CHAPTER II

PERTURBATION THEORY FOR LINEAR OPERATORS.

II.1. INTRODUCTION

The perturbation theory is a very useful technique for solving approximately the problems of physics. The Hamiltonian for the physical system is first decomposed into two parts. The first part should be a well-defined operator, leading to a problem which is exactly solvable. The effect of the remaining part of the Hamiltonian is then taken into account by an approximate method. This however, leads to sensible results provided the second term is a "small perturbation". An important problem in the perturbation theory is to assign a meaning to the term 'small perturbation', particularly when dealing with unbounded operators, which occur in most of the problems. Rellich[33-35] and Kato[36-38] initiated a thorough investigation of this problem and developed a general formalism of the perturbation theory of general linear operators.

In this chapter we briefly review some aspects of the Rellich-Kato theory, as applied to a Hilbert space, which will be used in the later parts of the thesis.

II.2. DEFINITIONS

Let $\mathcal{H}$ be a seperable Hilbert space with inner-product $\langle , \rangle$. For the physical space of square integrable functions

$$\langle u, v \rangle = \int u^*(x)\, v(x)\, dx \qquad \ldots (2.1)$$

Let T be a linear operator in $\mathcal{H}$. Let us denote by D (T) the domain of T. Among unbounded operators, the most important are the closed operators.

Definition 2.1. A linear operator T in $\mathcal{H}$ is called closed if for every sequence $u_n \in D(T)$ the existence of limits $u_n \to u$ and $Tu_n \to v$ implies $u \in$ D (T) and T $u = v$.

Clearly, closed operators are the immediate extensions of continuous ($\equiv$ bounded) operators in the following sense. Even though, for an unbounded operator, $u_n \to u$ does not imply $\{Tu_n\}$ to be convergent, but for those sequence for which $\{u_n\}$ and $\{Tu_n\}$ are both convergent, the requirement of continuity holds when T is closed. Most of the physical operators are found to be closed or can be made closed by a suitable choice of the corresponding domains.

Definition 2.2. T is said to be closable if T has a closed extension. Among closed extensions of T there is a smallest one, denoted by $\tilde{T}$, which is called the closure of T.

Let T be a closed operator. For any closable operator S such that $\tilde{S} = T$, its domain $D(S)$ is called a core of T.

As an example, we consider an anharmonic oscillator, described by the Hamiltonian

$$H = p^2 + x^2 + \beta x^4 \tag{2.2}$$

which has been studied by Simon[28]. To study the problem one needs to realize the well-defined operator from the formal one given by eqn. (2.2). Let us write

$$H(\alpha, \beta) = p^2 + \alpha x^2 + \beta x^4 . \tag{2.3}$$

Then $H(0, \beta)$, $\beta > 0$ can be shown to be a closed operator on the domain

$$\begin{aligned} D &= D(p^2) \cap D(x^4) \\ &= \left\{ \psi \in L^2 : \int x^8 |\psi|^2 dx < \infty ; \int p^4 |\hat{\psi}|^2 dp < \infty \right\} \end{aligned} \tag{2.4}$$

where $\hat{\psi}$ is the Fourier transform of ψ .

The adjoint, T^* of T is defined as follows:

Definition 2.3. If there exists a vector $\hat{v}$ $(\hat{v} \in D(T^*))$ so that

$$\langle v, Tu \rangle = \langle \hat{v}, u \rangle \tag{2.5}$$

for all $u \in D(T)$, then by definition $\hat{v} = T^* v$. Eqn. (2.5) defines a unique linear operator T^* if $D(T)$ is dense. The domain of T^* which follows from this definition need not be dense.

However, when $D(T^*)$ is dense, $(T^*)^*$ is defined and it follows that $(T^*)^* = \tilde{T}$, the closure of T. Hence T is closed iff $T = (T^*)^*$.

If $T \subset T^*$, T is called symmetric, T is said to be self-adjoint if $T = T^*$. If $T^{**} = T^*$, then T is essentially self-adjoint.

