Asymptotic Behaviour of the Eigenvalues of a Schrödinger Operator arising from a Simple Model of Predissociation

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Declaration

I hereby certify that this material, which I now submit for assessment of study leading to the award of Master of Science is entirely my own work and has not been taken from the work of others save and to the extent that such work has been cited and acknowledged within the text of my work.

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Go raibh maith agaibh.

Abstract

Within the perturbation theory of linear differential equations there has been considerable interest in recent years in calculating the imaginary part of an eigenvalue E which moves off the real axis when a small positive perturbation ε is switched on. Typically the perturbation in Re E is algebraic in ε, while that in Im E is exponentially small as $\varepsilon \to 0$. This phenomenon occurs in several physical applications including resonance theory in quantum mechanics, wave trapping by small islands, viscous fingering in fluid dynamics, and in energy losses at bends in optical fibres. In this thesis the problem arises from a model of molecular predissociation in quantum chemistry. It is more complicated than the above examples, firstly because there are two Schrödinger equations in the system and secondly because the small parameter appears in the coupling term.

In 1995 operator theoretic methods were used by Duclos and Meller [5] to obtain bounds on both the real and imaginary parts of the eigenvalue for such a problem, but gave no information about the associated eigenfunction. Here we consider a similar model proposed by Asch [2] and also use operator theoretic methods to get a bound on the resonances. We then improve on this bound by Fourier transforming the 2×2 system to a single second order equation whose solutions we approximate asymptotically by the classical analysis methods of Olver [13] as found in the paper of Dunster [6]. We then substitute the approximate solution plus its error term into the boundary condition at the origin to obtain an eigenvalue relation which yields another estimate for the perturbation in E. In the final chapter we report on other approaches which have been tried on this problem, outline the difficulties associated with each of them and make some suggestions for extending our results.

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Chapter 1

The Problem

1.1 Setting up the problem

The physical background to this problem is the model for predissociation for diatomic molecules proposed by Asch [2]. An outstanding problem is to obtain the exact behaviour of lifetime resonances for small values of the parameter $\hbar$ in this model. This thesis is an initial contribution to the research programme.

The problem we consider arises from a special case of a simple model for molecular predissociation (see [5]). Let H be the following 2×2 matrix Schrödinger operator acting on $L^2(\mathbb{R}) \oplus L^2(\mathbb{R})$

$$H = \begin{pmatrix} H^{(1)} & V^{(1,2)} \\ V^{(2,1)} & H^{(2)} \end{pmatrix} \qquad H^{(i)} = D^2 + V^{(i)} \tag{1.1.1}$$

where for any function $f \in L^2(\mathbb{R})$

$$Df = \frac{\hbar}{i} f'. \tag{1.1.2}$$

The $V^{(i)}$s are multiplication operators which are chosen as follows in the Asch model (see [2]):

$$V^{(1)} f = -f, \quad V^{(2)} f = x^2 f. \tag{1.1.3}$$

The coupling terms $V^{(i,j)}$ are generally functions of x and $\hbar$. We will take them to be simply of the form:

$$V^{(i,j)} = \hbar \tag{1.1.4}$$

where $\hbar = h/2\pi$, h being Planck's constant. This is the small parameter in the problem. It is the positioning of the small parameter in the coupling term which makes this singular perturbation problem non-standard. As $\hbar \to 0$, the system becomes uncoupled.

Let $H^{(d)}$ denote the diagonal part of H. It is well known that that $H^{(d)}$ is a selfadjoint operator with domain $\operatorname{dom} H^{(d)}$ given by

$$\operatorname{dom} H^{(d)} = \operatorname{dom} H^{(1)} \oplus \operatorname{dom} H^{(2)} = \mathcal{H}^2(\mathbb{R}) \oplus (\mathcal{H}^2(\mathbb{R}) \cap \operatorname{dom} V^{(2)}) \tag{1.1.5}$$

where $\mathcal{H}^2(\mathbb{R})$, the domain of D^2, is the usual Sobolev subspace of $L^2(\mathbb{R})$ which consists of functions whose first and second order weak derivatives are in $L^2(\mathbb{R})$ and $\operatorname{dom} V^{(2)}$ is the maximal domain of the multiplier operator $V^{(2)}$ defined by (1.1.3). Since the offdiagonal part is bounded and symmetric, H is also selfadjoint on $\mathcal{D}(H^d)$ (see [8, Ch. V, Thm. 4.3]). Furthermore, from [8, Ch. III, Sec 5.1] we see $\operatorname{dom} H = \operatorname{dom} H^{(d)}$.

Recall that if $X \neq \{0\}$ is a complex normed space and $T : \mathcal{D} \to \mathcal{X}$ is a linear operator with domain $\mathcal{D} \subset \mathcal{X}$ the resolvent of T is defined by

$$R(\lambda) = (T - \lambda I)^{-1} \tag{1.1.6}$$

where λ is a complex number and I is the identity operator on $\mathcal{D}$. A regular value λ of T is a complex number such that

(i) $R(\lambda)$ exists,

(ii) $R(\lambda)$ is bounded,

(iii) $R(\lambda)$ is defined on a set in which is dense in X.

The resolvent set $\rho(T)$ of T is the set of all regular value of T. Its complement $\sigma(T) = \mathbb{C} \setminus \rho(T)$ is called the spectrum of T, and $\lambda \in \sigma(T)$ is called a spectral value of T. Furthermore, the spectrum $\sigma(T)$ is partitioned into three disjoint sets as follows.

The point spectrum or discrete spectrum $\sigma_p(T)$ is the set such that $R(\lambda)$ does not exist. A $\lambda \in \sigma_p(T)$ is called an eigenvalue of T.

The continuous spectrum $\sigma_c(T)$ is the set such that $R(\lambda)$ exists and satisfies (iii) but not (ii), that is, $R(\lambda)$ is unbounded.

The residual spectrum $\sigma_r(T)$ is the set such that $R(\lambda)$ exists (and may be bounded or not) but does not satisfies (iii).

The spectrum of H^d, $\sigma(H^{(d)})$, is given by

$$\sigma(H^{(d)}) = \sigma(H^{(1)}) \cup \sigma(H^{(2)}) = [-1, \infty) \tag{1.1.7}$$

where $\sigma(H^{(1)}) = [-1, \infty)$ is a purely continuous spectrum and $\sigma(H^{(2)}) = (2\mathbb{N}+1)\hbar$ is a pure point spectrum. Thus $H^{(d)}$ has embedded eigenvalues in its continuous spectrum. When the offdiagonal part of H is turned on, the eigenvalues, E, become resonances.

One way to define these resonances is as follows. Let U_θ be the unitary implementation in $L^2(\mathbb{R})$ of the change of variable $\lambda_\theta : \mathbb{R} \to \mathbb{R}$, defined by $\lambda_\theta x \to \exp(\theta)x$, $\theta \in \mathbb{R}$, i.e.

$$\forall \psi \in L^2(\mathbb{R}), \quad U_\theta \psi(x) = e^{\theta/2}\psi(e^\theta x). \tag{1.1.8}$$

It then follows that

$$H_\theta^{(i)} = U_\theta H^{(i)} U_\theta^{-1} = e^{-2\theta} D^2 + V_\theta^{(i)} \tag{1.1.9}$$

where $V_\theta^{(i)}(x) = V^{(i)}(e^\theta x)$ and the coupling terms $V^{(i,j)}$, as given by (1.1.4), remain unchanged. In Kato, [8, Ch.VII], a family of operators $\{H_\theta\}_{\theta\in\Theta}$, $\Theta \subset \mathbb{C}$, is defined to be type A analytic if and only if dom H_θ is independent of θ and for all $\psi \in$ dom H_θ, $H_\theta\psi$ is analytic in Θ. By extending θ to the complex plane the two families of operators $\{H_\theta^{(i)}\}_{\theta\in\mathbb{R}}$, $i = 1, 2$, can be extended to families which are type A analytic in the above sense. More precisely $H_\theta^{(1)} = e^{2\theta}D^2 - 1$ is an analytic family of type A for $\theta \in \mathbb{C}$ and it is proved, in [4], that $H_\theta^{(2)}$ is type A analytic on $S_\alpha = \{\theta \in \mathbb{C}, |\mathrm{Im}\,\theta| < \alpha\}$ with $\alpha = \frac{\pi}{4}$. Therefore the family of operators given by

$$H_\theta = (U_\theta \oplus U_\theta) H (U_\theta \oplus U_\theta)^{-1} = \begin{pmatrix} H_\theta^{(1)} & \hbar \\ \hbar & H_\theta^{(2)} \end{pmatrix}, \quad \theta \in \mathbb{R} \tag{1.1.10}$$

is type A analytic when θ is extended to $S_{\frac{\pi}{4}}$.

Definition. *Any complex number E which is an eigenvalue of H_θ located in $\{z \in \mathbb{C}, \arg(z) \in (0, -2\mathrm{Im}\,\theta)\}$ for a given $\theta \in S_{\frac{\pi}{4}}$ is called* a resonance *of H.*

1.2 Strategy

We investigate the behaviour of the resonances E as $\hbar \to 0$. In Chapter 2 we use operator theoretic methods to show

$$\lambda = \lambda_0 + o(1), \quad (\hbar \to 0) \tag{1.2.1}$$

where $E = \lambda\hbar$ and $E_0 \in \sigma(H^{(2)})$. Then in Chapter 3 we show how applying the Fourier transform to (1.1.1) enables us to write the eigenvalue problem $H\Phi = E\Phi$, $\Phi = (\Phi_1, \Phi_2)^T$ as the following second-order ordinary differential equation in which the eigenvalue appears in a non-linear way:

$$\frac{d^2w}{dz^2} = (z^2 - \lambda + \psi(z, \lambda, \hbar))w \tag{1.2.2}$$

where we define

$$\psi(z, \lambda, \hbar) = \frac{-1}{z^2 - \lambda - \frac{1}{\hbar}}. \tag{1.2.3}$$

Then using the results of [6] we find asymptotic approximations to a solution of this equation from which we improve the result of Chapter 2 to

$$\lambda - \lambda_0 = \mathcal{O}(\hbar \ln(\hbar^{1/2})), \quad (\hbar \to 0). \tag{1.2.4}$$

in the specific for the case where $\theta = \iota\pi/24$.

Chapter 2

Stability of the resonances

2.1 The resolvent of H_θ

It is easily seen that when $\theta \in S_{\frac{\pi}{4}}$

$$\sigma(H_\theta^{(1)}) = \{-1 + xe^{-2\theta}; x \in \mathbb{R}_+\}. \tag{2.1.1}$$

Because $H_\theta^{(2)}$ is analytic of type A when θ is extended to $S_{\frac{\pi}{4}}$, then the discrete spectrum of $H_\theta^{(2)}$ remains unchanged (see [14]) i.e.

$$\sigma(H_\theta^{(2)}) = (2n+1)\hbar,\ n \in \mathbb{N}. \tag{2.1.2}$$

The spectrum of $H_\theta^{(d)}$, the diagonal part of H_θ, is depicted in Figure 2.1 for $\theta = i\beta$, with $\beta > 0$, the bold line being $\sigma(H_\theta^{(1)})$.

Let Γ be a contour around any eigenvalue $E_0 = (2n+1)\hbar$ of $H^{(2)}$ defined by

$$z \in \Gamma \iff |z - E_0| = \hbar\rho, \quad \text{with} \quad \rho \in (0,1] \tag{2.1.3}$$

where ρ small enough so that $\Gamma \cap \sigma(H^{(1)}) = \emptyset$. Thus we also require that

$$\hbar\rho < \sin(2\beta)(E_0 + 1) = \operatorname{dist}(E_0, \sigma(H^{(1)})). \tag{2.1.4}$$

Therefore, for any $z \in \Gamma$, we can define the resolvent of $H_\theta^{(d)}$ by

$$R_\theta^{(d)}(z) = (H_\theta^{(d)} - z)^{-1} = \begin{pmatrix} H_\theta^{(1)} - z & 0 \\ 0 & H_\theta^{(2)} - z \end{pmatrix}^{-1} \tag{2.1.5}$$

$$= \begin{pmatrix} R_\theta^{(1)}(z) & 0 \\ 0 & R_\theta^{(2)}(z) \end{pmatrix} \tag{2.1.6}$$

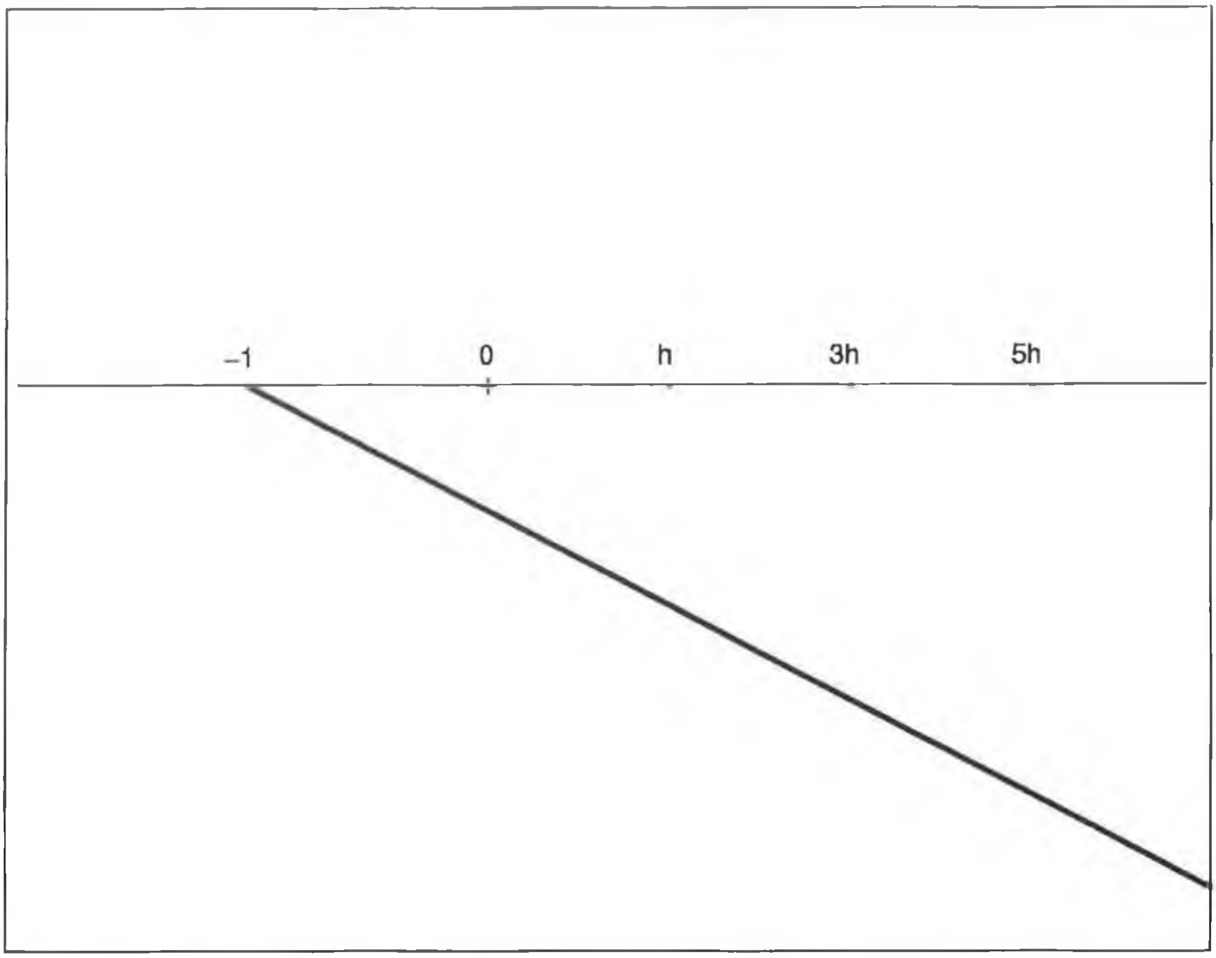

Figure 2.1: Spectrum of $H_\theta^{(d)}$

and its eigenprojector by

$$P_\theta^{(d)} = \frac{i}{2\pi}\int_\Gamma R_\theta^{(d)}(z)\,dz. \tag{2.1.7}$$

We note that $P_\theta^{(d)} = 0 \oplus P_\theta^{(2)}$ since $\sigma(H_\theta^{(1)})$ lies entirely outside Γ.

