr_o(z)[1 - Vr(z)]$, which is a trace class operator times a bounded operator, and so is in the trace class, z not in the spectrum of h_o. $r(z) - r_o(z)$ and $r_o(z)[-Vr_o(z)]^n$, $n \geq 1$ are analytic for z not in the spectrum of h_o. Applying theorem 3 we conclude that for $|z|$ large enough, z not in the spectrum of h_o, the Born expansion

$$r(z) - r_o(z) = \sum_{n=1}^{\infty} r_o(z)[-Vr_o(z)]^n$$

is valid, and

$$Tr[r(z) - r_o(z)] = \sum_{n=1}^{\infty} Tr[r_o(z)[-Vr_o(z)]^n] \quad .$$

The latter series converges uniformly and absolutely.

We can thus write for the spectral shift function

$$\xi(E) = -\frac{1}{2\pi i} \int_{C_E} Tr[r(z) - r_o(z)]$$

$$= -\frac{1}{2\pi i} \int_{C_E} \sum_{n=1}^{\infty} Tr[r_o(z)(-Vr_o(z))^n]$$

$$= \sum_{n=1}^{\infty} \left\{ -\frac{1}{2\pi i} \int_{C_E} Tr[r_o(z)(-Vr_o(z))^n] \right\}$$

$$= \sum_{n=1}^{\infty} \xi_n(E) \quad .$$

The interchange of integration and summation is justified by the uniform convergence of the series of traces. We have, for $n \geq 2$

$$\frac{d}{dz}\,[Vr_o(z)]^n \;=\; n[Vr_o(z)]^n r_o(z) \quad .$$

$[Vr_o(z)]^n$ and $[Vr_o(z)]^n r_o(z)$ are analytic and in the trace class for $n \geq 2$ and z not in the spectrum of h_o. From Theorem 2 of the previous chapter we conclude

$$\frac{d}{dz}\,\mathrm{Tr}[Vr_o(z)]^n \;=\; \mathrm{Tr}\,\frac{d}{dz}\,[Vr_o(z)]^n \quad ,$$

so that

$$\mathrm{Tr}[r_o(z)[-Vr_o(z)]^n] \;=\; \frac{(-1)^n}{n}\,\frac{d}{dz}\,\mathrm{Tr}[Vr_o(z)]^n \quad .$$

Hence we have for $n \geq 2$

$$\xi_n(E) \;=\; -\frac{1}{2\pi i}\int_{C_E} \frac{(-1)^n}{n}\,\frac{d}{dz}\,\mathrm{Tr}[Vr_o(z)]^n$$

$$= \frac{1}{2\pi i}\,\frac{(-1)^n}{n}\left\{\mathrm{Tr}[Vr_o(E+i0)]^n - \mathrm{Tr}[Vr_o(E-i0)]^n\right\} \quad .$$

We now look more closely at $\mathrm{Tr}[Vr_o(z)]^n$. We have had that $||[Vr_o(z)]^n||_1 = ||K^n||_1$, $K = V^{1/2} r_o(z) |V|^{1/2}$, for $n \geq 2$, and K^n is in the trace class for $n \geq 2$ for all z. Thus $[Vr_o(z)]^n$ is in the trace class for $n \geq 2$ and all z. Hence the limits as $\delta \to 0$ of $\mathrm{Tr}[Vr_o(E+i\delta)]^n$ and $\mathrm{Tr}[Vr_o(E-i\delta)]^n$ exist, $n \geq 2$. Further, $||K^2||_2 \to 0$ as $k \to \infty$, $\mathrm{Im}\, k \geq 0$, $z = k^2$. Hence $||K^n||_1 \to 0$ as $k \to \infty$, $\mathrm{Im}\, k \geq 0$, for $n \geq 3$. To see this note that for $n \geq 4$ and even $||K^n||_1 \leq ||K^2||_2 \cdot ||K^{n-2}||_2 \to 0$ as $k \to \infty$, while for $n \geq 3$ and odd $||K^n||_1 \leq ||K||_2 ||K^{n-1}||_2 \to 0$ as $k \to \infty$

since n-1 is equal to 2, or ≥ 4. Since $|\mathrm{Tr}\ K^n| \leq ||K^n||_1$, we have that $\mathrm{Tr}\ K^n \to 0$ as $k \to \infty$, $\mathrm{Im}\ k \geq 0$, $n \geq 3$. In particular, $\mathrm{Tr}[Vr_o(E + i0)]^n$ and $\mathrm{Tr}[Vr_o(E - i0)]^n$ both $\to 0$ as $E \to \infty$, $n \geq 3$. The same result also holds for $n = 2$, as is shown by Osborn and Bollé [1976], by direct calculation. We thus have, for $n \geq 2$, $\xi_n(\infty) = 0$. That is

$$\lim_{E \to \infty} (\xi(E) - \xi_1(E)) = \lim_{E \to \infty} \sum_{n=2}^{\infty} \xi_n(E) = 0 \ .$$