Self-adjoint operators are extremly well-behaved. Such operators are often useful to represent the time-evolution of a quantum mechanical system. If H is the Hamiltonian and it is self-adjoint then $U(t) = e^{iHt}$ is the unitary operator describing the corresponding dynamics of the system. A symmetric operator which is not essentially self-adjoint may admit infinite numbers of self-adjoint extensions or none.

For example, $H(0, \beta)$, $\beta > 0$ in eqn. (2.3) is a self-adjoint operator.

Next we consider the stability of a closed operator T under an unbounded perturbation. The simplest definition of 'small' perturbation for unbounded operators can be given for relatively bounded operators.

Definition 2.4. Let T and A be linear operators such that

i) $D(T) \subset D(A)$

ii) $\|Au\| \leq a\|u\| + b\|Tu\|$, $u \in D(T)$

where a, b are non-negative numbers. Then A is said to be relatively bounded with respect to T or simply T-bounded. The inifimum of such b is called the T-bound of A.

If T-bound of A is zero, we call A to be infinitesimally small w.r.t. T. Note that to prove estimates of the form (ii) it is sufficient to prove them on a core of T. We now state the fundamental stability theorem of Kato and Rellich.

Th. 2.1. Let T and A be as defined above and let A be T-bounded with T-bound $b < 1$. Then $S = T + A$ is closable iff T is closable; in this case the closures of T and S have the same domain. In particular, S is closed iff T is closed.

Cor.2.1. Any operator that is T-bounded with T-bound β is also S-bounded with S-bound $\leq \beta(1-b)^{-1}$, $b<1$. To explain the Kato-Rellich theorem, we note that the maximal multiplicative operator x^2 in eqn. (2.3) is H (0, β) - bounded with relative bound zero. Hence H(α, β), $\beta > 0$ is closed for any complex α. Moreover, for real α, $\beta > 0$, H (α, β) is a self-adjoint operator.

In perturbation theory the strength of the perturbing terms is usually expressed in terms of a parameter e.g. β in H (α, β) of eqn. (2.3). In such a case, we are often interested in the analyticity properties of the eigenvalues of the operator in that parameter. For this, we need to deal with a family of operators which depend holomorphically in the perturbation parameter. There are several useful criteria for a given family of operators to be holomorphic. Here we consider the holomorphic family of type A which is defined by the relative boundedness of the perturbation term with respect to the unperturbed operator.

Def. 2.5. A family T (α) of closed operators, defined for α in a domain D_0 of the complex plane, is said to be holomorphic of type A if

i) D (T (α)) = D is independent of α

and ii) T (α)u is holomorphic for $\alpha \in D_0$ $\forall$ $u \in D$.

In this case $T(\alpha)u$ has a Taylor expansion at each $\alpha \in D_0$. If, for example, $\alpha = 0$ belongs to D_0 we can write

$$T(\alpha)u = Tu + \alpha T_1 u + \alpha^2 T_2 u + \cdots, \quad u \in D \quad (2.6)$$

which converges in a disk $|\alpha| < r$ independent of u. $T = T(0)$ and T_n are linear operators with domain D.

A sufficient criterion for type A family is given by the following theorem.

Th.2.2. Let T be closable with $D(T) = D$. Let T_n, $n = 1,2,\ldots$ be linear operators with domains containing D, and let there be constants a,b, c ≥ 0 such that

$$\| T_n u \| \leq c^{n-1} \left(a \| u \| + b \| Tu \| \right), \quad u \in D. \quad (2.7)$$

Then the series (2.6) defines an operator $T(\alpha)$ with domain D for $|\alpha| < 1/c$. If $|\alpha| < (b+c)^{-1}$, $T(\alpha)$ is closable and the closures $\tilde{T}(\alpha)$ for such α form a holomorphic family of type A.

In many applications it happens that $T_2 = T_3 = \cdots = 0$. In this case one can choose $C = 0$ if

$$\| T_1 u \| \leq a \| u \| + b \| Tu \|, \quad u \in D.$$

Moreover, if it happens that the relative bound $b = 0$, then the corresponding holomorphic family is defined in the entire complex plane.