We now consider $R_\theta(z)$, the resolvent of H_θ. By writing $H_\theta = H_\theta^{(d)} + A$ where

$$A = \begin{pmatrix} 0 & \hbar \\ \hbar & 0 \end{pmatrix} \tag{2.1.8}$$

it can be seen that

$$(H_\theta - z)^{-1} = (H_\theta^{(d)} - z)^{-1}(1 + A(H_\theta^{(d)} - z)^{-1})^{-1}. \tag{2.1.9}$$

Thus by functional calculus

$$R_\theta(z) = R_\theta^{(d)}(z)(1 + AR_\theta^{(d)}(z))^{-1} \quad (2.1.10)$$

$$= R_\theta^{(d)}(z)(1 - (AR_\theta^{(d)}(z))^2)^{-1} - A(R_\theta^{(d)}(z))^2(1 - (AR_\theta^{(d)}(z))^2)^{-1} \quad (2.1.11)$$

where we have used the identity

$$\frac{1}{1+x} = \frac{1}{1-x^2} - \frac{x}{1-x^2}. \quad (2.1.12)$$

From (2.1.11), we see that $R_\theta(z)$ is defined for $z \in \Gamma$ provided

$$z \notin \sigma(H_\theta^{(d)}) \quad (2.1.13)$$

and

$$1 \notin \sigma((A(H_\theta^{(d)} - z)^{-1})^2) \quad (2.1.14)$$

It can be shown that a sufficient condition for both (2.1.13) and (2.1.14) to hold is

$$\|AR_\theta^{(d)}(z)\| = \hbar^2 \|R_\theta^{(1)}(z)R_\theta^{(2)}(z)\| \leq 1. \quad (2.1.15)$$

Because (2.1.15) implies that $z \notin \sigma(H_\theta^{(i)})$, $i = 1, 2$, (2.1.13) follows from this. To show that (2.1.14) is satisfied when (2.1.15) is we first recall that for any bounded operator A

$$\sup_{z \in \sigma(A)} |z| < \|A\|. \quad (2.1.16)$$

Thus $1 \notin \sigma((A(H_\theta^{(d)} - z)^{-1})^2)$ when $\|(W(H_\theta^{(d)} - z)^{-1})^2\| < 1$. As

$$(W(H_\theta^{(d)} - z)^{-1})^2 = \hbar^2 \begin{pmatrix} R_\theta^{(2)}(z)R_\theta^{(1)}(z) & 0 \\ 0 & R_\theta^{(1)}(z)R_\theta^{(2)}(z) \end{pmatrix} \quad (2.1.17)$$

$\|(W(H_\theta^{(d)} - z)^{-1})^2\| < 1$ when $\|\hbar^2 R_\theta^{(2)}(z)R_\theta^{(1)}(z)\| < 1$ and $\|\hbar^2 R_\theta^{(1)}(z)R_\theta^{(2)}(z)\| < 1$. These both follow from (2.1.15).

Next we must show (2.1.15) is true for all $z \in \Gamma$. For this we need the following lemma:

Lemma. *The resolvents $R_\theta^{(i)}$, $i = 1, 2$ are bounded as follows:*

$$\forall z \notin \sigma(H_\theta^{(1)}), \quad ||R_\theta^{(1)}(z)|| = \frac{1}{\text{dist}\,(z, \sigma(H_\theta^{(1)}))} \tag{2.1.18}$$

and

$$\exists C_{\Gamma,\theta} > 0, \quad \forall z \in \Gamma, \quad ||R_\theta^{(2)}(z)|| \leq \frac{C_{\Gamma,\theta}}{\hbar}. \tag{2.1.19}$$

Proof.

$$||R_\theta^{(1)}(z)|| = ||(e^{-2\theta}D^2 - 1 - z)^{-1}|| = |e^{2\theta}|\; ||(D^2 - e^{2\theta}(z+1))^{-1}|| \tag{2.1.20}$$

As $H_\theta^{(1)}$ is selfadjoint then

$$\begin{aligned} ||R_\theta^{(1)}(z)|| &= \frac{|e^{2\theta}|}{\text{dist}\,(\mathbb{R}_+, e^{2\theta}(z+1))} && \text{provided } z \notin \sigma(H_\theta^1) \\ &= \frac{1}{\text{dist}\,(\mathbb{R}_+, e^{2i\text{Im}\,\theta}(z+1))} && \text{dividing by } e^{2\text{Re}\,\theta} \\ &= \frac{1}{\text{dist}\,(-1 + e^{-2i\text{Im}\,\theta}\mathbb{R}_+, z)} = \frac{1}{\text{dist}\,(\sigma(H_\theta^{(1)}), z)}. \end{aligned}$$

We consider now $R_\theta^{(2)}(z) = (H_\theta^{(2)} - z)^{-1}$. For $z \in \Gamma$ we let $z = E_0 + \hbar\xi$ with $\xi \in \mathbb{C}$ on the circle $\gamma : |\xi| = \rho$. After the change of variable $x \to \sqrt{\hbar}x$, $\hbar R_\theta^{(2)}$ is unitarily equivalent to $(e^{-2\theta}\Delta^2 + e^{2\theta}V^{(2)} - (2n+1) - \xi)^{-1}$, where Δ is the Laplacian operator. Therefore $\hbar||R_\theta^{(2)}|| = ||(e^{-2\theta}\Delta^2 + e^{2\theta}V(2) - (2n+1) - \xi)^{-1}||$. This last operator is uniformly bounded on γ since γ is compact, belongs to the resolvent set of $-e^{-2\theta}\Delta^2 + e^{2\theta}V^2 - 2n - 1$ and the function $\mathbb{C} \setminus \text{spect}\, H^{(2)} : \xi \to (-e^{-2\theta}\partial_x^2 + e^{2\theta}x^2 - (2n+1) - \xi)^{-1}$ is continuous (even analytic). This bound depends only on Γ and θ and is denoted by $C_{\Gamma,\theta}$ ■

It then follows that, to ensure that $R_\theta(z)$ exists and is bounded on Γ, we need $\hbar^2||R_\theta^{(1)}(z)R_\theta^{(2)}(z)|| < 1$, which by the lemma will be true under the condition

$$\hbar < \frac{\text{dist}\,(\Gamma, \sigma(H_\theta^{(1)}))}{C_{\Gamma,\theta}}. \tag{2.1.21}$$

By taking $\hbar$ small enough such that (2.1.21) is satisfied we know that Γ belongs to the resolvent set of H_θ. Therefore we may define the corresponding eigenprojector of H_θ

$$P_\theta = \frac{\iota}{2\pi}\int_\Gamma R_\theta(z)\,dz. \tag{2.1.22}$$

2.2 Obtaining a bound on the resonances

Let

$$H_{\theta,a} = H_\theta^{(d)} + a\begin{pmatrix} 0 & \hbar \\ \hbar & 0 \end{pmatrix}, \quad 0 \le a \le 1. \tag{2.2.1}$$

Therefore

$$P_{\theta,a} = \frac{\iota}{2\pi}\int_\Gamma (H_{\theta,a} - z)^{-1}\,dz. \tag{2.2.2}$$

is a projection depending continuously on a. Also $P_{\theta,0} = P_\theta^{(d)}$ and $P_{\theta,1} = P_\theta$. Thus from [8, Ch. I, Lemma 4.10]

$$\dim P_\theta = \dim P_\theta^{(d)} = 1 \tag{2.2.3}$$

since $P_\theta^{(d)} = 0 \oplus P_\theta^{(2)}$ and the spectrum of $H_\theta^{(2)}$ is simple.

So we have shown that when (2.1.21) is satisfied there is one eigenvalue of H_θ, E, inside Γ. We let

$$\lambda = \frac{E}{\hbar} \tag{2.2.4}$$

so that inside Γ we have $|\lambda - \lambda_0| < \rho$. Also let $\hbar_\rho$ be the largest $\hbar$ satisfying (2.1.21) for each Γ defined by (2.1.3). Therefore for any $\rho \in (0,1]$, $|\lambda_0 - \lambda| < \rho$ for all $\hbar < \hbar_\rho$. We may then write

$$\lim_{\hbar\to 0} \lambda = \lambda_0 \tag{2.2.5}$$

or

$$\lambda = \lambda_0 + o(1), \quad (\hbar \to 0). \tag{2.2.6}$$

Chapter 3

Improving the bound on λ

3.1 Transforming the problem to a second order ODE

We define the semi-classical Fourier transform, $F_{sc} : L^2(\mathbb{R}) \to L^2(\mathbb{R})$, as follows

$$F_{sc}f(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\imath px/\hbar} f(x)\, dx. \tag{3.1.1}$$

Applying F_{sc} to the operator H_θ given by (1.1.10) where now $0 < \Im m\theta < \pi/4$ yields

$$\hat{H}_\theta = \begin{pmatrix} e^{-2\theta}V^{(2)} - 1 & \hbar \\ \hbar & e^{-2\theta}V^{(2)} + e^{2\theta}\hbar^2 D^2 \end{pmatrix} \tag{3.1.2}$$

where D is defined by (1.1.2) and $V^{(2)}$ by (1.1.3). The domain of this operator is given by

$$\operatorname{dom} \hat{H}_\theta = \operatorname{dom} V^{(2)} \oplus (\mathcal{H}^2(\mathbb{R}) \cap \operatorname{dom} V^{(2)}) \tag{3.1.3}$$

where $\mathcal{H}^2(\mathbb{R})$ is as in Section 1.1. As the Fourier transform preserves spectral properties, an eigenvalue E of $\hat{H}_\theta$ is a resonance of H as defined in Section 1.1.

We now consider the eigenvalue equation $H_\theta\Phi = E\Phi$, $\Phi = (\Phi_1, \Phi_2)^T$. As $\Phi_2 \in \mathcal{H}^2(\mathbb{R})$ we know

$$\lim_{x\to\infty} \Phi_2(x) = 0 \quad \text{and} \quad \lim_{x\to\infty} \Phi_2'(x) = 0 \tag{3.1.4}$$

where the dash denotes differentiation with respect to x. Also as H_θ commutes with the parity operator P, defined by

$$P\Phi(x) = \Phi(-x), \quad \Phi \in \operatorname{dom} \hat{H}_\theta, \tag{3.1.5}$$

we can choose Φ to be either even or odd. Thus

$$\Phi_2(0) = 0 \quad \text{or} \quad \Phi_2'(0) = 0. \tag{3.1.6}$$

We rewrite the eigenvalue equation as

$$\Phi_1 = \frac{-\hbar\Phi_2}{e^{-2\theta}p^2 - E - 1}, \tag{3.1.7}$$

$$-\hbar^2 e^{2\theta}\frac{d^2\Phi_2}{dp^2} + (e^{-2\theta}p^2 - E)\Phi_2 + \hbar\Phi_1 = 0. \tag{3.1.8}$$

Letting $z = e^{-\theta}\hbar^{-1/2}p$ and $w(z) = \Phi_2(e^{\theta}\hbar^{1/2}z) \in \mathcal{H}^2(e^{-\theta}\mathbb{R})$ gives

$$\frac{d^2w}{dz^2} = (z^2 - \lambda + \psi(z, \lambda, \hbar))w, \tag{3.1.9}$$

where again $\lambda = E/\hbar$ and

$$\psi(z, \lambda, \hbar) = \frac{-1}{z^2 - \lambda - \frac{1}{\hbar}}. \tag{3.1.10}$$

The boundary conditions in (3.1.4) and (3.1.6) become

$$\lim_{z\to\infty} w(e^{-\theta}z) = 0 \quad \text{and} \quad \lim_{z\to\infty} w'(e^{-\theta}z) = 0 \tag{3.1.11}$$

and

$$w(0) = 0 \quad \text{or} \quad w'(0) = 0. \tag{3.1.12}$$

depending on whether odd or even eigenfunctions are sought.

For definiteness, we will make the choice $\theta = \iota\pi/24$. We will construct an asymptotic approximation, complete with an error bound, to the solution of (3.1.9), subject to the following boundary conditions

$$w(0) = 0, \tag{3.1.13}$$

$$w(z) \to 0, \quad (z \to \infty e^{-\iota\pi/24}). \tag{3.1.14}$$

Note that if we ignore ψ in (3.1.9), the resulting comparison equation is similar to the parabolic cylinder function equation (A.0.1). Thus it is natural to follow the analysis of [6] as this furnishes us with solutions in terms of parabolic cylinder functions whose asymptotic properties are well understood. This result is in turn employed to explore the behaviour of λ as $\hbar \to 0$ and improve the result of Chapter 2.

3.2 Summary of Dunster's results

In [6] the differential equation

$$\frac{d^2W}{d\zeta^2} = (u^2\zeta^2 + \beta\zeta + \psi(u,\zeta))W \tag{3.2.1}$$

where u is real and positive and β bounded (real or complex), is considered. The independent variable ζ lies in some complex domain, possibly bounded, in which $\psi(u,\zeta)$ is holomorphic and $o(u/\ln u)$ as $u \to \infty$. Solutions to (3.2.1) are constructed in terms of parabolic cylinder functions, including explicit error bounds. We note later that the bounds obtained by Dunster are sharper than those originally obtained by Olver [12] because he takes the more realistic comparison equation (3.2.2).

First Dunster defined four 'approximants', $\nu_j(\beta, \sqrt{u}\zeta)$, $(j = 1,2,3,4)$, which are exact solutions to the 'comparison' equation

$$\frac{d^2W}{d\zeta^2} = (u^2\zeta^2 + \beta\zeta)W. \tag{3.2.2}$$

The first of these is written in terms of the parabolic cylinder function $U(a,x)$ (see Appendix A)

$$\nu_1(\beta,z) = e^{(1+\beta)/4}U\left(\frac{\beta}{2}, \sqrt{2}z\right) \tag{3.2.3}$$

and the second in terms of a confluent hypergeometric function (again see Appendix A)

$$\nu_2(\beta,z) = e^{(1-\beta)\pi\iota/4}e^{z^2/2}\mathrm{U}\left(\frac{1}{4}+\frac{\beta}{4}, \frac{1}{2}, -z^2\right). \tag{3.2.4}$$

The remaining two are given in terms of $\nu_1(\beta,z)$ and $\nu_2(\beta,z)$

$$\nu_3(\beta,z) = \nu_1(\beta,z) - \frac{2\pi e^{(\beta-1)\pi\iota/4}}{\Gamma(\frac{3}{4}+\frac{\beta}{4})\Gamma(\frac{1}{4}+\frac{\beta}{4})}\nu_2(\beta,z), \tag{3.2.5}$$

$$\nu_4(\beta,z) = \frac{e^{(1-3\beta)\pi\iota/4}2^{(1-\beta)/2}\sqrt{\pi}}{\Gamma(\frac{1}{2}-\frac{\beta}{2})}\nu_1(\beta,z) - e^{\beta\pi\iota}\nu_2(\beta,z). \tag{3.2.6}$$

Of particular interest to us is $\nu_1(\beta, z)$, which has the following asymptotic behaviour

$$\nu_1(\lambda, z) \sim z^{(\lambda-1)/2} e^{-z^2/2} \quad (z \to \infty \,|\arg(z)| \leq \frac{3}{4}\pi - \sigma), \tag{3.2.7}$$

where σ is an arbitrarily small constant. Also $\nu_1(\beta, z)$ is recessive at infinity in the sector $|\arg z| < \pi/4$. In addition we note that the Wronskian of $\nu_1(\beta, z)$ and $\nu_2(\beta, , z)$ is given by

$$\mathcal{W}(\nu_1(\lambda, z), \nu_2(\lambda, z)) = 2. \tag{3.2.8}$$

Dunster then goes to rigorously prove that

$$W_j(u, \zeta) = \nu_j(\beta, \sqrt{u}\zeta) + \epsilon_j(u, \zeta), \quad (j = 1, 2, 3, 4) \tag{3.2.9}$$

are exact solutions to (3.2.1) and obtains bounds for the error terms $\epsilon_j(u, \zeta)$. This involves a standard method whereby (3.2.9) is substituted in (3.2.1) to yield

$$\frac{\partial^2 \epsilon_j(u, \zeta)}{\partial \zeta^2} - (u^2\zeta^2 + \beta\zeta)\epsilon_j(u, \zeta) = \psi(u, \zeta)(\nu_j(\beta, \sqrt{u}\zeta) + \epsilon_j(u, \zeta)) \tag{3.2.10}$$

which is rewritten as an integral equation using variation of parameters. A bound on $\epsilon_j(u, \zeta)$ can be found from [13, Ch. 6, Thm. 10.2].