Recalling the relation

$$\xi(E) - N(E) = \frac{1}{2\pi} \int_b^E \mathrm{tr}\ q(x)dx \ ,$$

where the integral $\int_b^E$ is taken over the continous spectrum, and putting

$$\xi(E) = \xi_1(E) + \sum_{n=2}^{\infty} \xi_n(E) \ ,$$

we obtain

$$N + \frac{1}{2\pi} \int_b^E \mathrm{tr}\ q(x)dx - \xi_1(E) = \sum_{n=2}^{\infty} \xi_n(E) \ .$$

We can calculate $\xi_1(E)$. We have

$$\xi_1(E) = -\frac{1}{2\pi i} \int_{C_E} \mathrm{Tr}[r_o(z)[-Vr_o(z)]dz$$

$$= \frac{1}{2\pi i} \int_{C_E} \frac{i\tilde{v}}{8\pi\sqrt{z}}\, dz$$

$$= \frac{1}{2\pi i} \cdot \frac{i\tilde{v}}{8\pi} \cdot \int_{C_E} \frac{dz}{\sqrt{z}}$$

$$\xi_1(E) = \frac{1}{2\pi i} \frac{i\tilde{v}}{8\pi} (-4\sqrt{E})$$

$$= -\frac{\tilde{v}}{4\pi^2} \sqrt{E} \cdot = -\frac{1}{2\pi} \int_0^E \frac{\tilde{v}}{4\pi} \frac{dx}{\sqrt{x}}$$

(Using $h_o = p^2/2\mu$ instead of $h_o = p^2$, we obtain $\xi_1(E) = -\frac{2}{\pi^2} (\frac{\mu}{2})^{3/2} \tilde{v} \sqrt{E}$).

We have $b = 0$, and all points from 0 to E are in the continuous spectrum in this situation so that

$$N + \frac{1}{2\pi} \int_0^E [\mathrm{tr}\, q(x) + \frac{\tilde{v}}{4\pi} \frac{1}{\sqrt{x}}]dx = \sum_{n=2}^{\infty} \xi_n(E) ,$$

with $\sum_{n=2}^{\infty} \xi_n(E) = -\frac{1}{2\pi i} \int_{C_E} \mathrm{Tr}[r(z) - r_o(z) + r_o(z)Vr_o(z)]dz$. Since $\lim_{E \to \infty} \sum_{n=2}^{\infty} \xi_n(E) = 0$, we have (Osborn and Bollé [1976])

$$N + \frac{1}{2\pi} \int_0^{\infty} [\mathrm{tr}\, q(x) + \frac{\tilde{v}}{4\pi} \frac{1}{\sqrt{x}}]dx = 0 .$$

Chapter 8

PARTICLE IN A PERIODIC POTENTIAL WITH AN IMPURITY

8.1 *Introduction*

We now consider the case of a particle in a periodic potential, with an impurity potential superimposed. The Hamiltonian is $h = h_o + V$, $h_o = p^2 + W$, W periodic.

8.2 The Resolvent Operator

In the case $h_o = p^2$ we can obtain an explicit form for the resolvent operator $r_o(z) = (p^2 - z)^{-1}$ in the position representation, i.e., $< s|r_o(z)|t > = \frac{1}{4\pi} \frac{e^{ik|s-t|}}{|s-t|}$ (Appendix 1). In the case $h_o = p^2 + W$ we cannot obtain an explicit form for the resolvent operator $r_o(z) = (h_o - z)^{-1}$. We have, using the crystal momentum representation

$$< s|r_o(z)|t > = \int_B \sum_n \int_{B'} \sum_{n'} < s|k,n > < k,n|r_o(z)|k',n' > < k',n'|t >$$

$$= \int_B \sum_n \int_{B'} \sum_{n'} \psi_n(k,s)[E_n(k) - z]^{-1} < k,n|k',n' > \psi^*_{n'}(k',t)$$