Considering the example of anharmonic oscillator, we see that since x^2 is $H(0, \beta)$ - bounded with relative bound zero, $H(\alpha, \beta)$ is a holomorphic family of type A in α for each fixed $\beta > 0$. $H(\alpha, \beta)$ is also a holomorphic family of type A in $\beta > 0$ for each fixed α. Moreover, using an estimate of the form

$$a\left[\|(p^2+x^2)\psi\|^2 + \|\beta x^4\psi\|^2\right] < \|(p^2+x^2+\beta x^4)\psi\|^2 + b\|\psi\|^2,$$
$$a < 1, \quad \psi \in D,$$

it can be shown that x^4 is $H(1, \beta)$-bounded and hence $H(1, \beta)$ is again a holomorphic family of type A for complex β in the plane cut along the negative real axis.

II.3. DEGENERACY OF EIGENVALUES.

The eigenvalue problem which is of interest to us in the present work involves a study of (i) the nature of spectrum (discrete or continuous) and (ii) the degeneracy, if any, of a discrete eigenvalue. The study of the eigenvalue problem of a closed operator T is greatly facilitated by introducing the concept of the corresponding resolvent operator.

Def.2.6. If $(T-z)$ is invertible with

$$R(z) = R(z, T) = (T-z)^{-1} \tag{2.8}$$

bounded, z is said to belong the resolvent set of T. The operator-valued function R(z) thus defined on the resolvent set $\mathbb{P}(T)$ is called the resolvent of T. Thus R(z) has domain $\mathcal{H}$ and range D(T), for any $z \in \mathbb{P}(T)$.

The complementary set $\Sigma(T)$ of $\mathbb{P}(T)$ is called the spectrum of T. Thus $z \in \Sigma(T)$, if either (T-z) is not invertible or it is invertible, but has range smaller than $\mathcal{H}$. The part $\Sigma_p(T)$ of $\Sigma(T)$ for which (T-z) is not invertible is known as the point spectrum. The complement $\Sigma_c(T)$ of $\Sigma_p(T)$ in $\Sigma(T)$, is the continuous spectrum of T.

Since we are interested in this work only in discret~~e~~ spectrum, we will henceforth assume that the operator T is such that i~~t~~s spectrum $\Sigma(T)$ consists wholly of point spectra. In such a case it happens usually that the spectrum $\Sigma(T)$ contains a bounded part Σ' separated from the set Σ'' in such a way that a rectifiable, simple closed curve Γ can be drawn so as to enclose an open set containing Σ' in its interior and Σ'' in its exterior. In this case, we have the following decomposition theorem.

Th. 2.3. Let $\Sigma(T)$ be seperated into two parts Σ', Σ'' in the way described above. Then we have a decomposition of T according to a decomposition $\mathcal{H} = M' \oplus M''$ of the space in such a way that the spectra of the parts $T_{M'}$, $T_{M''}$ coincide with Σ', Σ'' respectively and $T_{M'}$ is bounded. Thus $\Sigma(T_{M'}) = \Sigma'$

where $\Sigma(T_{M''})$ may contain $z = \infty$.

Suppose, for example, that λ be an isolated point of the spectrum $\Sigma(T)$. Obviously, $\Sigma(T)$ is divided into two parts Σ', Σ'' in the sense of the above theorem. Σ' consists of the single point λ; any closed curve enclosing λ but no other point of $\Sigma(T)$ may be chosen as Γ. Then the bounded operator

$$P = -(2\pi i)^{-1}\int_{\Gamma} R(z)\,dz \qquad (2.9)$$

is a projection on $M' = PH$ along $M'' = (1-P)H$. The point λ is called a (descrite) eigenvalue of T if the range space of P, M', is finite - dimensional. In this case dim M' is called the algebraic multiplicity of the eigenvalue λ of T and P is called the corresponding eigen-projection.

An eigenvalue λ of T is non-degenerate if the corresponding algebraic multiplicity has the value 1. Otherwise, it is degenerate. It should be noted that the non-degeneracy means something more than the statement that the equation $Tu = \lambda u$ has only one solution ($\equiv$ geometric multiplicity one). When T is self-adjoint, however, non-degenerate has the usual meaning of $Tu = \lambda u$ having a unique solution.

