Very-High-Precision Calculations in Physics

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O my Lord! Increase me further in knowledge.

(Holy Quran, Surah Ta Ha, 20:114.)

I dedicate this work and give special thanks to my lovely husband, Asif Mushtaq, for being there for me throughout the entire doctorate program.
I dedicate this work to the beloved parents of both of us

Preface

This thesis is submitted by the author as part of the requirements for the degree Philosophiae Doctor at the Norwegian University of Science and Technology (NTNU). It is the conclusion of a little more than four years of work.

My supervisor has been Professor Kåre Olaussen. The work has been performed at the Norwegian University of Science and Technology.

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Part I. Introduction

1. Physical background

1.1. What is the most accurate number in physics?

What is the most accurately known number in physics? It can be argued that theoretically this is the ratio between the perimeter and diameter of a circular disk, also known as π , quite recently computed to about 10^{13} decimals [1]. This precision is not quite matched by experimental observations. It can also be criticized for not taking into account the discrete and quantum nature of matter, or — at this accuracy — even the tiny non-euclidean nature of surrounding space.

Experimentally the best accuracy is probably what can be obtained by use of optical frequency combs [2], currently with a relative accuracy of a few parts in 10^{17} (i.e. 17 decimals). This is expected to improve by a few orders of magnitude during the next decades, cf. Fig 2 of reference 2. Hence, there are situations where it makes sense to compute physical quantities to 20 decimals precision or better — provided that the physical model is known accurately enough.

The latter is usually not the case. The physical quantity where experimental and theoretical values are in best agreement is probably the magnetic moment of the electron. This quantity is measured to about 13 decimals [3], with the computation of the theoretical contributions from Quantum Electrodynamics (QED) recently completed to fifth order in the fine structure constant α [4]. This leads to agreement between experiment and theory to about 13 decimals without adjustable parameters. Also the QED contributions to the muon magnetic moment has been computed to fifth order in α [5], but for this quantity the theoretical contributions from other sources (like hadronic contributions to vacuum polarization) are larger, and the experimental uncertainty is also larger.

1.2. The role of ordinary differential equations in physics

Most of physics can be described locally in space and time, hence mathematically by differential equations. Differential equations therefore form a central part of theoretical physics, both on the elementary and advanced level. In most cases the relevant equations are *partial*. But by symmetry reductions, or more systematically for linear equations by the method of separation of variables, they can be reduced to ordinary differential equations. This greatly increases the prospects of finding solutions, and of understanding the properties of such solutions.

There is a powerful and quite complete method of solving ordinary linear homogeneous equations, starting with works by Fuchs [6] and Frobenius [7]. In this method the solution is expanded in a convergent (generalized) power series, a Frobenius series, around ordinary or

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regular singular points of the equation in the complex plane. This method can be combined with analytic continuation to extend the solution beyond the radius of convergence of each power series.

1.2.1. Schrödinger equation in one dimension

The Schrödinger equation is a partial differential equation that governs the time evolution of quantum mechanical wave-functions $\Psi(q,t)$, where q denotes the position(s) of the particle(s). It gives a good description of the quantum motion of non-relativistic particles interacting instantaneously with each other. In the one-dimensional single-particle case it reads

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q^2} + V(q) \right] \Psi(q, t) = i\hbar \frac{\partial \Psi(q, t)}{\partial t}. \tag{1.1}$$

This equation can be reduced to an ordinary differential equation by separation of variables. Assuming a solution in product form,

$$\Psi(q,t) = \psi(q) T(t).$$

and substituting into equation (1.1), one finds $T(t) = e^{-iEt/\hbar}$, and

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q^2} + V(q) \right] \psi(q) = E \ \psi(q).$$

We assume the potential to be a low-order even polynomial,

$$V(q) = \sum_{n=0}^{N} \nu_n q^{2n}.$$
 (1.2)

For numerical computations one must use dimensionless quantities. We first introduce a dimensionless length $x = q/\lambda$ such that the Schrödinger equation becomes

$$\left[-\frac{\partial^2}{\partial x^2} + x^{2N} + \sum_{n=0}^{N-1} v_n x^{2n} \right] \psi(x) = \varepsilon \psi(x), \tag{1.3}$$

with $\lambda^{2N+2} = \hbar^2/2mV_N$, $v_n = 2mV_n\lambda^{2n+2}/\hbar^2$, and $\varepsilon = 2mE\lambda^2/\hbar^2$. Here the scaling coefficient λ has been chosen to give unit coefficients in front of the $\partial^2/\partial x^2$ and the x^{2N} terms. Other choices may sometimes be more convenient, in particular it is natural to generalize to the case where

$$-\frac{\partial^2}{\partial x^2} \to -s^2 \frac{\partial^2}{\partial x^2},$$

with s^2 usually a small number. It is common to think of it as $\hbar^2/2m$, but since this quantity is not dimensionless it is not a true small parameter of the equation.