$$= \int_B \sum_n \frac{\psi_n(k,s)\psi^*_n(k,t)}{E_n(k) - z} \quad .$$

We have used the orthonormalization $< k,n|k',n' > = \delta_{nn'}\delta(k-k')$, and put $< x|k,n > = \psi_n(x,k)$, a Bloch wave. In order to calculate $< s|r_o(z)|t > = r_o(z,s,t)$ we need to know the Bloch functions $\psi_n(k,x)$, and the band functions $E_n(k)$, for the given periodic potential W. Such

information is not available except in the form of numerical solutions. (Slater [1952] has given an exactly soluble example in three dimensions, but this remains an isolated example). Information concerning $< s|r_o(z)|t >$ must be sought by numerical methods, or by general analytical methods which do not depend on knowledge of an explicit form for $< s|r_o(z)|t >$.

The resolvent $r_o(z) = (h_o - z)^{-1}$ of $h_o = p^2 + W$ is related to the resolvent $r_{oo}(z) = (p^2 - z)^{-1}$ of $h_{oo} = p^2$ (Hamiltonian of a free particle) by

$$r_o(z) = r_{oo}(z) - r_{oo}(z)Wr_o(z) \quad ,$$

for z not in the spectrum of $r_o(z)$ or $r_{oo}(z)$. We can use this relation to obtain information on operators such as $Vr_o(z)$. We have

$$Vr_o(z) = Vr_{oo}(z) - Vr_{oo}(z)Wr_o(z) \quad .$$

Now $Vr_{oo}(z)$ is in the Schmidt class for z not in the spectrum of h_{oo} and $v(x) \in L^2$ (Appendix 1). Since $Wr_o(z)$ is bounded for z not in the spectrum of h_o, $Vr_{oo}(z)Wr_o(z)$ is in the Schmidt class for Im $z \neq 0$. Thus $Vr_o(z)$ is in the Schmidt class for Im $z \neq 0$. The same argument applies to $V^{1/2}r_o(z)$, $|V|^{1/2}r_o(z)$.

8.3 The Operator $K = V^{1/2}r_o(z)|V|^{1/2}$

Since we do not have an explicit form for $r_o(z)$, we cannot show directly (as we did in the case $h_o = p^2$) that K is in the Schmidt class. However, as in the preceding section, we have

$$\begin{aligned} K &= V^{1/2}[r_{oo}(z) - r_{oo}(z)Wr_o(z)]|V|^{1/2} \\ &= V^{1/2}r_{oo}(z)|V|^{1/2} - V^{1/2}r_{oo}(z)Wr_o(z)|V|^{1/2} \quad . \end{aligned}$$

The first term (which is the operator K in case $h_o = p^2$) will be denoted by A. We have seen that A is in the Schmidt class for all z. Put $W = |W|^{1/2}W^{1/2}$. W is multiplication by the periodic function w(x), $|W|^{1/2}$ is multiplication by $|w(x)|^{1/2}$, and $W^{1/2}$ is multiplication by $|w(x)|^{1/2}\text{sign}(w(x))$. Then

$$K = A - V^{1/2}r_{oo}(z)|W|^{1/2}W^{1/2}r_o(z)|V|^{1/2}$$

$$= A - BL \quad ,$$

with $B = V^{1/2}r_{oo}(z)|W|^{1/2}$ and $L = W^{1/2}r_o(z)|V|^{1/2}$. The operators $V^{1/2}r_{oo}(z)$ and $r_o(z)|V|^{1/2}$ are in the Schmidt class for Im $z \neq 0$, and the operators $|W|^{1/2}$ and $W^{1/2}$ are bounded, so that B and L are in the Schmidt class for Im $z \neq 0$. Thus BL is in the Schmidt class. K then is also in the Schmidt class for Im $z \neq 0$, being the sum of the Schmidt class operators A and -(BL).

We proceed similarly for K^2. We have

$$K^2 = (A - BL)^2 = A^2 - ABL - BLA + (BL)^2 \quad .$$

K^2 is in the Schmidt class for Im $z \neq 0$, since K is. We have

$$||K^2||_2 = ||A^2 - ABL - BLA + (BL)^2||_2$$

$$\leq ||A^2||_2 + ||ABL||_2 + ||BLA||_2 + ||(BL)^2||_2 \quad .$$

We have further

$$||ABL||_2 \leq ||AB||_2||L||_2 \quad ,$$

$$||BLA||_2 = ||ABL||_2$$

$$||(BL)^2||_2 \leq ||BLB||_2||L||_2 = ||B^2L||_2||L||_2 \leq ||B^2||_2||L||_2^2 \quad .$$