In order to apply this theorem a universal weight function is defined as follows

$$\varepsilon(z) = \begin{cases} |e^{z^2/2}| = e^{\mathrm{Re}\, z^2/2} & |z| \leq 1 \\ |z|^{\mathrm{Re}\,(-\lambda)/2} |e^{z^2/2}| = e^{\frac{1}{2}\mathrm{Re}\,(z^2 - \lambda \ln |z|)} & |z| > 1 \end{cases} \tag{3.2.11}$$

The complex plane is divided up into four non-overlapping domains given by

$$\begin{aligned} \Delta_1 &= \{z : \mathrm{Re}\,(z) \geq 0, \varepsilon(z) \geq 1\}, \quad \Delta_2 = \{z : \mathrm{Im}\,(z) \leq 0, \varepsilon(z) \leq 1\} \\ \Delta_3 &= \{z : \mathrm{Re}\,(z) \leq 0, \varepsilon(z) \geq 1\}, \quad \Delta_4 = \{z : \mathrm{Im}\,(z) \geq 0, \varepsilon(z) \leq 1\} \end{aligned} \tag{3.2.12}$$

The boundaries of these regions are the level curves satisfying $\varepsilon(z) = 1$. It can be seen that inside the unit circle the boundaries are the level curves are given by

$$\mathrm{Re}\, z = \pm \mathrm{Im}\, z \tag{3.2.13}$$

while outside the unit circle the boundaries are the curves which satisfy

$$\text{Re } (-\lambda \ln |z| + z^2) = 0. \tag{3.2.14}$$

As

$$-\lambda \ln |z| + z^2 \sim z^2, \quad (|z| \to \infty, |z| \to 1) \tag{3.2.15}$$

then the boundaries outside the circle approach the lines defined in (3.2.13) when $|z| \to \infty$ and $|z| \to 1$.

For each of the four approximants Dunster then defines a weight function $\varepsilon_j(z)$ to reflect their exponential growth or decay at infinity. For $j = 1, 3$

$$\varepsilon_j(z) = \begin{cases} \varepsilon(z) & z \in \Delta_j \cup \Delta_{j+1} \cup \Delta_{j-1}, \\ \varepsilon^{-1}(z) & z \in \Delta_{j+2}, \end{cases} \tag{3.2.16}$$

and for $j = 2, 4$

$$\varepsilon_j(z) = \begin{cases} \varepsilon(z) & z \in \Delta_j \cup \Delta_{j+1} \cup \Delta_{j-1}, \\ \varepsilon^{-1}(z) & z \in \Delta_{j+2}, \end{cases} \tag{3.2.17}$$

Next a modulus function, $M_j(\beta, z)$, is defined as follows

$$M_j(\beta, z) = \{\varepsilon^2_{j+1}(z)|\nu^2_{j+1}(\beta, z)| + \varepsilon^2_{j+2}(z)|\nu^2_{j+2}(\beta, z)| + \varepsilon^2_{j+3}(z)|\nu^2_{j+3}(\beta, z)|\}^{1/2}, \tag{3.2.18}$$

where it can be seen that

$$M_j(\lambda^{(1)}, z) = O(\{1 + |z|\}^{-1/2}) \tag{3.2.19}$$

uniformly in the complex plane. The following constants are also needed

$$\kappa_0 = \max_{1 \leq, j, k, l \leq 4} \left[\sup_{z \in \Delta_j \cup \Delta_k} \{(1 + |z|) M_l^2(\lambda^{(1)}, z)\} \right], \tag{3.2.20}$$

$$\kappa = \max_{1 \leq, j, k, l \leq 4} \left[\sup_{z \in \Delta_j \cup \Delta_k} \{(1 + |z|) \varepsilon_j(z) M_l(\lambda^{(1)}, z) |\nu_j(z)|\} \right]. \tag{3.2.21}$$

where in both cases $j \neq k \neq l$.

Finally, for each solution given by (3.2.9), Dunster defines subdomains $Z_j(\alpha_j) \subset \Delta$ in which lie integration paths L_j on which the weight functions $\varepsilon_j(\sqrt{u}\zeta)$ are monotonic, where α_j is an arbitrary reference point. On choosing an $\alpha_j \in \Delta$ such that $\sqrt{u}\alpha_j \in \Delta_j$, he defines $Z_j(\alpha_j)$ to be the set of points for which there exists a path L_j linking ζ to α_j, having the properties:

(i) L_j is a finite chain of R_2 arcs.

(iia) If $\sqrt{u}\zeta \in \Delta_j \cup \Delta_{j\pm1}$, then as t passes along L_j, from ζ to α_j, $(-1)^{j-1}\mathrm{Re}\,(ut^2)$ and $(-1)^{j-1}\mathrm{Re}\,(ut^2 + \beta\ln(\sqrt{u}|t|))$ are nondecreasing when $\sqrt{u}|t| \leq 1$ and $\sqrt{u}|t| > 1$ respectively.

(iib) If $\sqrt{u}\zeta \in \Delta_{j+2}$, then as t passes along L_j, from ζ to α_j, $(-1)^{j-1}\mathrm{Re}\,(ut^2)$ and $(-1)^{j-1}\mathrm{Re}\,(ut^2 + \beta\ln(\sqrt{u}|t|))$ are nonincreasing for the segment in $\{t : \sqrt{ut} \in \Delta_{j+2}, \sqrt{u}|t| \leq 1\}$ and $\{t : \sqrt{ut} \in \Delta_{j+2}, \sqrt{u}|t| > 1\}$, respectively, and nondecreasing for the segment in $\{t : \sqrt{ut} \in \Delta_j, \sqrt{u}|t| \leq 1\}$ and $\{t : \sqrt{ut} \in \Delta_j, \sqrt{u}|t| > 1\}$, respectively.

We recall that an arc with parametric equation $z = z(\tau)$ is said to be an R_2 arc if $z''(\tau)$ is continuous and $z'(\tau)$ does not vanish [13, p 147]

Now, using the aforementioned theorem from [13], Dunster obtains a bound for $\epsilon_j(u, \zeta)$ and states this result in the following theorem.

Theorem 3.2.1. *Under the conditions of this section, the differential equation*

$$\frac{d^2W}{d\zeta^2} = (u^2\zeta^2 + \beta\zeta + \psi(u, \zeta))W \tag{3.2.22}$$

has, for each positive value of u, *solutions* $W_j(u, \zeta)$, $(j = 1, 2, 3, 4)$, *which are holomorphic* *in Δ, given by*

$$W_j(u,\zeta) = \nu_j(\beta, \sqrt{u}\zeta) + \epsilon_j(u,\zeta), \tag{3.2.23}$$

where

$$\frac{|\epsilon_j(\beta,\zeta)|}{M_l(\sqrt{u}\zeta)} \leq \frac{\kappa}{\kappa_0}\varepsilon_j^{-1}(\sqrt{u}\zeta)\left[\exp\left\{\frac{\kappa_0}{|\mathcal{W}(\nu_j,\nu_k)|}\int_{\alpha_j}^{\zeta}\frac{|\psi(u,t)\,dt|}{1+\sqrt{u}|t|}\right\}-1\right] \tag{3.2.24}$$

for $\zeta \in Z_j(\alpha_j)$. The suffix k is determined by the subdomain Δ_k in which $\sqrt{u}\zeta$ lies, except when $\sqrt{u}\zeta \in \Delta_j$, in which case k is chosen arbitrarily different from j subject to $\mathcal{W}(\nu_j,\nu_k) \neq 0$. The auxiliary suffix l is an integer chosen different from j and k.

Dunster notes that uniform asymptotic solutions to (3.2.1) can be found in terms of Bessel functions if we consider $u^2\zeta^2$ to be the dominant term and apply Theorem 3 of [12]. However he points out that the error terms would only be $\mathcal{O}(1)$ as $u \to \infty$. In special cases the error bound in (3.2.24) can be shown to be $\mathcal{O}(u^{-1})$ as $u \to \infty$.

It is then remarked that the condition $\psi(u,\zeta) = o(u/\ln u)$ as $u \to \infty$ is needed for the error bounds to be meaningful in this limit. However, in our specific application, we can compute an explicit bound on the integral in the error bound and thus can forego this condition.

3.3 Recovering E_0 from the differential equation

First we solve the comparison equation

$$\frac{d^2w}{dz^2} = (z^2-\lambda)w, \tag{3.3.1}$$

subject to the boundary conditions (3.1.13) and (3.1.14).

Equation (3.3.1) is of the form (3.2.2) with $u = 1$ and $\beta = -\lambda$. Therefore (3.3.1) has as a solution

$$\nu_1(\lambda, z) = e^{(1-\lambda)/4}U\left(-\frac{\lambda}{2}, \sqrt{2}z\right) \tag{3.3.2}$$

which we can see from (3.2.7) satisfies condition (3.1.14). From (A.0.6) we see that at the origin

$$\nu_1(\lambda, 0) = e^{(1-\lambda)/4} \frac{\sqrt{\pi}}{2^{-\lambda/4+1/4}\Gamma(\frac{3}{4} - \frac{\lambda}{4})}. \tag{3.3.3}$$

So (3.1.13) is satisfied when

$$\frac{3}{4} - \frac{\lambda}{4} = -k, \quad (k = 0, 1, 2, 3, ...) \tag{3.3.4}$$

or

$$\lambda = 2n + 1 \quad (n \text{ odd}). \tag{3.3.5}$$

Therefore, from (2.2.4) we have

$$E = (2n + 1)\hbar \quad (n \text{ odd}). \tag{3.3.6}$$

Equivalently, if we solved (3.3.1) subject to $w'(0) = 0$ and (3.1.14) we would find

$$E = (2n + 1)\hbar \quad (n \text{ even}). \tag{3.3.7}$$

Combining (3.3.5) and (3.3.7) gives the spectrum of $H_\theta^{(2)}$

$$\sigma(H_\theta^{(2)}) = (2n + 1)\hbar, \quad n \in \mathbb{N}. \tag{3.3.8}$$

Again we will denote E_0 as any eigenvalue of $H_\theta^{(2)}$ and λ_0 as $E_0/\hbar$. We consider λ_0 to be an unperturbed eigenvalue of the problem where $\psi(z, \lambda, \hbar)$ is the perturbation.

3.4 Approximation to a solution of the differential equation

In this section we use the result of [6] outlined in Section 3.2 to construct a solution to

$$\frac{d^2w}{dz^2} = (z^2 - \lambda + \psi(z, \lambda, \hbar))w, \tag{3.4.1}$$

subject to

$$w(0) = 0, \tag{3.4.2}$$

$$w(z) \to 0, \quad (z \to \infty e^{-\iota\pi/24}) \tag{3.4.3}$$

where

$$\psi(z,\lambda,\hbar) = \frac{-1}{z^2 - \lambda - \frac{1}{\hbar}}. \tag{3.4.4}$$

The solution will be in terms of the parabolic cylinder function $U(a,x)$ plus an error term which is bounded on a path on which (3.4.3) is satisfied.

We note that $\psi(z,\lambda,\hbar)$ has two poles at

$$z = p_{1,2} = \pm\sqrt{\lambda + \frac{1}{\hbar}}. \tag{3.4.5}$$

From Chapter 2 we know that $\lambda \to \lambda_0$ as $\hbar \to 0$, so $p_{1,2} \to \pm\infty$ respectively on the real axis as $\hbar \to 0$. Therefore we position these points just off the real axis in Figure 3.1.

We look for such a solution in the domain Δ which is the z-plane cut from p_1 to ∞ along the horizontal line $\text{Im } z = \text{Im } p_1$ and from p_2 to ∞ along the line $\text{Im } z = \text{Im } p_2$. Also circles surrounding $z = p_1$ and $z = p_2$ of radius $\frac{1}{2}\delta$ have been removed (see Figure 3.1).

We choose σ to be a small positive constant such that the circles do not intersect with the line

$$L_1 : z(\tau) = \tau e^{-\iota\pi/24}, \quad (0 \le \tau < \infty). \tag{3.4.6}$$

Now $\psi(z,\lambda,\hbar)$ is holomorphic in Δ.

Equation (3.4.1) is of the form (3.2.1) with $u = 1$ and $\beta = -\lambda$. From Chapter 2 we know each λ is bounded in a circle about a specific λ_0 for $\hbar$ satisfying (2.1.21). Thus for these values of $\hbar$ we can apply the results of Section 3.2 to (3.4.1).