The solutions of equation (1.3) be expanded in a power series in x^2 . The radius of convergence of this power series is infinite. One may make an analytic continuation to expand the solution around another point x_0 , but this will destroy the explicit parity

symmetry of the problem. The latter leads to a doubling of expansion coefficients in the power series, and a significant increase in the number of coefficients describing the polynomial potential. The advantage for a numerical evaluation is that the power series may converge faster, and with a smaller loss of precision due to roundoff errors.

1.2.2. Schrödinger equation in higher dimensions

The real world is not one-dimensional, but can in many situations be treated as quite symmetric. F.i., the Schrödinger equation for a *D*-dimensional rotationally symmetric system,

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V(q) \right] \Psi(q, t) = i\hbar \frac{\partial}{\partial t} \Psi(q, t), \tag{1.4}$$

allows for a separation of variables,

$$\Psi(\mathbf{q},t) = \psi(q) \,\mathcal{Y}^{(\ell)}(\hat{\mathbf{q}}) \,T(t). \tag{1.5}$$

Here $q \equiv |\boldsymbol{q}|$, and $\mathcal{Y}^{(\ell)}(\boldsymbol{\hat{q}})$ is the generalization of the spherical harmonics to D dimensions. They are independent of the length of \boldsymbol{q} (i.e., scale invariant), hence $\boldsymbol{q} \cdot \nabla \mathcal{Y}^{(\ell)}(\boldsymbol{\hat{q}}) = 0$. The functions

$$\mathcal{P}^{(\ell)}(\boldsymbol{q}) \equiv q^{\ell} \, \mathcal{Y}^{(\ell)}(\hat{\boldsymbol{q}})$$

are homogeneous polynomials of order ℓ in the components of the vector q, which are also solutions of the Laplace equation

$$\nabla^2 q^{\ell} \mathcal{Y}^{(\ell)}(\hat{\boldsymbol{q}}) = (\nabla^2 q^{\ell}) \mathcal{Y}^{(\ell)}(\hat{\boldsymbol{q}}) + q^{\ell} \nabla^2 \mathcal{Y}^{(\ell)}(\hat{\boldsymbol{q}}) = 0. \tag{1.6}$$

It follows from these relations that

$$\boldsymbol{\nabla}^2 \left[\boldsymbol{\mathcal{Y}}^{(\ell)}(\boldsymbol{\hat{q}}) \right] = - \left(q^{-\ell} \, \boldsymbol{\nabla}^2 q^{\ell} \right) \, \boldsymbol{\mathcal{Y}}^{(\ell)}(\boldsymbol{\hat{q}}) = -\ell(\ell + D - 2) \, q^{-2} \, \boldsymbol{\mathcal{Y}}^{(\ell)}(\boldsymbol{\hat{q}}),$$

and

$$\nabla^2 \mathcal{Y}^{(\ell)}(\hat{q}) \, \psi(q) = \mathcal{Y}^{(\ell)}(\hat{q}) \, \left[\psi''(q) + (D-1)q^{-1}\psi'(q) - \ell(\ell+D-2) \, q^{-2}\psi(q) \right].$$

Hence, the separation of variables (1.5) leads to the radial equation

$$\left[-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial q^2} + \frac{D-1}{q} \frac{\partial}{\partial q} + \frac{\ell(\ell+D-2)}{q^2} \right) + V(q) \right] \psi(q) = E \, \psi(q). \tag{1.7}$$

This equation has a regular singular point at q = 0, but it still has a generalized series solution which can be found by the Frobenius method [7].