Thus, for Im $z \neq 0$, we have

$$||K^2||_2 \leq ||A^2||_2 + 2||L||_2||AB||_2 + ||L||_2^2||B^2||_2 .$$

We now turn to an examination of the operators A^2, AB, and B^2. We had $A = V^{1/2}r_{oo}(z)|V|^{1/2}$, and $B = V^{1/2}r_{oo}(z)|W|^{1/2}$. Thus we have

$$A^2 = V^{1/2}r_{oo}(z)Vr_{oo}(z)|V|^{1/2} ,$$

$$AB = V^{1/2}r_{oo}(z)Vr_{oo}(z)|V|^{1/2} ,$$

$$B^2 = V^{1/2}r_{oo}(z)|W|^{1/2}V^{1/2}r_{oo}(z)|W|^{1/2} .$$

These operators are all of the form $(V_1r_{oo}(z)V_2)^2 = V_1r_{oo}(z)V_2V_1r_{oo}(z)V_2$, where V_1 is a localized potential (i.e., $V^{1/2}$) and V_2 is either a localized potential (i.e., $|V|^{1/2}$), or a bounded periodic potential (i.e., $|W|^{1/2}$). The product V_2V_1 is then a localized potential, since V_1 will cause the product to decrease at infinity essentially as V_1. The matrix elements in the position representation of an operator of the form $J^2 = (V_1r_{oo}(z)V_2)^2$ are, as in the previous chapter,

$$< s|J^2|t > = < s|V_1r_{oo}(z)V_2V_1r_{oo}(z)V_2|t >$$

$$= v_1(s)v_2(t) < s|r_{oo}(z)V_2V_1r_{oo}(z)|t > .$$

We have, as in the previous chapter,

$$< s|r_{oo}(z)V_2V_1r_{oo}(z)|t > = \int\int dx\, dy < s|r_{oo}(z)|x > < x|V_2V_1|y > < y|r_{oo}(z)|t >$$

$$= \int dx < s|r_{oo}(z)|x > v_2(x)v_1(y)\delta(x-y) < y|r_{oo}(z)|t >$$

$$= \frac{1}{(4\pi)^2} \int dx\, v_2(x)v_1(x) \frac{e^{ik|s-x|}}{|s-x|} \frac{e^{ik|x-t|}}{|x-t|}$$

$$< s|r_{oo}(z)V_2V_1r_{oo}(z)|t > \;=\; \frac{1}{(4\pi)^2}\; I(s,t,z) \quad .$$

Then

$$< s|J^2|t > \;=\; v_1(s)v_2(t)\;\frac{1}{(4\pi)^2}\; I(s,t,z) \quad .$$

Now put $v_2(x)v_1(x) = u(x)$. $v_1(x)$ is a localized function, while $v_2(x)$ is either a localized function or a bounded periodic potential. Hence $u(x)$ is a localized function. It is thus possible, in accordance with the discussion given in the preceding chapter, to choose $u(x)$ so that $I(s,t,z)$ tends to zero uniformly in s and t as $k \to \infty$, $\mathrm{Im}\, k \geq 0$. Such being the case, we have for the Schmidt norm of J

$$||J^2||_2^2 \;=\; \int\int ds\, dt|\, < s|J^2|t > \,|^2$$

$$= \frac{1}{(4\pi)^2} \int\int ds\, dt|v_1(s)|^2|v_2(t)|^2|I(s,t,z)|^2 \quad .$$

Then, as in the preceding chapter

$$\lim_{\substack{k \to \infty \\ \mathrm{Im}\, k \geq 0}} ||J^2||_2^2 \;=\; 0 \quad .$$

This result then holds for A^2 (as we already know), and for AB and B^2 as well:

$$\lim_{\substack{k \to \infty \\ \mathrm{Im}\, k \geq 0}} ||AB||_2 \;=\; 0 \quad , \qquad \lim_{\substack{k \to \infty \\ \mathrm{Im}\, k \geq 0}} ||B^2||_2 \;=\; 0 \quad .$$

Returning now to the inequality for $||K^2||_2$, which holds for $\mathrm{Im}\, k > 0$:

$$||K^2||_2 \leq ||A^2||_2 + 2||L||_2||AB||_2 + ||L||_2^2||B^2||_2 \quad .$$

Since $||A^2||_2$, $||AB||_2$, $||B^2||_2$ all $\to 0$ as $k \to \infty$, Im $k \geq 0$, we conclude that

$$\lim_{\substack{k \to \infty \\ \text{Im } k > 0}} ||K^2||_2 = 0 \quad .$$

Note that we have not demonstrated that the inequality for $||K^2||_2$ holds for Im $k = 0$, so that we cannot conclude that $||K^2||_2 \to 0$ as $k \to \infty$ for Im $k = 0$. The reason for this is that, while A is in the Schmidt class for all z, B and L are in the Schmidt class only for Im $k > 0$ (see Appendix 1).