From (3.2.11) we see that for this particular case the universal weight function $\varepsilon(z)$ is given by

$$\varepsilon(z) = \begin{cases} |e^{z^2/2}| = e^{\text{Re } z^2/2} & |z| \le 1 \\ |z|^{\text{Re }(-\lambda)/2}|e^{z^2/2}| = e^{\frac{1}{2}\text{Re } e(z^2 - \lambda \ln|z|)} & |z| > 1 \end{cases} \tag{3.4.7}$$

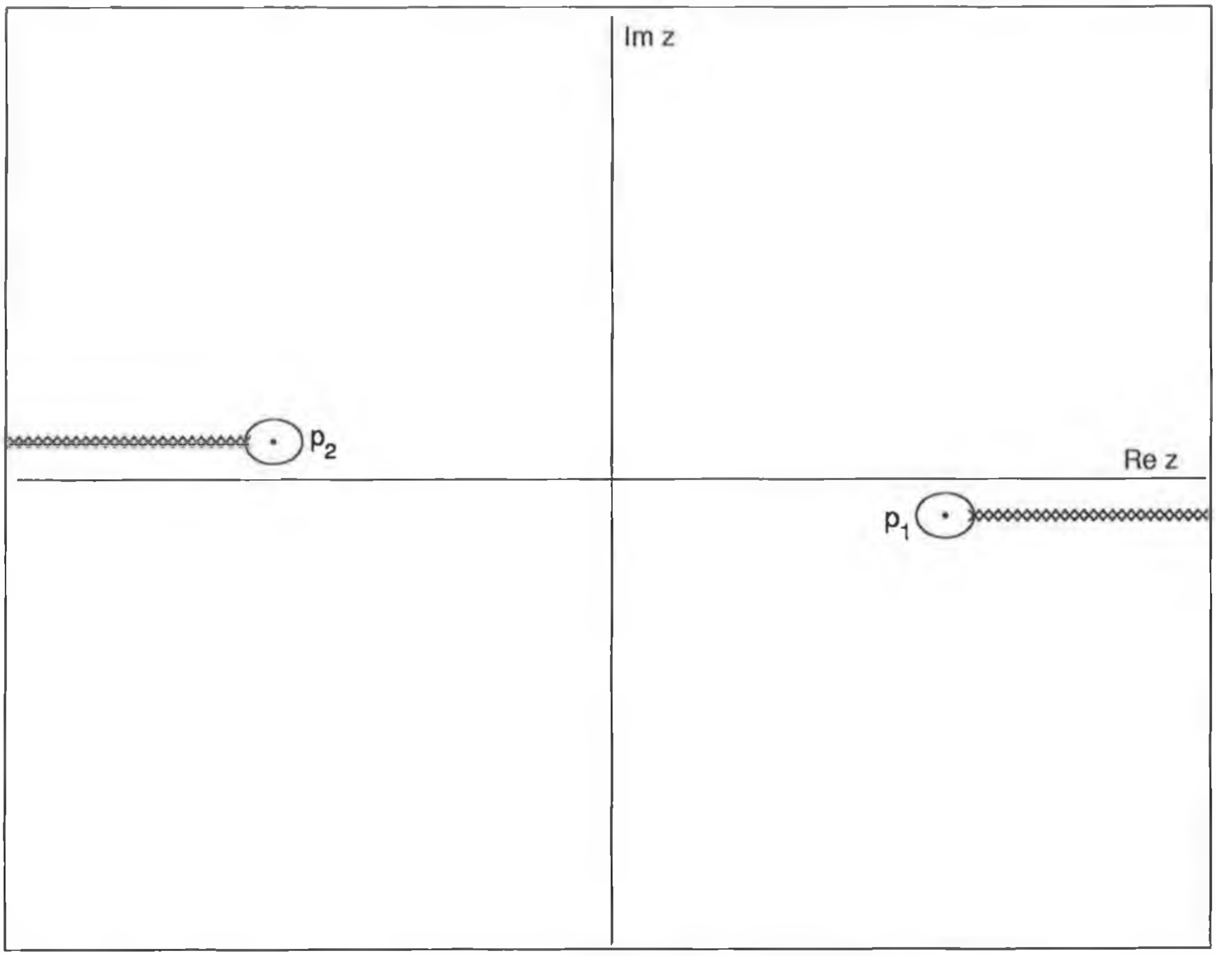

Figure 3.1: Δ with branch cuts

In order to draw the level curves of $\varepsilon(z)$ we must approximate λ by $\lambda_0 = 2n + 1$, n odd. For the lowest such value , $\lambda_0 = 3$, the level curves satisfying $\varepsilon(z) =$ constant are drawn in Figures 3.2 to 3.4 each showing a different region of the complex z-plane. The bold lines indicate the level curves $\varepsilon(z) = 1$ which are the boundaries of the domains Δ_j, $(j = 1, 2, 3, 4)$, defined by (3.2.12). The dashed curves indicate other level curves.

In Δ_1 and Δ_3, $\varepsilon(z)$ increases as Re $z \to 0$ while $\varepsilon(z)$ decreases as Im $z \to \infty$ in Δ_2 and Δ_4. The line L_1 is also shown in each case. Note that the vertical and horizontal axes are not necessarily of the same scale in each figure.

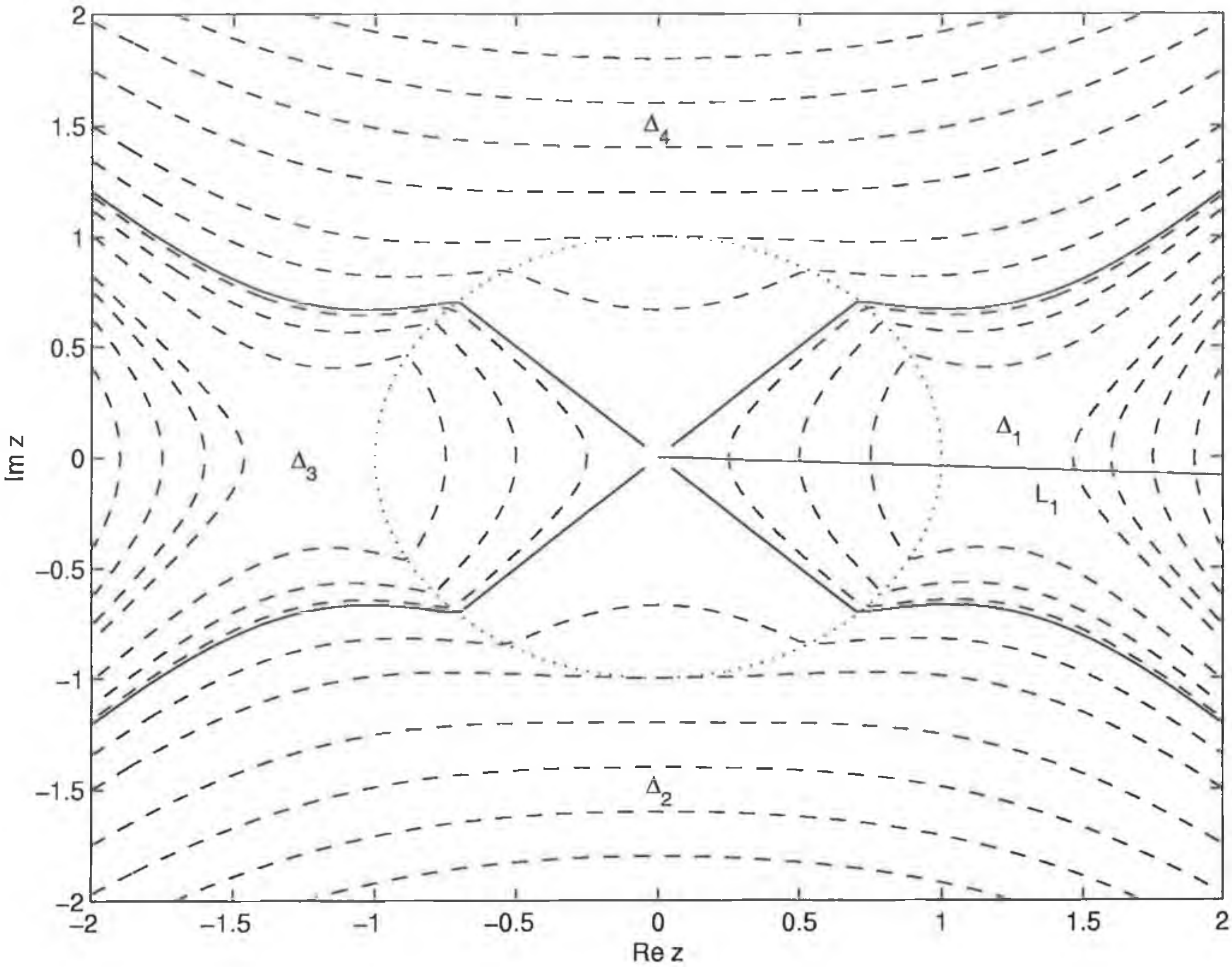

Figure 3.2: Domains Δ_j with level curves $\varepsilon(z) = \text{constant}$ for $\lambda \approx 3$.

Let

$$\alpha_1 = e^{-\iota\pi/24} \tag{3.4.8}$$

be our reference point. In order to apply Theorem 3.2.1 for $j = 1$ to (3.4.1)-(3.4.3) we must find a path in Δ_1 connecting the origin to α_1 along which $\mathrm{Re}\, z^2$ and $\mathrm{Re}\,(z^2 - \lambda \ln|z|)$ are nondecreasing as z passes from the origin to α_1. This is equivalent to a path on which $\varepsilon(z)$ is nondecreasing as z passes from the origin to α_1.

While L_1 would appear an obvious candidate from Figures 3.2 to 3.3, we notice from Figure 3.4 that near the unit circle the level curves become simple closed curves which L_1

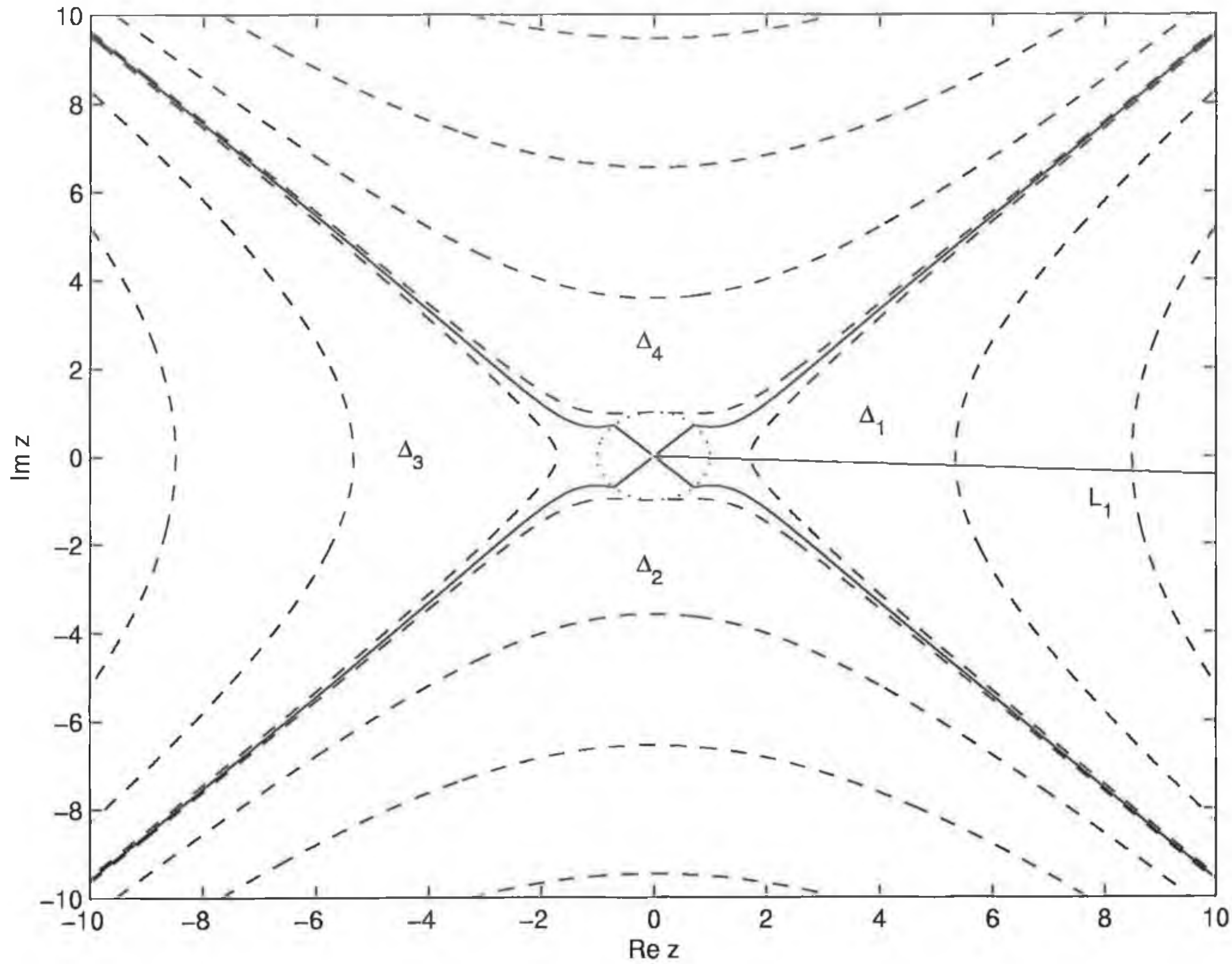

Figure 3.3: Domains Δ_j with level curves $\varepsilon(z) = $ constant for $\lambda \approx 3$.

passes through. Thus $\varepsilon(z)$ is not nondecreasing as z moves to α_1 on L_1. Also note that $\varepsilon(z)$ has a saddle point in Δ_1 at

$$z_s = \left(\frac{1}{2}\text{Re }\lambda\right)^{\frac{1}{2}} \tag{3.4.9}$$

See Appendix C for the derivation of this result. With this in mind we introduce the following five curves in Δ_1:

l_1: This curve starts at the origin and is identical to L_1. It terminates inside the unit circle where L_1 intersects with the level curve $\varepsilon(z) = A$ which is not a simple closed curve and intersects L_1 at only one point (A is a positive constant).

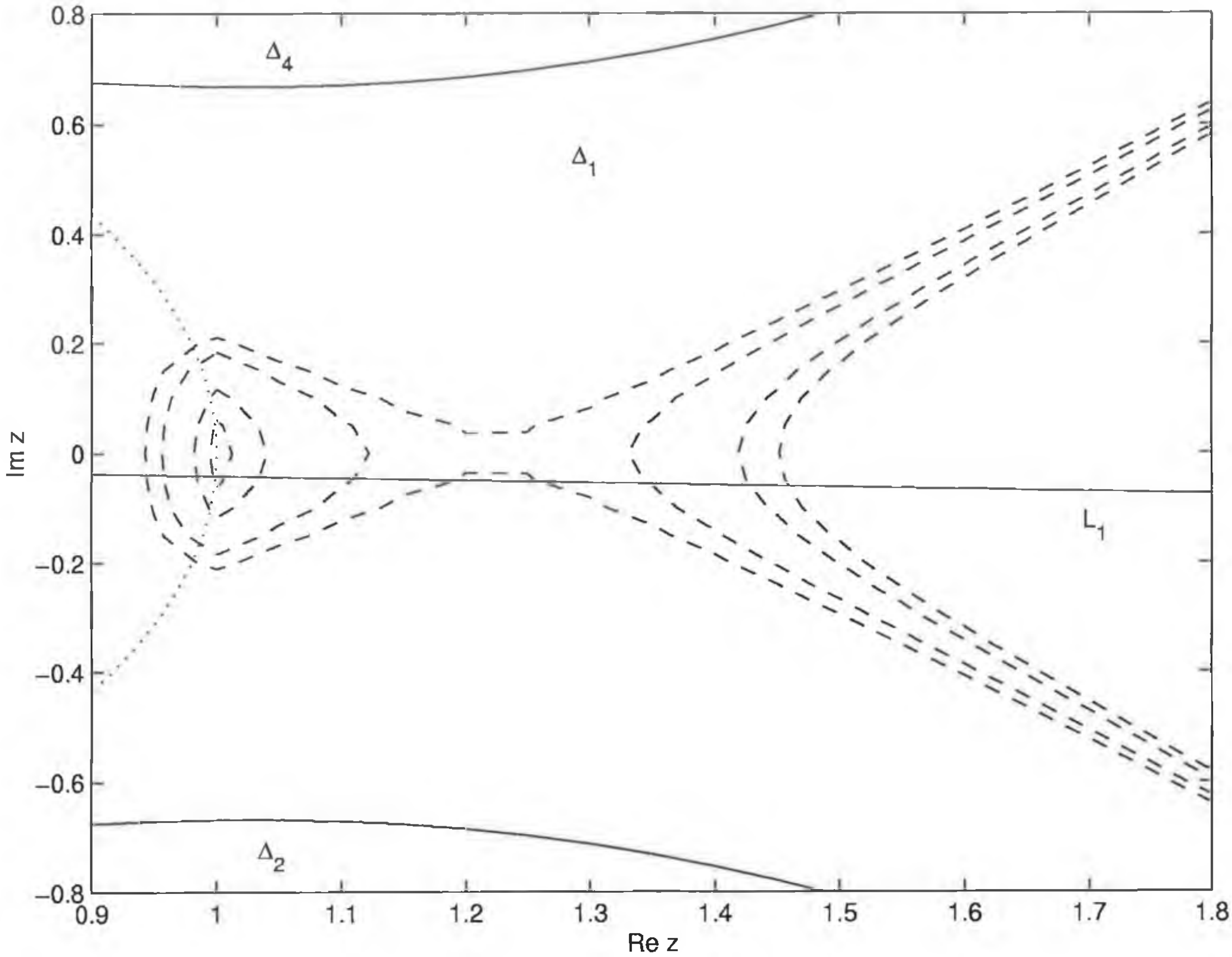

Figure 3.4: Domains Δ_j with level curves $\varepsilon(z)$ = constant for $\lambda \approx 3$.