A closed operator T whose resolvent $R(z)$ is compact for each $z \in P(T)$ is known as an operator with compact resolvent. Most differential operators that appear in physics are of this type. The spectrum of such an operator consists entirely of discrete eigenvalues.

Finally, the eigenvalues of a holomorphic family of operators $T(\alpha)$ are given by analytic functions $\lambda_n(\alpha)$ in the following sense. If $\lambda_n(\alpha_0)$ is a non-degenerate eigenvalue of $T(\alpha_0)$ then there exists a neighbourhood of α_0 and an analytic function $\lambda_n(\alpha)$ defined in that neighbourhood so that $\lambda_n(\alpha)$ is a non-degenerate eigenvalue for all α in that neighbourhood and no other eigenvalue of $T(\alpha)$ is near $\lambda_n(\alpha)$. If, on the otherhand, there is an m-fold degeneracy, then there are $\leq m$ eigenvalues $\lambda_K(\alpha)$ for α near α_0 which coalesce to $\lambda_n(\alpha_0)$ at $\alpha = \alpha_0$. The λ_k's are analytic near $\alpha = \alpha_0$ and have at most an algebraic branch point there.

We note that anharmonic oscillator energy levels $E_n(\alpha, \beta)$ are analytic functions of α, β for real values of α and $\beta > 0$. This follows from the self-adjointness of the corresponding Hamiltonian $H(\alpha, \beta)$ given in (2.3).

II.4. DIVERGENCE OF ENERGY SERIES

In most of the cases of singular perturbations, as illustrated by the anharmonic oscillator problem in the preceding section, the expansion series of an eigenvalue in the perturbation parameter is found to diverge. Simon gave rigorous proof of this fact for the anharmonic oscillator problem. Since the proof has become a standard tool for similar models of singular perturbation theory, we review the main arguments of the proof. In particular it will be shown that the energy level $E_n(1,\beta)$ of the anharmonic oscillator

$$H(1,\beta) = p^2 + x^2 + \beta x^4$$

has a divergent Rayleigh-Schrodinger perturbation series and the divergence is due to an essential singularity of the function at $\beta = 0$. An analysis of the global analytic structure of $E_n(1,\beta)$ will also be done.

First, we note that the energy levels $E_n(\alpha,\beta)$ of the Hamiltonian (2.3) satisfy the scaling relation,

$$E_n(\alpha,\beta) = \lambda E_n(\alpha\lambda^{-2}, \beta\lambda^{-3}). \quad (2.10)$$

It means, in particular, that

$$E_n(1,\beta) = \beta^{1/3} E_n(\beta^{-2/3}, 1) . \quad (2.11)$$

Thus the investigation of the singularity structure of $E_n(1, \beta)$ can be done by looking at the function $E_n(\alpha, 1)$, when the analysis is a little simpler. From eqn. (2.11) it can be shown by using the principle of analytic continuation near $\alpha = \infty$ that $E_n(1, \beta)$ is non-analytic at $\beta = 0$. This result proves the divergence of the corresponding perturbation series in β. However, this does not preclude the existence of a series expansion in the powers of $\beta^{1/3}$.

To exclude such a possibility, one needs to investigate the singularities of $E_n(1, \beta)$ away from $\beta = 0$. The Herglotz property

$$\operatorname{Im} E_n / \operatorname{Im} \beta > 0 \tag{2.12}$$

that is satisfied by the function $E_n(1, \beta)$ asserts that $E_n(1, \beta)$ has no isolated poles or essential singularities. Moreover, algebraic branch points have no negative powers in their Puiseux series.

A characterization of non-isolated singularities can be given by the following 'lifting' theorem.

Th. 2.4. Let $\gamma : [0, 1] \rightarrow C$ be a curve in the α-plane.

Let $E_n(\alpha, 1)$ have analytic continuation along γ into interval $[0, 1)$. If the values $E_n(\gamma(t), 1)$

have a finite limit point as $t \to 1$ then $E_n(\alpha, 1)$ has an isolated singularity at $\alpha_0 = \gamma(1)$.