8.4 The Trace of $r_o(z)Vr_o(z)$

Since $r_o(z)V^{1/2}$ and $|V|^{1/2}r_o(z)$ are both in the Schmidt class for z not in the spectrum of h_o, then $r_o(z)V^{1/2}|V|^{1/2}r_o(z) = r_o(z)Vr_o(z)$ is in the trace class for z not in the spectrum of h_o. Since we do not have an explicit form for $r_o(z)$, we cannot derive an explicit form for $\mathrm{Tr}[r_o(z)Vr_o(z)]$, as we could for the case $h_o = p^2$. For the same reason it is not possible to show that the functional dependence of $\mathrm{Tr}[r_o(z)Vr_o(z)]$ in general allows a continuation on to the real axis. These problems seem to be difficult.

8.5 The Born Expansion and Levinson's Theorem

We now apply Theorem 4, in the same way it was applied to the case $h_o = p^2$ in the previous chapter. $K = V^{1/2}r_o(z)|V|^{1/2}$ is in the Schmidt class for Im $k > 0$. $r_o(z)$ is bounded for z not in the spectrum of h_o. $||K^2||_2 < 1$ for $|z|$ large enough, Im $z \neq 0$. The series of trace norms

$\sum_{n=2}^{\infty} ||r_o(z)[-Vr_o(z)]^n||_1$ converges for $|z|$ large enough, Im $z \neq 0$. Also, $r_o(z)[-Vr_o(z)]$ is in the trace class for z not in the spectrum of h_o, so that the series of trace norms $\sum_{n=1}^{\infty} ||r_o(z)[-Vr_o(z)]^n||_1$ converges.

We now apply Theorem 3, in the same way as in the preceding chapter for the case $h_o = p^2$. The argument given in the preceding chapter is unchanged, leading to the conclusion that, for Im $z \neq 0$, the Born expansion

$$r(z) - r_o(z) = \sum_{n=1}^{\infty} r_o(z)[-Vr_o(z)]^n$$

is valid, and

$$\mathrm{Tr}[r(z) - r_o(z)] = \sum_{n=1}^{\infty} \mathrm{Tr}[r_o(z)[-Vr_o(z)]^n] \quad .$$

The last series converges uniformly and absolutely.

We can thus write for the spectral shift function

$$\xi(E) = \sum_{n=1}^{\infty} \left\{ -\frac{1}{2\pi i} \int_{C_E} \mathrm{Tr}[r_o(z)[-Vr_o(z)]^n] \right\}$$

$$= \sum_{n=1}^{\infty} \xi_n(E) \quad .$$

The result $\frac{d}{dz}[Vr_o(z)]^n = n[Vr_o(z)]^n r_o(z)$ depends only on the analyticity of $[Vr_o(z)]^n$ and on the Hilbert identity. It is thus valid in this case. The argument given in the preceding chapter leading to the result

$$\mathrm{Tr}[r_o(z)[-Vr_o(z)]^n] = \frac{(-1)^n}{n} \frac{d}{dz} \mathrm{Tr}[Vr_o(z)]^n$$

is unchanged. Hence, for $n \geq 2$ we have

$$\xi_n(E) = -\frac{1}{2\pi i} \int_{C_E} \frac{(-1)^n}{n} \frac{d}{dz} \mathrm{Tr}[Vr_o(z)]^n$$

$$= \frac{1}{2\pi i} \frac{(-1)^n}{n} \left\{ \mathrm{Tr}[Vr_o(E + i0)]^n - \mathrm{Tr}[Vr_o(E - i0)]^n \right\}$$

We have written $[Vr_o(E + i0)]^n$ and $[Vr_o(E - i0)]^n$, although at this stage we have not demonstrated the existence of these limits onto the real axis. A further question, should the limits exist, is their behaviour as $E \to \infty$. Considerable work has been done on these problems with inconclusive results so far. These questions are difficult to deal with because we lack an explicit form for $r_o(z)$, and hence general results can only be obtained by further assumptions, or by complex analytical approximation techniques. We have obtained partial results in this direction, and regard this as an important direction for future research.