$\underline{l_2}$: l_2 starts at the point where l_1 ends and is identical to the level curve $\varepsilon(z) = A$. It ends when this curve intersects with the unit circle.

$\underline{l_3}$: This curve starts where l_2 ends and is identical to the level curve $\varepsilon(z) = A$ outside the unit circle. It terminates at some finite point $\bar{z}$ such that $|\bar{z}| > |z_s|/(\cos(\pi/12))^{1/2}$.[1]

$\underline{l_4}$: This is a straight line, along which Re z remains constant, starting at $\bar{z}$ and ending at a point $\hat{z} \in L_1$ (Im $\bar{z} <$ Im $\hat{z}$). Obviously $\hat{z}$ depends on the choice of $\bar{z}$.

$\underline{l_5}$: l_5 starts at $\hat{z}$ and is identical to L_1 as they both go to ∞.

[1]This is required to show $\varepsilon(z)$ is nondecreasing on l_4 (see Appendix B).

We then let

$$L_1^\star = l_1 + l_2 + l_3 + l_4 + l_5. \tag{3.4.10}$$

As we are constructing a solution in terms of the approximant $\nu_1(\lambda, z)$, from (3.2.16) we define its weight function by

$$\varepsilon_1(z) = \begin{cases} \varepsilon(z) & z \in \Delta_1 \cup \Delta_2 \cup \Delta_4, \\ \varepsilon^{-1}(z) & z \in \Delta_3, \end{cases} \tag{3.4.11}$$

To see if we can apply Theorem 3.2.1 to (3.4.1) for $z \in L_1^\star$, we must show that $L_1^\star$ is a finite chain of R_2 arcs and as z travels along $L_1^\star$ to α_1 Re z^2 and Re$(-\lambda + \ln|z|)$ are nondecreasing for $|z| \leq 1$ and $|z| > 1$ respectively. In Appendix C we show that both of these conditions are satisfied.

Therefore, for $\lambda_0 = 3$, Theorem 3.2.1 gives the following solution for (3.4.1)

$$W_1(z, \lambda, \hbar) = \nu_1(\lambda, z) + \epsilon_1(z, \lambda, \hbar) \tag{3.4.12}$$

where

$$\nu_1(\lambda, z) = e^{(1-\lambda)/4} U\left(-\frac{\lambda}{2}, \sqrt{2}z\right). \tag{3.4.13}$$

We also have the following bound on $\epsilon_1(z, \lambda, \hbar)$ when $z \in L_1^\star$,

$$\frac{|\epsilon_1(z, \lambda, \hbar)|}{M_3(z)} \leq \frac{\kappa}{\kappa_0} \varepsilon_1^{-1}(z) \left[\exp\left\{\frac{\kappa_0}{2} \int_{\alpha_1}^{z} \frac{|\psi(t, \lambda, \hbar)\, dt|}{1 + |t|}\right\} - 1\right] \tag{3.4.14}$$

where $M_3(z)$, κ_0 are κ are given by (3.2.18), (3.2.20) and (3.2.21) respectively.

In Figures 3.5 and 3.6, the Δ_j domains for $\lambda \approx 7$ and $\lambda \approx 11$ are drawn. It can be seen that in both these cases it is impossible to find a path on connecting the origin to α_1 on which $\varepsilon(z)$ is monotonic increasing or decreasing. Thus Theorem 3.2.1 employed above can no longer be applied for $\lambda_0 \geq 7$. While it is possible that the proof of the theorem could be modified so the monotonicity condition is relaxed, that is beyond the scope of this thesis.

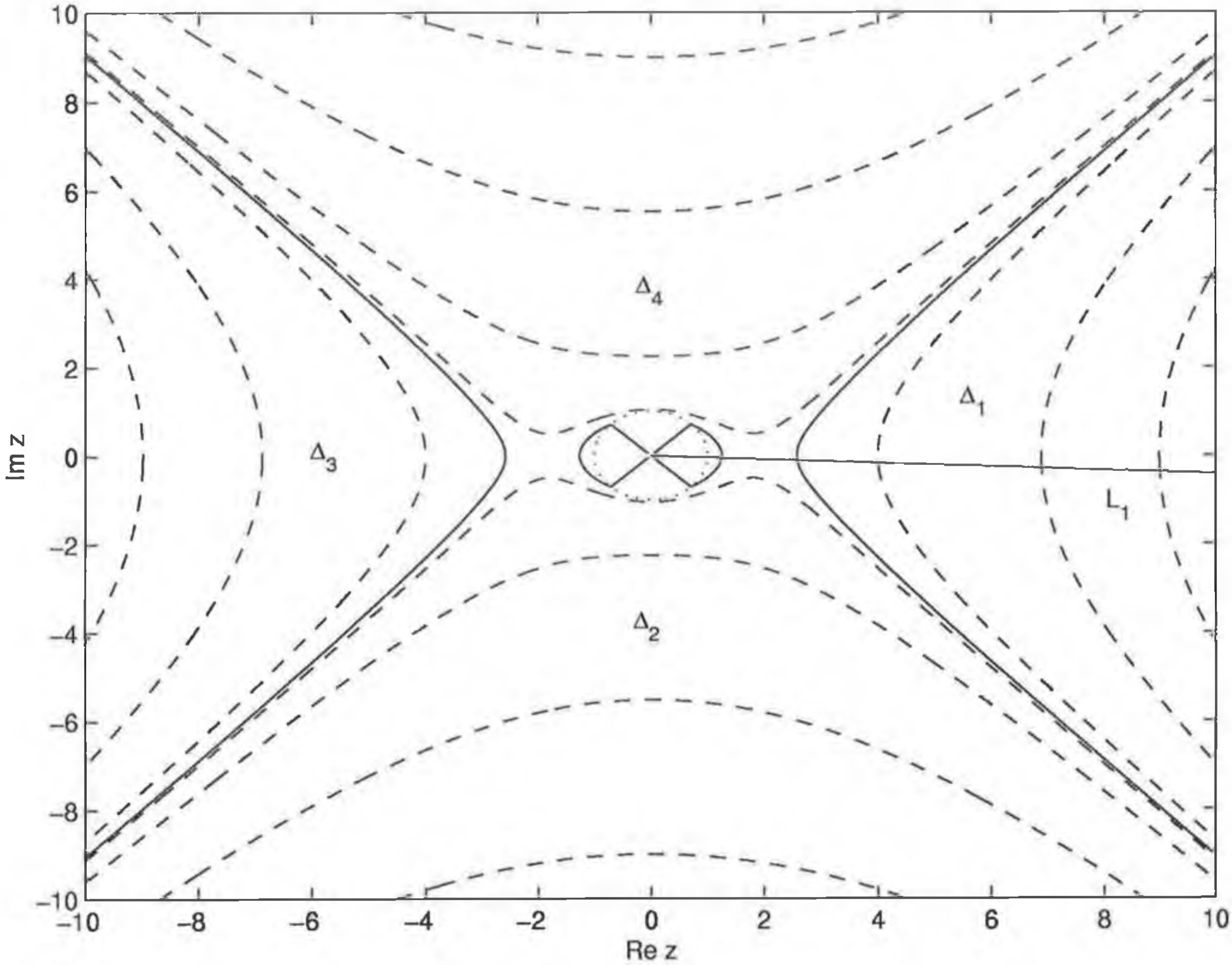

Figure 3.5: Domains Δ_j with level curves $\varepsilon(z) =$ constant for $\lambda \approx 7$.

3.5 Further analysis of the error bound

In this section we examine the bound given by (3.4.14) at the point $z = 0$ when $\hbar \to 0$.

From (3.4.14) we have

$$\epsilon_1(0, \lambda, \hbar) \leq \frac{\kappa}{\kappa_0} \frac{M_3(0)}{\varepsilon_1(0)} \left[\exp\left\{ \frac{\kappa_0}{2} \int_{\alpha_1}^{0} \frac{|\psi(t, \lambda, \hbar)\, dt|}{1 + |t|} \right\} - 1 \right]. \tag{3.5.1}$$

From (3.4.11) and (3.2.19) respectively, we see that at $z = 0$

$$\varepsilon_j(0) = 1 \quad (j = 1, 2, 3, 4) \tag{3.5.2}$$

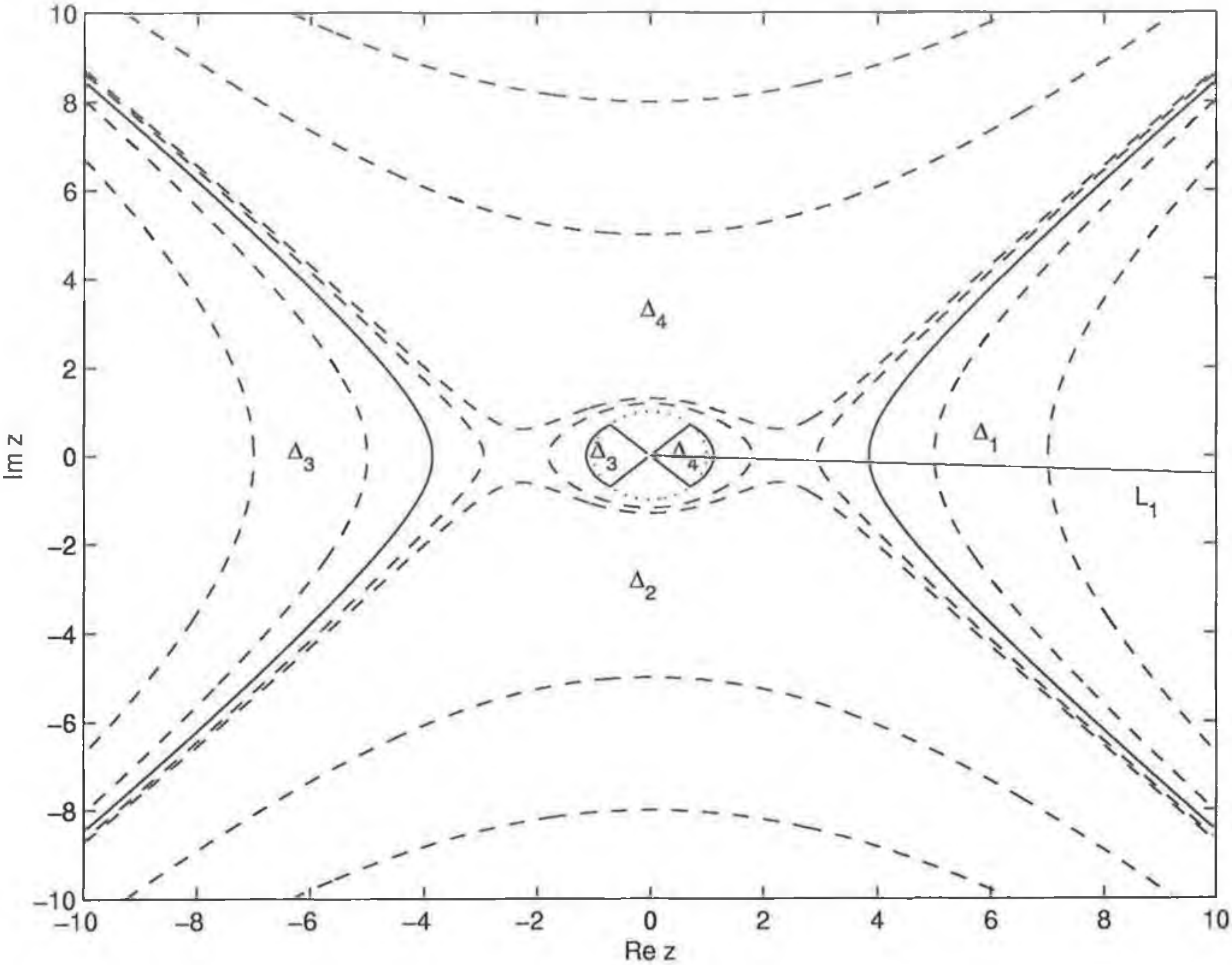

Figure 3.6: Domains Δ_j with level curves $\varepsilon(z)$ = constant for $\lambda \approx 11$.

and

$$M_3(\lambda, 0) = \mathcal{O}(1). \tag{3.5.3}$$

Therefore, as κ and κ_0 are constants

$$\frac{\kappa}{\kappa_0}\frac{M_3(\lambda, 0)}{\varepsilon_1(0)} \leq A \tag{3.5.4}$$

for some positive constant[2] A.

[2] A is an absolute constant which need not have the same value each time it appears.

We now consider the integral in (3.4.14) for small $\hbar$ on the path L_1^*. We let

$$\int_0^{e^{-\iota\pi/24}\infty} \frac{|\psi(t,\lambda,\hbar)\,dt|}{1+|t|} = \int_{l_1+l_2+l_3+l_4} \frac{|\psi(t,\lambda,\hbar)\,dt|}{1+|t|} + \int_{l_5} \frac{|\psi(t,\lambda,\hbar)\,dt|}{1+|t|} \tag{3.5.5}$$

where the l_s are all defined in Section 3.4. We look at each of these integrals in turn.