The theorem tells us that if we have a non-isolated singularity, whenever we approach it in some direction, the values $E_n(\alpha, 1)$ must approach ∞ . A non-isolated singularity may either be a limit point of isolated singularities (algebraic branch points) or a part of a natural boundary. Since at an algebraic branch point eigenvalues cross, α_0 can only be a limit point of such singularities of one level $E_n(\alpha, 1)$ which goes to ∞ as $\alpha \to \alpha_0$, crossing infinitely many levels along the way. Using the Herglotz property and the non-analyticity of $E_n(1, \beta)$ at $\beta = 0$ the following stronger result can also be obtained.

Th. 2.5. $E_n(1, \beta)$ has a global cubic branch point at $\beta = 0$ which is the limit point of algebraic branch points (or natural boundaries or logarithmic branch points).

By global cubic branch point we mean the following: if a curve $\gamma : [0, 1] \to C$ circles around complex conjugate branch points in complex conjugate ways and $\gamma(0) = \gamma(1)$ then $E_n(1, \beta)$ is continuable along γ and

$$E_n(1, \gamma(0)) = E_n(1, \gamma(1))$$

if γ winds about $\beta = 0$ three times. Moreover, in no case does $E_n(1, \beta)$ return back to its original value if γ winds $\beta = 0$ less than thrice. This theorem tells us that the (Rayleigh-Schrodinger) perturbation series for $E_n(1, \beta)$ is totally divergent.

The nature of the distribution of the infinite number of algebraic branch points (and natural boundaries) in the three-sheeted Riemann surface is quite complicated and not fully understood. However, two important results have been derived.

1. Loeffel and Martin[39] and Loeffel et al[41] were able to develop an argument which showed that the region $|\arg\alpha| < 2\pi/3$ in the α-plane were free from any singularity. Hence it follows from the scaling relation (2.11) that $E_n(1, \beta)$ is analytic in the first-sheet of the β-plane cut along the negative real axis.

2. Simon showed that the branch points approaching $\beta = 0$ on the three-sheeted surface have an asymptotic phase $\pm 3\pi/2$. This means that the branch points that approach $\beta = 0$ do so by spiralling into $\arg\beta = 3\pi/2$. The proof of this result rests on the estimate

$$a\left[\|(p^2+x^2)\psi\|^2 + |\beta|^2\|x^4\psi\|^2\right] < \|(p^2+x^2+\beta x^4)\psi\|^2 + b\|\psi\|^2 \tag{2.13}$$

where $a < 1 - |\beta|^{-1}|\mathrm{Re}\,\beta|$, $\mathrm{Im}\,\beta \neq 0$, $b = b(a)$ and $\psi \in D(p^2) \cap D(x^4)$.

It thus follows that H $(1, \beta)$ is a holomorphic family of type A (with compact resolvents) in β in the cut plane $|\arg \beta| < \pi$. The estimate is also used to prove the norm convergence of the resolvents

$$\| R_\gamma(|\beta|, E) - R_\gamma(0, E) \| \to 0 \quad \text{as} \quad |\beta| \to 0+ \tag{2.14}$$

where

$$R_\gamma(|\beta|, E) = [H(\gamma, |\beta|) - E]^{-1} \tag{2.15}$$

The convergence in (2.14) is uniform in γ as long as γ belongs to compact subsets of the complex plane cut along the negative real axis. In eqn. (2.15) $|\beta|$ is taken because by a scaling of the phase of β one can always study $p^2 + x^2 + \beta x^4$ by looking instead at $p^2 + \gamma' x^2 + |\beta| x^4$ where $\gamma' = \exp(-\frac{2}{3} i \arg \beta)$.

It then follows immediately that

Th. 2.6. Let n be given and $\theta < 3\pi/2$. Then, there is a B so that $E_n(1, \beta)$ is analytic in $\{\beta$ on the three-sheeted surface : $0 < |\beta| < B$, $|\arg \beta| < \theta\}$.

Determination of the asymptotic phase of the singularities is now a simple corollary to the above theorem.