SUMMARY

We have dealt with the time delay associated with scattering from an impurity in a periodic medium. This problem has not been treated in the literature previously. In order to lay the foundations for the analysis of time delay we have discussed first of all the free motion, i.e., motion in a periodic potential, and then discussed the scattering problem for an impurity in a periodic medium. In particular, the absolute continuity of the spectrum of the free Hamiltonian was established. The scattering problem was treated from the point of view of time-dependent theory. Proofs were given of the partial isometry and intertwining properties of the wave operators, and of the existence and asymptotic completeness of the wave operators.

With these results in hand, we gave the definition of the time delay for one-body scattering from an impurity. The existence and uniqueness of the time delay operator for a region Σ_R were demonstrated. The concept of the direct integral of Hilbert spaces was used in this discussion. The spectral property of time delay was established, which involved a study of the limit as the size of the region used in the definition of time delay approached all of space. The result obtained was shown to be consistent with a less abstract approach using the crystal momentum representation.

A detailed discussion of the spectral shift function associated with the Hamiltonians h_o and h (the free and perturbed Hamiltonians respectively) led to a general time delay form of Levinson's theorem. This was related to the convergence of the Born expansion. Mathematical theorems were derived, which isolated the nature of the various properties required in relating the convergence of the Born expansion to the time delay and

Levinson's theorem. These theorems were applied to the case of a free particle, treated previously by Osborn and Bollé, and to the case of a particle scattering from an impurity in a periodic potential.

APPENDIX 1

A1.1 *Introduction*

In this appendix we gather together several results related to the resolvent of a free particle, $r_o(z) = (p^2 - z)^{-1}$.

A1.2 $< x|r_o(z)|y >$

The matrix elements of $r_o(z)$ in the position representation are

$$< x|r_o(z)|y > = \int dp\, dq < x|p >< p|r_o(z)|q >< q|y >$$

$$= \int dp\, dq \; \frac{e^{ipx}}{(2\pi)^{3/2}} \cdot \frac{\delta(p-q)}{p^2 - z} \; \frac{e^{-iqy}}{(2\pi)^{3/2}}$$

$$= \frac{1}{(2\pi)^3} \int dp \; \frac{e^{ip(x-y)}}{p^2 - z}$$

$$= \frac{1}{(2\pi)^3} \int p^2 dp d\Omega \; \frac{e^{ip|x-y|\cos\theta}}{p^2 - z}$$

$$= \frac{2\pi}{(2\pi)^3} \int \frac{p^2 dp}{p^2 - z} \cdot \frac{2\sin p|x-y|}{p|x-y|}$$

$$= \frac{4\pi}{(2\pi)^3} \; \frac{2\pi}{i|x-y|} \int_{-\infty}^{\infty} \frac{p e^{ip|x-y|}}{p^2 - z} \, dp \; .$$

The integral over p can be done by the method of residues, yielding $+ \pi i \, e^{ik|x-y|}$, $k^2 = z$. Thus

$$< x|r_o(z)|y > = \frac{2\pi \cdot \pi i}{(2\pi)^3 i} \cdot \frac{e^{ik|x-y|}}{|x-y|} = \frac{1}{4\pi} \; \frac{e^{ik|x-y|}}{|x-y|} \; .$$

(If we had used $\frac{p^2}{2\mu}$ instead of p^2 we obtain 2μ times the above result, with $k^2 = 2\mu z$, i.e. $< x|r_o(z)|y > = \frac{\mu}{2\mu} \frac{e^{ik|x-y|}}{|x-y|}$).

A1.3 $Vr_o(z)$

The Schmidt norm of $Vr_o(z)$ is given by

$$||Vr_o(z)||_2^2 = Tr[[Vr_o(z)]^\dagger \; Vr_o(z)] = \int dx < x|[Vr_o(z)]^\dagger \; [Vr_o(z)]|x >$$

$$= \frac{1}{(4\pi)^2} \int\int dx\, dy \; \frac{e^{ik|x-y|}}{|x-y|} \cdot \frac{e^{ik|y-x|}}{|y-x|} \; |v(y)|^2$$

$$= \frac{1}{(4\pi)^2} \int dy|v(y)|^2 \int dx \left| \frac{e^{ik|x-y|}}{|x-y|} \right|^2$$

$$= \frac{1}{(4\pi)^2} \int dy|v(y)|^2 \cdot \frac{2\pi}{Im\ k}$$

$$= \frac{1}{8\pi} \frac{1}{Im\ k} \int dy|v(y)|^2 \; .$$

Tus if $v(y) \in L^2$, $Im\ k > 0$, then $Vr_o(z)$ is in the Schmidt class. The same calculation applies to $V^{1/2}r_o(z)$ and $|V|^{1/2}r_o(z)$, with $v(y) \in L^1$.