On $l_2 + l_2 + l_3 + l_4$, $|z|$ is bounded. If we let $z = x + \iota y$ then

$$|x| < A, |y| < B, \quad x + \iota y \in l_2 + l_2 + l_3 + l_4 \tag{3.5.6}$$

where B is also a positive constant. Using the well-known inequality $|z_1 + z_2| \geq ||z_1| - |z_2||$ we see that

$$\frac{|\psi(z,\lambda,\hbar)|}{1+|z|} = \frac{1}{|z^2-\lambda-\frac{1}{\hbar}||1+|z||} \leq \frac{1}{|z^2-\lambda-\frac{1}{\hbar}|} \tag{3.5.7}$$

$$= \frac{\hbar}{|1+(\lambda\hbar-\hbar z^2)|} \leq \frac{\hbar}{|1-|\lambda\hbar-\hbar z^2||} \tag{3.5.8}$$

and

$$|\lambda\hbar - \hbar z^2| \leq ||\lambda| + |z^2||\hbar \leq |\lambda + A^2 + B^2|\hbar. \tag{3.5.9}$$

Recall that we know $\lambda \to \lambda_0$ as $\hbar \to 0$. Thus let $\hbar_1$ be the largest $\hbar$ such that $|\lambda| \leq 3\lambda_0/2$, i.e.

$$|\lambda\hbar - \hbar z^2| \leq \left(\frac{3}{2}\lambda_0 + A^2 + B^2\right)\hbar \tag{3.5.10}$$

when $\hbar \leq \hbar_1$. Next let

$$\hbar_0 = \min\left\{\hbar_1, \frac{1}{2\left(\frac{3}{2}\lambda_0 + A^2 + B^2\right)}\right\}. \tag{3.5.11}$$

Therefore for $\hbar \leq \hbar_0$ we have

$$|\lambda\hbar - \hbar z^2| \leq \frac{1}{2} \tag{3.5.12}$$

and

$$\frac{|\psi(z,\lambda,\hbar)|}{1+|z|} \leq 2\hbar. \tag{3.5.13}$$

So

$$\int_{l_1+l_2+l_3+l_4} \frac{|\psi(t,\lambda,\hbar)\,dt|}{1+|t|} \leq 2\hbar \int_{l_2+l_2+l_3+l_4} |dt|, \quad \hbar \leq \hbar_0 \tag{3.5.14}$$

or

$$\int_{l_1+l_2+l_3+l_4} \frac{|\psi(t,\lambda,\hbar)\,dt|}{1+|t|} = \mathcal{O}(\hbar), \quad (\hbar \to 0). \tag{3.5.15}$$

Along l_5, $z(\tau) = e^{-\iota\pi/24}\tau$ so

$$\int_{l_5} \frac{|\psi(t,\lambda,\hbar)\,dt|}{1+|t|} = \int_{\bar{\tau}}^{\infty} \frac{d\tau}{|e^{-\iota\pi/12}\tau^2 - (\lambda+\hbar^{-1})|(1+|\tau|)} \tag{3.5.16}$$

where $\bar{z} = e^{-\iota\pi/24}\bar{\tau}$. Letting $b = e^{-\iota\pi/24}\sqrt{\lambda+\hbar^{-1}}$ yields

$$\int_{l_5} \frac{|\psi(t,\lambda,\hbar)\,dt|}{1+|t|} = \int_{\bar{\tau}}^{\infty} \frac{d\tau}{|\tau^2-b^2|(1+|\tau|)} \leq \int_0^{\infty} \frac{d\tau}{|\tau^2-b^2|(1+|\tau|)} \tag{3.5.17}$$

$$= \int_0^{\frac{|b|}{2}} \frac{d\tau}{|\tau^2-b^2|(1+|\tau|)} + \int_{\frac{|b|}{2}}^{\infty} \frac{d\tau}{|\tau^2-b^2|(1+|\tau|)}. \tag{3.5.18}$$

As $|\tau^2 - b^2| \geq ||\tau|^2 - |b|^2| \geq |b|^2/2$ on $[0, |b|/2]$

$$\int_0^{\frac{|b|}{2}} \frac{d\tau}{|\tau^2-b^2|(1+|\tau|)} \leq \frac{2}{|b|^2}\int_0^{\frac{|b|}{2}} \frac{d\tau}{1+\tau} = \frac{2}{|b|^2}\ln\left(1+\frac{|b|}{2}\right) \tag{3.5.19}$$

$$= \frac{2\hbar}{|\lambda\hbar+1|}\ln\left(1+\frac{|\sqrt{|\lambda\hbar+1|}|}{2\sqrt{\hbar}}\right). \tag{3.5.20}$$

Letting $x = \tau/|b|$ in the second integral in (3.5.18) gives

$$\int_{\frac{|b|}{2}}^{\infty} \frac{d\tau}{|\tau^2-b^2|(1+|\tau|)} = \frac{1}{|b|}\int_{\frac{1}{2}}^{\infty} \frac{dx}{\left|x^2-\frac{b^2}{|b|^2}\right|(1+|b|x)}. \tag{3.5.21}$$

As $1+|b|x \geq |b|/2$ on $[1/2, \infty)$

$$\int_{\frac{|b|}{2}}^{\infty} \frac{d\tau}{|\tau^2-b^2|(1+|\tau|)} \leq \frac{2}{|b|^2}\int_{\frac{1}{2}}^{\infty} \frac{dx}{\left|x^2-\frac{b^2}{|b|^2}\right|} \tag{3.5.22}$$

$$= \frac{2\hbar}{|\lambda\hbar+1|}\int_{\frac{1}{2}}^{\infty} \frac{dx}{|x^2-e^{-\iota\pi/12}|} + o(1), \quad (\hbar \to 0) \tag{3.5.23}$$

where we have used the Lebesgue dominated convergence theorem.

Combining (3.5.20) and (3.5.23) we see from (3.5.18) that

$$\int_{l_5} \frac{|\psi(t,\lambda,\hbar)\,dt|}{1+|t|} = \mathcal{O}(\hbar\ln(\hbar^{1/2})), \quad (\hbar \to 0). \tag{3.5.24}$$

Thus from (3.5.15) and (3.5.24)

$$\int_0^{\alpha_1} \frac{|\psi(t,\lambda,\hbar)\,dt|}{1+|t|} = \mathcal{O}(\hbar \ln(\hbar^{1/2})), \quad (\hbar \to 0) \tag{3.5.25}$$

or

$$\left| \int_{\alpha_1}^0 \frac{|\psi(t,\lambda,\hbar)\,dt|}{1+|t|} \right| \leq A|\hbar \ln(\hbar^{1/2})|, \quad (\hbar \to 0). \tag{3.5.26}$$

Combining (3.5.1) with (3.5.4) and (3.5.26) gives

$$\epsilon_1(0,\lambda,\hbar) \leq A(e^{A\hbar \ln(\hbar^{1/2})} - 1), \quad (\hbar \to 0). \tag{3.5.27}$$

Expanding the exponential in (3.5.27) gives

$$e^{A\hbar \ln(\hbar^{1/2})} - 1 = \sum_{s=0}^{\infty} \left(\frac{A^s}{s!}\right) (\hbar \ln(\hbar^{1/2}))^s - 1 = \mathcal{O}(\hbar \ln(\hbar^{1/2})), \quad (\hbar \to 0) \tag{3.5.28}$$

which, taken with (3.5.27), implies

$$|\epsilon_1(0,\lambda,\hbar)| \leq A|\hbar \ln(\hbar^{1/2})|, \quad (\hbar \to 0). \tag{3.5.29}$$

3.6 Behaviour of λ as $\hbar \to 0$

We now compute a bound on λ for small $\hbar$. From (3.4.1) and (3.4.2) we see

$$\nu_1(\lambda, 0) + \epsilon_1(0,\lambda,\hbar) = 0. \tag{3.6.1}$$

We expand $\nu_1(\lambda, 0)$ as a Taylor series about $\lambda = \lambda_0$ to get

$$\nu_1(\lambda, 0) = \sum_{s=0}^{\infty} \frac{\nu_1^s(\lambda, 0)}{s!}(\lambda - \lambda_0)^s \tag{3.6.2}$$

which has an infinite radius of convergence as $\nu_1(\lambda, 0)$ is analytic for all λ (see (A.0.6)). As $\nu_1(\lambda_0, 0) = 0$ (see Section 3.3) (3.6.1) becomes

$$\nu_1'(\lambda_0, 0)(\lambda - \lambda_0) + f(\lambda) = -\epsilon_1(0,\lambda,\hbar) \tag{3.6.3}$$

where

$$f(\lambda) = \sum_{s=2}^{\infty} \frac{\nu_1^s(\lambda, 0)}{s!}(\lambda - \lambda_0)^s \tag{3.6.4}$$

Taking the modulus of both sides of (3.6.3) yields

$$|\lambda - \lambda_0||\nu_1'(\lambda_0, 0) + f(\lambda)| = |\epsilon_1(0, \lambda, \hbar)| \tag{3.6.5}$$

or

$$|\lambda - \lambda_0| = \frac{|\epsilon_1(0, \lambda, \hbar)|}{|\nu_1'(\lambda_0, 0) + f(\lambda)|}. \tag{3.6.6}$$

Since $\lambda \to \lambda_0$ as $\hbar \to 0$, for all $C_1 > 0$ there exists $\hbar_{C_1} > 0$ such that for all $\hbar < \hbar_{C_1}$, $|\lambda - \lambda_0| < C_1$. This is turn means that for all $C_2 > 0$ there exists $\hbar_{C_2} > 0$ such for all $\hbar < \hbar_{C_2}$, $|f(\lambda)| < C_2$. Choosing $C_2 = \frac{1}{2}|\nu_1'(\lambda_0, 0)|$ means

$$\begin{aligned} |\nu_1'(\lambda_0, 0) + f(\lambda)| &\geq ||\nu_1'(\lambda_0, 0)| - |f(\lambda)|| \qquad (3.6.7) \\ &\geq \frac{1}{2}|\nu_1'(\lambda_0, 0)|. \qquad (3.6.8) \end{aligned}$$

From (3.6.6) and (3.6.8) we have

$$|\lambda - \lambda_0| \leq \frac{|\epsilon_1(0, \lambda, \hbar)|}{\frac{1}{2}|\nu_1'(\lambda_0, 0)|}, \quad \hbar < \hbar_{C_2}. \tag{3.6.9}$$

As $\nu_1'(\lambda_0, 0) \neq 0$ (see (A.0.7)) combining (3.6.9) with (3.5.29) gives

$$|\lambda - \lambda_0| \leq A|\hbar \ln(\hbar^{1/2})|, \quad (\hbar \to 0) \tag{3.6.10}$$

or

$$\lambda - \lambda_0 = \mathcal{O}(\hbar \ln(\hbar^{1/2})), \quad (\hbar \to 0). \tag{3.6.11}$$

Recall we chose $\theta = \iota\pi/24$ in Section 3.1 and the derivation of 3.6.11 followed from this. However, this result will hold for all $0 < \theta < \pi/4$ although the choice of paths $l_s, (s = 1, 2, 3, 4, 5)$, would have to be different when θ is close to $-\arg p_1$ because of the branch cut emanating from this point. Alternatively the direction of the branch cut could be changed.

Note that we have proved this result only for the lowest unperturbed eigenvalue λ_0. As noted in Section 3.4 the result for higher eigenvalues is more complicated.

Chapter 4

Other strategies considered

4.1 Matched Asymptotics

The change of variable made in Section 3.1 to take (3.1.7) and (3.1.8) to (3.1.9) was made specifically to give an equation in this form in order to apply the results of [6]. However this was not the only option considered. Below we describe other formulations of the problem we worked with and their shortcomings.

Initially we tried using matched asymptotics which was successfully employed in [10] to find the exponentially small imaginary part of the eigenvalue in a simpler problem. A very readable introduction to this method can be found in [3, Ch. 10]. By letting $z = e^{-\theta}x$ and $\phi(z) = \Phi_2(e^{\theta}z) \in \mathcal{H}^2(e^{-\theta}\mathbb{R})$ in (3.1.7) and (3.1.8), the problem can be written as

$$-\hbar^2\frac{d^2\phi}{dz^2} + f(z)\phi = 0, \tag{4.1.1}$$

where

$$f(z) = \frac{(z^2 - z_1^2)(z^2 - z_2^2)}{(z^2 - z_p^2)} \tag{4.1.2}$$

and

$$\phi(0) = 0, \quad \phi(z) \to 0 \quad (z \to \infty e^{-\theta}). \tag{4.1.3}$$

The zeros of $f(z)$, known as turning points $\pm z_1$ and $\pm z_2$ are given by

$$z_1 = \sqrt{\frac{1}{2} + E - \frac{1}{2}\sqrt{1+4\hbar^2}}, \quad z_2 = \sqrt{\frac{1}{2} + E + \frac{1}{2}\sqrt{1+4\hbar^2}} \tag{4.1.4}$$

and the poles $\pm z_p$ by

$$z_p = \sqrt{1+E}. \tag{4.1.5}$$

Because $\lambda \to \lambda_0$ as $\hbar \to 0$ and $E = \lambda\hbar$, it follows that $E \to 0$ as $\hbar \to 0$. Therefore $z_1, z_p \to 1$ as $\hbar \to 0$.

We divide the half-plane Re $z > 0$ into five sections as shown in Figure 4.1. The L-G approximation (see Appendix D) which is valid in region I and satisfies the boundary condition at infinity is

$$\phi_I(z) = Af^{-1/4}(z)\exp\left[-\frac{1}{\hbar}F(z)\right] \tag{4.1.6}$$

where

$$F(z) = \int_{z_0}^{z} \sqrt{f(t)}\,dt \tag{4.1.7}$$

for some fixed point z_0 which we will pick later. This of course breaks down in the region II containing the pole p and the turning point z_2, but close to these points, by setting $\xi = z - p$, we see that the approximate equation is the Whittaker equation whose small solution (in the sector containing $\infty e^{-\theta}$) is $W_{k,\frac{1}{2}}(\xi)$, which may be matched [1] to the L-G solutions in the overlap between regions I and II.

Taking into account the changes in the solution given by the Whittaker function as we cross the Stokes line emanating from the turning point at z_2, we then match it to the L-G solution valid in region III, which is away from the turning points z_1 and z_2. Near the simple turning point at z_1, our first attempt was to approximate the solution by the Airy function. But since $\pm z_1 \to 0$ as $\hbar \to 0$ we are in the situation of coalescing turning points, for which a suitable model is the parabolic cylinder function. It is plausible on physical grounds that the turning point at $-z_1$ will also have an influence on the solution at zero. The L-G solution in region III was matched to a parabolic cylinder function in the overlap region between regions III and IV. Due account of Stokes phenomenon was again taken as we went around z_1 and finally a combination of two parabolic cylinder functions was

[1] By matching we mean selecting the solution in II which has the same functional form as the solution in I in the overlap

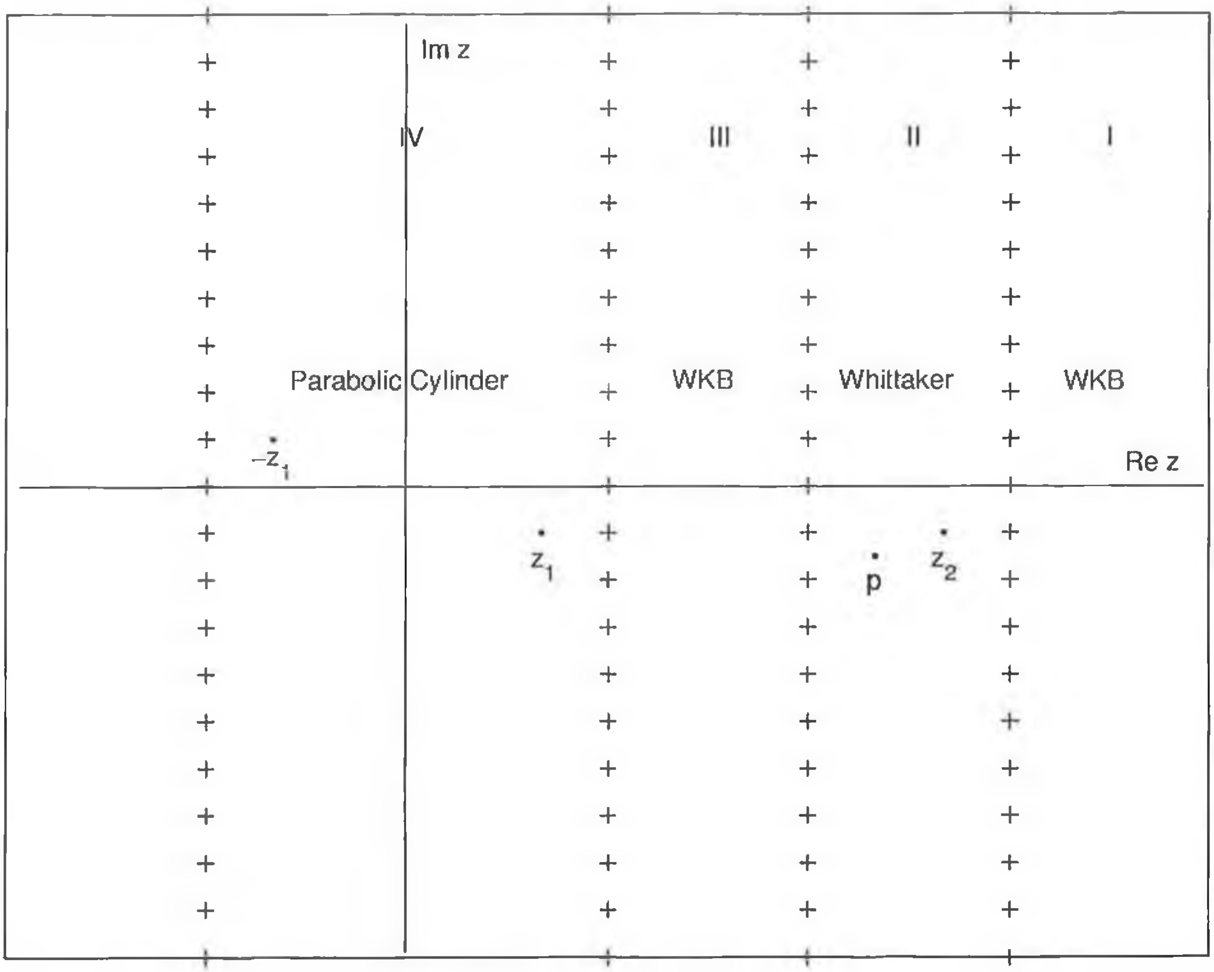

Figure 4.1: Regions for solution to (4.1.1)

substituted into the boundary condition at $z = 0$. This gave us an implicit eigenvalue relation which unfortunately failed to yield an estimate for the imaginary part of E.

We then decided to apply the more rigorous method of Olver which give error bounds and regions of validity. By making the following change of variable $z = e^{-\theta/2}p$, where now $\theta = -\iota \arg E$, (3.1.7) and (3.1.8) are taken to

$$\frac{d^2w}{dz^2} = (\mu^4 f(z, \lambda) + g(z, \lambda, \theta))w \tag{4.1.8}$$

where $w(z) = \Phi_2(e^{-\theta/2}z)$, $\mu = \hbar^{-1/2}e^{-\theta/2}$ and $\lambda = |E|$. The functions f and g are given by

$$f(z,\lambda) = z^2 - \lambda, \quad g(z,\lambda,\theta) = \frac{-1}{z^2 - e^{\theta} - \lambda}. \tag{4.1.9}$$

Also f has two turning points on the real axis at

$$z_{1,2} = \pm\sqrt{\lambda} \tag{4.1.10}$$

and g has two poles at

$$p_{1,2} = \pm\sqrt{\lambda + e^{-\theta}}. \tag{4.1.11}$$

Next, using the methods of [11], we attempted to construct a L-G asymptotic approximation , complete with an error bound, to the solution of (4.1.8) which is subject to

$$w(0) = 0, \quad w(z) \to 0, \quad (z \to \infty e^{-\theta/2}). \tag{4.1.12}$$

However any L-G approximation will not be valid at the turning points $z = z_{1,2}$. This leads to difficulty in showing that a L-G expansion satisfying the second condition of (4.1.12) is valid at the origin. We considered following the method of [7] to derive an approximation, which is valid in a neighbourhood of the turning points, for a solution to (4.1.8) which is originally defined by a L-G solution satisfying the condition at infinity. This would involve applying the theory of [6], but as we have seen in Chapter 3, direct application of these results, without the use of L-G approximations, yield our results.

A further attempt at asymptotic matching is currently being made by rewriting (3.4.1) as

$$-\frac{d^2w}{dz^2} + \left(\frac{(z^2-\lambda)(z^2-\lambda-\hbar^{-1})}{(z^2-\lambda-\hbar^{-1})}\right) w = 0 \tag{4.1.13}$$

with boundary conditions as in Section 3.4. This equation has a simple poles at $\pm p$, where

$$p = \sqrt{\lambda + \frac{1}{\hbar}} \tag{4.1.14}$$

and turning points at $\pm z_1, \pm z_2$ where

$$z_1 = \sqrt{\lambda - \hbar + \mathcal{O}(\hbar^3)}, \quad (\hbar \to 0) \tag{4.1.15}$$

$$z_1 = \sqrt{\lambda - \frac{1}{\hbar} + \mathcal{O}(\hbar)} \quad (\hbar \to 0). \tag{4.1.16}$$

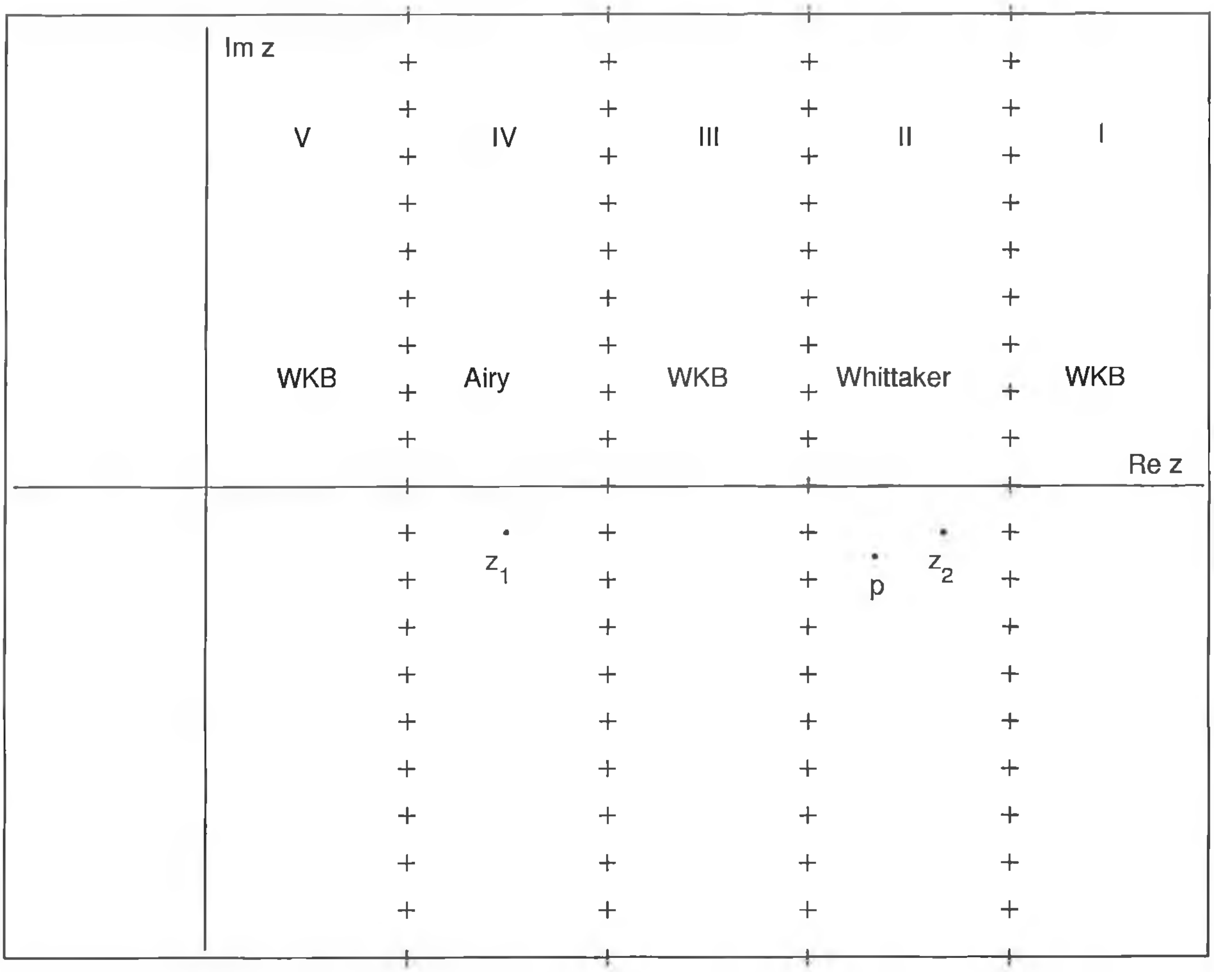

Figure 4.2: Regions for solution to (4.1.13)

This formulation has the advantage that the turning points nearer the origin remain fixed at a distance $\mathcal{O}(1)$ from the origin, while the pole p and its associated turning point z_2 tend to $+\infty$ as $\hbar \to 0$. This means that there is no contribution as $z \to 0+$ from the turning point at $-z_1$.

This time the half-plane Re $z > 0$ is divided into five sections as shown in 4.2. The same strategy of L-G/Whittaker/L-G matching is followed in regions I/II/III, but now we match to the simpler Airy function in the region IV about the isolated simple turning point z_1. The final matching will be to L-G approximation valid in the region V containing the origin.

4.2 Perturbed Operators

By applying the perturbation theory for operators described in [8] to the operator H_θ

$$E = \sum_{m=0}^{\infty} E_{2m}(\hbar) \tag{4.2.1}$$

where $E_0 = 2n + 1$, $n \in \mathbb{N}$ as before, Duclos has shown that

$$e_2 = \mathcal{O}(\hbar), \quad e_4 = \mathcal{O}(\hbar^2), \quad (\hbar \to 0). \tag{4.2.2}$$

While this result is an improvement on that obtained in Chapter 3, this method employed give no information on the eigenfunction. The methods in Chapter 3 have the advantage of also giving an approximation to the transformed eigenfunction for small $\hbar$.

4.3 Extending the results of Chapter 3

In [6] the results which are summarised in Chapter 3 are extended to give solutions in terms of a power series of n terms times a parabolic cylinder function plus an error term. Again a bound is supplied for the error term in certain region of the complex domain. Such a solution exists for any nonnegative integer n, $n = 0$ giving (3.2.9).

The work in this thesis can be extended by applying this result for $n \geq 1$ to (3.4.1). It may then be possible to obtain term by term an asymptotic series representation for λ as $\hbar \to 0$. This result would be an improvement on that of Duclos given in the previous section.

Appendix A

The parabolic cylinder function $U(a,x)$

In Chapter 3 we introduced the parabolic cylinder function $U(a,x)$. From [1, Ch. 19] we see this is a standard solution to the parabolic cylinder equation

$$\frac{d^2y}{dx^2} = \left(\frac{1}{4}x^2 + a\right)y \tag{A.0.1}$$

which is given by

$$U(a,x) = 2^{-\frac{1}{4}-\frac{a}{2}}e^{-\frac{x^2}{4}}\mathrm{U}\left(\frac{a}{2}+\frac{1}{4}, \frac{1}{2}, \frac{1}{2}x^2\right) \tag{A.0.2}$$

where $\mathrm{U}(a,b,x)$ is the hypergeometric function, a solution to Kummer's equation

$$x\frac{d^2w}{dx^2} + (b-x)\frac{dw}{dx} - aw = 0. \tag{A.0.3}$$

The hypergeometric function $\mathrm{U}(a,b,x)$ is defined by

$$\mathrm{U}(a,c,x) = \frac{1}{\Gamma(a)}\int_0^\infty t^{a-1}(1+t)^{c-a-1}e^{-xt}\,dt \quad (|\arg(x)| < \frac{1}{2}\pi,\ \Re e(a) > 0)) \tag{A.0.4}$$

and by analytic continuation elsewhere. We can also describe $U(a,x)$ in terms of the Hermite polynomials:

$$U(a,x) = e^{-\frac{x^2}{4}}H_{-a-1/2}(x). \tag{A.0.5}$$

In addition we note that $U(a,x)$ and its derivative $U'(a,x)$ have the following values when $x = 0$

$$U(a,0) = \frac{\sqrt{\pi}}{2^{\frac{1}{2}a+\frac{1}{4}}\Gamma(\frac{3}{4}+\frac{1}{2}a)}, \tag{A.0.6}$$

$$U'(a,0) = -\frac{\sqrt{\pi}}{2^{\frac{1}{2}a-\frac{1}{4}}\Gamma(\frac{1}{4}+\frac{1}{2}a)}. \tag{A.0.7}$$

Appendix B

The path $L_1^\star$

B.1 Showing $l_s (s = 1, 2, 3, 4, 5)$ are R_2 arcs

Recall that in Chapter 3 we defined an arc with parametric equation $z = z(\tau)$ to be an R_2 arc if $z''(\tau)$ is continuous and $z'(\tau)$ does not vanish. For each l_s, except l_3, we parameterise the curve and show that it satisfies these conditions. We deal with l_3 differently.

l_1, l_5: As both l_1 and l_5 lie on L_1 we deal with them together. From their respective definitions in Section 3.4 we see

$$l_1 : z(\tau) = \tau e^{-\iota\pi/24}, \quad 0 \leq \tau \leq \tau_1 \tag{B.1.1}$$

where $z(\tau_1)$ lies on the level curve on which we choose to terminate l_1 and

$$l_5 : z(\tau) = \tau e^{-\iota\pi/24}, \quad \hat{\tau} \leq \tau \leq \infty \tag{B.1.2}$$

where $z(\hat{\tau}) = \hat{z}$. From these representations we see that l_1 and l_5 are R_2 arcs as both necessary conditions are satisfied.

l_2: As l_2 is a level curve of $\varepsilon(z)$ and $|z| < 1$ on l_2

$$\varepsilon(z) = |e^{z^2/2}| = A, \quad z \in l_2. \tag{B.1.3}$$

Writing $z = x + \iota y$ gives

$$\varepsilon(z) = e^{\frac{1}{2}(x^2 - y^2)} = A, \quad z \in l_2. \tag{B.1.4}$$

Taking the natural logarithm of both sides gives upon rearranging

$$\frac{x^2}{2 \ln A} - \frac{y^2}{2 \ln A} = 1, \quad z \in l_2 \tag{B.1.5}$$

which is the equation of a hyperbola. Thus l_2 can be parameterised by

$$l_2 : z(\tau) = (2 \ln A)^{1/2} \sec \tau + \iota (2 \ln A)^{1/2} \tan \tau, \quad \tau_2 \leq \tau \leq \tau_3 \tag{B.1.6}$$

where $-\pi/2 < \tau_2, \tau_3 < 0$, $z(\tau_2) \in L_1$ and $z(\tau_3) = 1$. Therefore

$$z'(\tau) = (2\ln A)(\sec\tau\tan\tau + \iota\sec^2\tau) \tag{B.1.7}$$

and

$$z''(\tau) = (2\ln A)(\sec\tau\tan^2\tau + \sec^3\tau + 2\iota\sec^2\tau\tan\tau) \tag{B.1.8}$$

From (B.1.7) and (B.1.8) we see that for $-\pi/2 < \tau_2, \tau_3 < 0$, l_2 is an R_2 arc as both necessary conditions are satisfied.

l_3: As l_3 is difficult to parameterise we continue as follows. Consider any level curve $\varepsilon(z) = A$ on $\mathbb{C} \setminus B^c(0,1)$ where $B^c(0,1)$ is the closed ball of radius 1 centered on the origin. On $\mathbb{C} \setminus B^c(0,1)$

$$\varepsilon(z) = e^{\frac{1}{2}\mathrm{Re}\,(z^2 - \lambda\ln|z|)} \tag{B.1.9}$$

so

$$\varepsilon(z) = a \Leftrightarrow \mathrm{Re}\,(z^2 - \lambda\ln|z|) = 2\ln A \tag{B.1.10}$$

Upon letting $z = x + \iota y$, this becomes

$$F(x,y) = 0 \tag{B.1.11}$$

where

$$F(x,y) = x^2 - y^2 - \mathrm{Re}\,\lambda\ln\sqrt{x^2+y^2} - 2\ln A \tag{B.1.12}$$

with dom $F = \mathbb{R}^2 \setminus B^c(0,1)$ which is an open subset of $\mathbb{R}^2$. As it can be seen $F(x,y)$ is twice continuously differentiable on $\mathbb{R}^2 \setminus B^c(0,1)$, we apply the form of the implicit function theorem given in [9, Ch. XVII, Thm. 4.6] with $n = p = 2$. If $F_y \neq 0$, where F_y is the partial derivative of F with respect to y, the equation $F(x,y) = 0$ defines y implicitly as a twice continuously differentiable function of x, say $y = g(x)$. This function gives a parameterisation for l_3 with x the parameter and $g''(x)$ is continuous. Thus if $F_y \neq 0$ and

$$g'(x) = \frac{dy}{dx} = -\frac{F_x}{F_y} \neq 0 \tag{B.1.13}$$

l_3 is an R_2 arc. So we must show F has no critical points in $\mathbb{R}^2 \setminus B^c(0,1)$.

$$\frac{\partial F}{\partial x} = 2x - \mathrm{Re}\,\lambda\frac{x}{x^2+y^2}, \quad \frac{\partial F}{\partial y} = -2y - \mathrm{Re}\,\lambda\frac{y}{x^2+y^2} \tag{B.1.14}$$

(x, y) is a critical point of F if and only if $F_x = F_y = 0$ i.e.

$$x\left(2 - \frac{\mathrm{Re}\,\lambda}{x^2+y^2}\right) = 0 \qquad \text{(B.1.15)}$$

$$y\left(-2 - \frac{\mathrm{Re}\,\lambda}{x^2+y^2}\right) = 0. \qquad \text{(B.1.16)}$$

Since $(0,0) \notin \mathrm{dom}\, F$ this system of equations is equivalent to

$$x = 0 \text{ and } y^2 = -\frac{1}{2}\mathrm{Re}\,\lambda \qquad \text{or} \qquad y = 0 \text{ and } x^2 = \frac{1}{2}\mathrm{Re}\,\lambda. \qquad \text{(B.1.17)}$$

The second combination in (B.1.17) give z_s in (3.4.9). Therefore F has critical points if and only if

$$2\ln A = \frac{1}{2}\mathrm{Re}\,\lambda\left(1 - \ln\left|\frac{\mathrm{Re}\,\lambda}{2}\right|\right) \qquad \text{(B.1.18)}$$

Hence we choose A such that (B.1.18) is not satisfied. Then l_3 is an R_2 arc.