In particular, if P(R) is the projection on a region Σ_R, then $P(R)r_o(z)$ behaves, as far as the calculation of its Schmidt norm is concerned, in the same way as $Vr_o(z)$, with V being the potential which is zero outside Σ_R, and unity inside Σ_R.

A1.4 $V_1 r_o(z) V_2$

The Schmidt norm of $V_1 r_o(z) V_2$ is given by

$$||V_1 r_o(z) V_2||_2^2 = \int\int dx\, dy\, |\langle x|V_1 r_o(z)|y\rangle|^2$$

$$= \int\int dx\, dy\, |v_1(x) r_o(z,x,y) v_2(y)|^2$$

$$= \frac{1}{(4\pi)^2} \int\int dx\, dy\, |v_1(x)|^2 |v_2(y)|^2 \frac{e^{-2\mathrm{Im}\, k|x-y|}}{|x-y|^2}$$

$V_1 r_o(z) V_2$ is in the Schmidt class for $v_1(x)$, $v_2(y)$ sufficiently localized. Suppose now that $v_2(y)$ is only a bounded function (that is, does not necessarily $\to 0$ in some way at infinity). Put $x-y = q$. Then

$$||V_1 r_o(z) V_2||_2^2 = \frac{1}{(4\pi)^2} \int dx\, |v_1(x)|^2 \cdot \int dq\, |v_2(x-q)|^2 \frac{e^{-2\mathrm{Im}\, k\, q}}{q^2}$$

We have for the q integral, with $B = \sup |v_2(x-q)|^2$

$$\int dq\, |v_2(x-q)|^2 \frac{e^{-2\mathrm{Im}\, k\, q}}{q^2} \leq B \int dq\, \frac{e^{-2\mathrm{Im}\, k\, q}}{q^2} = B\, \frac{2\pi}{\mathrm{Im}\, k} .$$

Thus

$$||V_1 r_o(z) V_2||_2^2 = \frac{1}{(4\pi)^2}\, B\, \frac{2\pi}{\mathrm{Im}\, k} \int dx\, |v_1(x)|^2 .$$

If $\int dx\, |v_1(x)|^2$ is finite, then $V_1 r_o(z) V_2$ is in the Schmidt class for $\mathrm{Im}\, k > 0$, but not for $\mathrm{Im}\, k = 0$.

APPENDIX 2

A2.1 *Introduction*

In this appendix we examine the limit as $R \to \infty$ of $(2i \text{ Im } z)\text{Tr}[|r_o(z)|^2\Gamma(R)]$.

A2.2 $\lim_{R \to \infty} (2i \text{ Im } z)\text{Tr}[|r_o(z)|^2\Gamma(R)]$

We have had the result (formula of Osborn and Tsang)

$$2i \text{ Im Tr}[r(z) - r_o(z)] = (2i \text{ Im } z) \sum_i \frac{1}{|E_i - z|^2}$$

$$+ \lim_{R \to \infty} (2i \text{ Im } z)\text{Tr}[|r_o(z)|^2\Gamma(R)] \ .$$

We have also had the result

$$\text{Tr}[r(z) - r_o(z)] = \int_{-\infty}^{\infty} \frac{d\xi(\lambda)}{\lambda - z} \ ,$$

with $\xi(\lambda)$ a real function. Thus

$$2i \text{ Im Tr}[r(z) - r_o(z)] = 2i \int_{-\infty}^{\infty} \text{Im}\left[\frac{1}{\lambda - z}\right] d\xi(\lambda)$$

$$= 2i \int_{-\infty}^{\infty} \frac{\text{Im } z}{|\lambda - z|^2} \, d\xi(\lambda)$$

The function $\xi(\lambda)$ is the spectral shift function, and gives the shift in the spectrum of h_o due to the perturbation V, i.e., $\xi(\lambda)$ gives the difference between the spectrum of h_o and $h = h_o + V$. We have in fact written

$$\xi(\lambda) = \sigma(\lambda) - \sigma_o(\lambda) \ ,$$

$\sigma(\lambda)$ and $\sigma_o(\lambda)$ being the spectral functions of h and h_o respectively. Now h_o is spectrally absolutely continuous, so that $\sigma_o(\lambda)$ is a non-decreasing absolutely continuous function of λ. $\sigma(\lambda)$ is also a non-decreasing function of λ, and can be written (as can any non-decreasing function) as the sum of three functions:

$$\sigma(\lambda) = \sigma_1(\lambda) + \sigma_2(\lambda) + \sigma_3(\lambda) \quad .$$