$\underline{l_4}$: l_4 is the straight line connecting $\bar{z}$ and $\hat{z}$ which we can parameterise by

$$l_4 : z(\tau) = \tau(\hat{z} - \bar{z}) + \bar{z}, \quad 0 \le \tau \le 1 \qquad \text{(B.1.19)}$$

From this representation we see that l_4 is an R_2 arc as both necessary conditions are satisfied.

B.2 Showing that Re z^2 and Re $(-\lambda + \ln|z|)$ are nondecreasing on l_s

$\underline{l_1}$: On l_1, $|z| < 1$ so we must show that Re z^2 is nondecreasing as z moves from the origin to the level curve $\varepsilon(z) = A$ on l_1. Let

$$f(z) = \mathrm{Re}\, z^2, \quad z \in l_1. \qquad \text{(B.2.1)}$$

From (B.1.1) this becomes

$$f(\tau) = \cos\left(\frac{\pi}{12}\right)\tau^2, \quad 0 \le \tau \le \tau_1. \qquad \text{(B.2.2)}$$

Therefore

$$f'(\tau) = 2\cos\left(\frac{\pi}{12}\right)\tau, \quad 0 \le \tau \le \tau_1. \qquad \text{(B.2.3)}$$

As $f'(\tau) > 0$ for all $\tau \in (0, \tau_1]$, then Re z^2 is increasing on l_1.

$\underline{l_1,\ l_5}$: As both of these are level curves of $\varepsilon(z)$, from (3.4.7) we see that Re z^2 and Re $(-\lambda +$ ln $|z|)$ are nondecreasing on l_2 and l_3 respectively.

$\underline{l_4}$: On l_4 $|z| > 1$ so we must show Re $(-\lambda + \ln|z|)$ is nondecreasing as z moves from $\bar{z}$ to $\hat{z}$ along l_4. Let

$$f(z) = \text{Re}\,(-\lambda + \ln|z|) = \text{Re}\, z^2 + \ln|z|^{-\text{Re}\,\lambda}, \quad z \in l_4. \tag{B.2.4}$$

By writing $z = x + \iota y$, this becomes

$$f(x,y) = x^2 - y^2 + \ln(x^2 + y^2)^{-\text{Re}\,\lambda/2}, \quad z \in l_4. \tag{B.2.5}$$

As z moves along l_4 from $\bar{z}$ to $\hat{z}$, x remains constant while y is negative but increasing. Thus y^2 is decreasing and $-y^2$ is increasing. So $x^2 + y^2$ and $(x^2+y^2)^{\text{Re}\,\lambda/2}$ are both decreasing hence $(x^2+y^2)^{-\text{Re}\,\lambda/2}$ and $\ln(x^2+y^2)^{-\text{Re}\,\lambda/2}$ are both increasing. Also as $-y^2$ is increasing, $x^2 - y^2$ is increasing on l_4. Hence $f(x,y)$ is increasing on l_4.

$\underline{l_5}$: On l_5 $|z| > 1$ so we must show Re $(-\lambda + \ln|z|)$ is nondecreasing as z moves from $\hat{z}$ to ∞ along l_5. Again let $f(z)$ be given by (B.2.4). From (B.1.2) this becomes

$$f(\tau) = \cos\left(\frac{\pi}{12}\right)\tau^2 + \ln \tau^{-\text{Re}\,\lambda}, \quad \hat{\tau} \le \tau \le \infty. \tag{B.2.6}$$

Therefore

$$f'(\tau) = 2\cos\left(\frac{\pi}{12}\right)\tau - \frac{\text{Re}\,\lambda}{\tau}, \quad \hat{\tau} \le \tau \le \infty. \tag{B.2.7}$$

In Section 3.4 we chose $\hat{z}$ such that

$$|\hat{z}|^2 = \hat{\tau}^2 > \frac{\text{Re}\,\lambda}{2\cos\left(\frac{\pi}{12}\right)}. \tag{B.2.8}$$

Therefore for $\tau \in [\bar{\tau}, \infty)$, $f'(\tau) > 0$. Thus Re $(-\lambda + \ln|z|)$ is nondecreasing on l_5.

Drawing the level curves

We use the Mathlab package to draw the level curves in Figures 3.2 to 3.6. To draw Figures 3.2 to 3.4 we first define $\varepsilon(z)$ as follows (where we have renamed it weight1):

function Z1=weight1(X1,Y1);

$R1 = (X. * X + Y. * Y <= 1);$

inner1 $= exp(0.5 * (X.^2 - Y.^2));$

outer1 $= (exp(0.5 * (X.^2 - Y.^2))) * (X.^2 + Y.^2)^(- 3/4);$

$Z1 = R1. *$ (inner1) $+ (1 - R1). *$ (outer1);

We input the following to draw the level curves in Figure 3.2:

$[X1, Y1]$ =meshgrid$(-2 : 0.05 : 2, -2 : 0.05 : 2);$

$[X2, Y2]$ =meshgrid$(-1 : 0.05 : 1, -1 : 0.05 : 1);$

$Z1$ =weight1$(X1, Y1);$

$Z2$ =sqrt$((X2).^2 + (Y2).^2);$

$V3aa = [1.0317, 1.1331, 1.3248, 1.6487, 1.7771, 1.9974, 2.3215];$

$V3ab = [0.8, 0.6065, 0.3703, 0.2266, 0.1374, 0.0819];$

$V = [1, 1];$

contour$(X1, Y1, Z1, V)$;hold on

contour$(X1, Y1, Z1, V3aa,' --')$;hold on

contour$(X1, Y1, Z1, V3ab,' --')$;hold on

contour$(X2, Y2, Z2, V,' :')$;hold on

$N = 1/100; a = 0 : N : 2;$plot$(a, -a/24)$;hold on

xlabel('Re z'); ylabel('Im z');

The vector $V3aa$ gives the values which the level curves take in Δ_1 and Δ_3, the first entry being the value of $\varepsilon(z)$ on the curves nearest the unit circle. Similarly for $V3ab$ and the curves in Δ_2 and Δ_4, again the first entry being the value of $\varepsilon(z)$ on the curves nearest the unit circle. This will be the same in all the following cases. Also if the last letter is a in the name of a vector then the level curves which take on the values in that vector lie in Δ_1 and Δ_3. Similarly if the last letter is b the curves are in Δ_2 and Δ_4.

Figure 3.3 is drawn by the above commands with the following changes:

$[X1, Y1]$ =meshgrid$(-10 : 0.05 : 10, -10 : 0.05 : 10)$;

$V3ba = [1.9246, 1.2410 + e005, 1.7745e + 014]$;hold on

$V3bb = [0.6065, 2.3755e - 004, 2.8785e - 011, 1.1782e - 021]$;hold on

contour$(X1, Y1, Z1, V3ba,' --')$;hold on

contour$(X1, Y1, Z1, V3bb,' --')$;hold on

$N = 1/100$;$a = 0 : N : 10$;plot$(a, -a/24)$;hold on

For Figure 3.4, the required amendments are

$[X1, Y1]$ =meshgrid$(0.9 : 0.05 : 1.8, -0.8 : 0.05 : 0.8)$;

$V3ca = [1.64, 1.64, 1.58, 1.56]$;hold on

contour$(X1, Y1, Z1, V3ca,' --')$;hold on

contour$(X1, Y1, Z2, V,' :')$;hold on

$N = 1/100$;$a = 0.9 : N : 0.18$;plot$(a, -a/24)$;hold on

In order to draw Figure 3.5 we redefine weight1 as follows:

function Z1=weight1(X1,Y1);

$R1 = (X. * X + Y. * Y <= 1)$;

inner1 $= exp(0.5 * (X.^2 - Y.^2))$;

outer1 $= (exp(0.5 * (X.^2 - Y.^2))) * (X.^2 + Y.^2)^(- 7/4)$;

$Z1 = R1. * (\text{inner1}) + (1 - R1). * (\text{outer1});$

We then use similar instructions to Figure 3.3, making the following changes:

$V7a = [23.2887, 2.1535 + e007, 1.5494e + 014]$;hold on

$V7b = [0.5, 0.0047, 5.9331e - 010, 1.1782e - 021]$;hold on

contour$(X1, Y1, Z1, V7a,' --')$;hold on

contour$(X1, Y1, Z1, V7b,' --')$;hold on

Finally, for Figure 3.6, weight1 is defined as

function Z1=weight1(X1,Y1);

$R1 = (X. * X + Y. * Y <= 1);$

inner1 $= exp(0.5 * (X.^2 - Y.^2));$

outer1 $= (exp(0.5 * (X.^2 - Y.^2))) * (X.^2 + Y.^2)^(- 11/4);$

$Z1 = R1. * (\text{inner1}) + (1 - R1). * (\text{outer1});$

and then as above, changing the following:

$V11a = [38.4013, 9.8214.e + 005]$;hold on

$V11b = [0.2, 0.1, 5.3332e - 010, 1.3664e - 019]$;hold on

contour$(X1, Y1, Z1, V11a,' --')$;hold on

contour$(X1, Y1, Z1, V11b,' --')$;hold on

Appendix D

Basics of Asymptotics

D.1 Poincaré Asymptotics

Let $x_0 \in \mathbb{R}$ or be a point at infinity.

1. A function f is asymptotic to g as $x \to x_0$ if

$$\lim_{x \to x_0} \frac{f(x)}{g(x)} = 1. \tag{D.1.1}$$

   We write this as $f(x) \sim g(x)$ as $x \to x_0$.

2. A function f is of order less than g as $x \to x_0$ if

$$\lim_{x \to x_0} \frac{f(x)}{g(x)} = 0. \tag{D.1.2}$$

   We write this as $f(x) = o(g(x))$ as $x \to x_0$.

3. A function f is of order not exceeding g as $x \to x_0$ if

$$\lim_{x \to x_0} \frac{f(x)}{g(x)} < A, \quad 0 < |A| < \infty. \tag{D.1.3}$$

   We write this as $f(x) = O(g(x))$ as $x \to x_0$.

Notice that $f(x) = o(g(x))$ implies $f(x) = O(g(x))$ but the converse of this is not true. These asymptotic relations can be extended to the complex plane, though we must proceed with caution when doing so. If $z \in \mathbb{C}$, it may not make sense to say $f(z) \sim g(z)$ as $z \to z_0$ if $\lim_{z \to z_0} f(z)/g(z)$ is non-unique when $z \to z_0$ is taken along arbitrary paths in the complex plane. This difficulty can be eliminated by insisting that all paths lie within a particular sector of the complex plane in which the limit is unique. If $\mathbf{S}$ is a sector of the complex plane given by $\alpha \leq \arg(z - z_0) \leq \beta$, then

$$f(z) \sim g(z), \quad z \to z_0, \quad z \in \mathbf{S} \tag{D.1.4}$$

if

$$\lim_{z \to z_0} \frac{f(z)}{g(z)} = 1, \quad z \in \mathbf{S}. \tag{D.1.5}$$

The validity of the symbols O and o in the complex plane also depends on the sector of definition. For a more detailed introduction to the basic concepts of asymptotics see [3] and [13].

Suppose, as is the case for solutions of some second-order ordinary differential equations, that a function has a compound asymptotic representation given by two series, each multiplied by an exponential, $e^{S_1(z)}$ and $e^{S_2(z)}$. Along directions in the complex plane given by $\mathrm{Re}\,[S_1(z)] = \mathrm{Re}\,[S_2(z)]$, the two exponentials are comparable in magnitude. These are known as principal curves. Inside a sector defined by these lines, where $\mathrm{Re}\,[S_1(z)] > \mathrm{Re}\,[S_2(z)]$, $e^{S_1(z)}$ is said to be dominant and produces the leading asymptotic behaviour, while $e^{S_2(z)}$ is said to be subdominant or recessive. As z moves closer to a principal curve, $e^{S_2(z)}$ grows in magnitude, until z crosses the principal curve and now $e^{S_2(z)}$ is dominant and $e^{S_1(z)}$ recessive. Along lines $\mathrm{Im}\,[S_1(z)] = \mathrm{Im}\,[S_2(z)]$, now called Stokes lines, is where one of the exponentials is maximally dominant over the other.

Stokes observed that the coefficient, now known as a Stokes multiplier, multiplying the recessive term seems to change suddenly as z crosses a Stokes line. This is known as Stokes phenomenon. For further discussion see [3, Sec. 3.7] and [13, P. 240].

D.2 Liouville-Green approximate solutions

Named after Liouville and Green, this method gives an approximation to the solution of a second-order linear differential equation of the form

$$\frac{d^2w}{dz^2} = u^2 f(z) w \tag{D.2.1}$$

in a domain where $f(z)$ is holomorphic and does not vanish. The L-G approximation to the general solution of (D.2.1) is

$$w(z) \sim A f^{-1/4}(z) \exp\left\{u \int f^{1/2}(t)\,dt\right\} + B f^{-1/4}(z) \exp\left\{-u \int f^{1/2}(t)\,dt\right\}, \quad (u \to \infty). \tag{D.2.2}$$

The constants A and B are obtained given by initial or boundary conditions. Again a very comprehensible introduction to these ideas can be found in [3, Ch. 10].

A more rigorous approach is employed in [13] for the more general equation

$$\frac{d^2w}{dz^2} = (u^2 f(z) + g(z))w \tag{D.2.3}$$

in a simply connected D domain where $f(z)$ and $g(z)$ are holomorphic and $f(z)$ does not vanish. The function $f(z)$ is known as the dominant term. It is seen that (D.2.3) has the following solutions

$$w_j(z) = f^{-1/4}(z) \exp\left\{(-1)^{j+1} \int f^{1/2}(z)\, dz\right\} \{1 + \varepsilon_j(z)\}, \quad (j = 1, 2) \tag{D.2.4}$$

where the error terms, $\varepsilon_j(z)$, are bounded in certain regions of the **D**. For further details see [13, Ch. 6].

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