$\sigma_1(\lambda)$ is a jump function (i.e., constant except for a countable set of jumps); $\sigma_2(\lambda)$ is an absolutely continuous function; $\sigma_3(\lambda)$ is a singular continuous function (i.e., a function whose derivative is zero almost everywhere). This decomposition of $\sigma(\lambda)$ corresponds exactly to the decomposition of the Hilbert space $\mathcal{H}$ into corresponding subspaces with respect to h:

$$\mathcal{H} = \mathcal{H}_p \oplus \mathcal{H}_{ac} \oplus \mathcal{H}_{sc} \quad .$$

We assume that the singularly continuous spectrum is empty, i.e., $\sigma_3(\lambda) \equiv 0$. Then $\sigma(\lambda) = \sigma_1(\lambda) + \sigma_2(\lambda)$, so that

$$\xi(\lambda) = [\sigma_1(\lambda) - \sigma_o(\lambda)] + \sigma_2(\lambda) \quad ,$$

which is the sum of the absolutely continuous function $\sigma_1(\lambda) - \sigma_o(\lambda) = \xi_{ac}(\lambda)$, and the jump function $\sigma_2(\lambda) = \xi_p(\lambda)$.

Returning now to the stieltjes integral

$$2i \int_{-\infty}^{\infty} \frac{\text{Im } z}{|\lambda - z|^2} \, d\xi(\lambda) \quad ,$$

the jump function component $\xi_p(\lambda)$ of $\xi(\lambda)$ yields a discrete sum over the

jumps of $\xi_p(\lambda)$, and an integral with respect to the absolutely continuous component $\xi_{ac}(\lambda)$ of $\xi(\lambda)$. Since $\xi_{ac}(\lambda)$ has a derivative almost everywhere we can write

$$2i \operatorname{Im} \operatorname{Tr}[r(z) - r_o(z)] = (2i \operatorname{Im} z) \sum_i \frac{1}{|\lambda_i - z|^2}$$

$$= 2i \int_{-\infty}^{\infty} \frac{\operatorname{Im} z}{|\lambda - z|^2} \frac{d\xi_{ac}(\lambda)}{d\lambda} d\lambda \ .$$

We now compare this with the formula of Osborn and Tsang, given at the beginning of this appendix. We conclude that

$$\lim_{R \to \infty} (2i \operatorname{Im} z) \operatorname{Tr}[|r_o(z)|^2 \Gamma(R)] = 2i \int_{-\infty}^{\infty} \frac{\operatorname{Im} z}{|E - z|^2} \frac{d\xi_{ac}(E)}{dE} dE \ .$$

Further, we had the result

$$\operatorname{Tr}[|r_o(z)|^2 \Gamma(R)] = \int |r_o(E,z)|^2 \operatorname{tr} \frac{q(E,R)}{2\pi} dE \ ,$$

with $r_o(E,z) = (E - z)^{-1}$. Hence

$$\lim_{R \to \infty} 2i \int \frac{\operatorname{Im} z}{|E - z|^2} \operatorname{tr} \frac{q(E,R)}{2\pi} dE = 2i \int_{-\infty}^{\infty} \frac{\operatorname{Im} z}{|E - z|^2} \frac{d\xi_{ac}(E)}{dE} dE \ .$$

Both integrals are in fact over the absolutely continuous spectrum. This shows the existence of a function

$$f(E) = \frac{d\xi_{ac}(E)}{dE}$$

such that

$$\lim_{R \to \infty} 2i \int \frac{\mathrm{Im}\, z}{|E - z|^2} \, \mathrm{tr}\, \frac{q(E,R)}{2\pi} \, dE = 2i \int \frac{\mathrm{Im}\, z}{|E - z|^2} \, f(E) dE \quad .$$

We write $f(E) = \frac{1}{2\pi} \, \mathrm{tr}\, q(E)$ to bring out the idea that $f(E)$ is the value of $\mathrm{tr}\, q(E,R)$ in the limit $R \to \infty$, in the sense, and only in the sense, of the foregoing discussion. In the foregoing sense then we can speak of a limiting operator $q(E)$ for $q(E,R)$ as $R \to \infty$.

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