Separations of variables can be applied to many other coordinate systems. F.i., in three dimensions the Schrödinger equation in zero potential can be separated in ellipsoidal

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coordinates (ξ_1, ξ_2, ξ_3) , related to Cartesian coordinates by

$$x = \sqrt{\frac{(\xi_1^2 - a^2)(\xi_2^2 - a^2)(\xi_3^2 - a^2)}{a^2(a^2 - b^2)}},$$

$$y = \sqrt{\frac{(\xi_1^2 - b^2)(\xi_2^2 - b^2)(\xi_3^2 - b^2)}{b^2(b^2 - a^2)}}, \quad \xi_1 > a > \xi_2 > b > \xi_3 > 0,$$

$$z = \frac{\xi_1 \xi_2 \xi_3}{ab},$$

$$(1.8)$$

plus 10 degenerate forms of these coordinates [8]. The separated equations have five regular singular points, at $\pm a$, $\pm b$, and ∞ [9]. The Schrödinger equation remains separable if we add a potential of the form

$$V = \frac{(\xi_2^2 - \xi_3^2)u(\xi_1) + (\xi_1^2 - \xi_3^2)v(\xi_2) + (\xi_1^2 - \xi_2^2)w(\xi_3)}{(\xi_1^2 - \xi_2^2)(\xi_1^2 - \xi_3^2)(\xi_2^2 - \xi_3^2)}.$$
 (1.9)

The degenerate forms often lead to situations where two or more regular singular points merge to irregular singular points (confluent singularities).

1.2.3. The Fokker-Planck equation

There are of course many other fields of physics where equations similar to the Schrödinger equation occur. One such example is the Fokker-Planck equation [10, 11] describing the time evolution of a probability distribution $\rho(\mathbf{r},t)$ of a diffusing particle in a force field $\mathbf{F}(\mathbf{r}) = -\nabla U(\mathbf{r})$,

$$\frac{\partial}{\partial \tau} \rho(\mathbf{r}, \tau) = \frac{1}{2} \nabla^2 \rho(\mathbf{r}, \tau) - \nabla \cdot [\mathbf{F}(\mathbf{r}) \rho(\mathbf{r}, \tau)]. \tag{1.10}$$

By writing $\rho(\mathbf{r}) = e^{-U(\mathbf{r})} \Psi(\mathbf{r}, t)$ we obtain a "Schrödinger equation", in imaginary time $\tau = it$, for $\Psi(\mathbf{r}, \tau)$,

$$-\frac{\partial}{\partial \tau} \Psi(\mathbf{r}, \tau) = -\frac{1}{2} \nabla^2 \Psi(\mathbf{r}, \tau) + V(\mathbf{r}) \Psi(\mathbf{r}, \tau), \qquad (1.11)$$

with a potential $V(\mathbf{r}) \equiv \frac{1}{2} [\mathbf{F}(\mathbf{r}) \cdot \mathbf{F}(\mathbf{r}) + \nabla \cdot \mathbf{F}(\mathbf{r})]$. For this reason we have denoted the equations we study in Paper I [35] and Paper II [36] as *Schrödinger type* equations instead of just Schrödinger equations.

2. The projects of this thesis

Although the projects of this thesis are inspired by all the points in section 1.1, they are nearest to the first one. In the first project [35] the ground state energy of the anharmonic oscillator was computed to the accuracy of one million decimal digits. There are certainly no experimental results which require such accuracy, or physical systems which is modeled to that accuracy by the given Hamiltonian. That project was an attempt to explore the borders of applicability of our method, using standard computers of the time.

The practical applications of very-high-precision calculations is that they provide essentially exact results, and hence may be useful for testing theoretical conjectures or the accuracy of approximation methods. One may also think of practical problems where numerical accuracy to several tens of decimals may be useful.

2.1. Properties of the used algorithms

Most projects of this thesis are based on an algorithm for solving Schrödinger type equations to very high precision. Despite the numerical character of this topic, the focus of all investigations has been to explore analytic questions. How do the required resources, like computer memory and CPU cycles, scale with the wanted precision? With standard numerical methods, based on discretization of the Schrödinger differential operator, the error $\varepsilon \equiv 10^{-D}$ scales like a low power of the discretization step [16],

$$\varepsilon \sim (\Delta x)^n$$
,

usually with $1 \leq n \leq 6$. Hence the number N of computational steps would grow exponentially with the wanted precision,

$$N \sim 10^{D/n}$$

In contrast, in the algorithm used here the number of computational steps grows asymptotically linearly with the wanted precision D as $D \to \infty$,

$$N \approx N_0 + \text{const} \times D$$
.

This algorithm works for Schrödinger type equations with polynomial potentials in one dimension, and can be extended to a much larger class of ordinary differential equations. Note that in many situations the offset N_0 can be quite large, making it computationally very expensive to obtain the first few decimals of accuracy. Hence, our algorithm may not be suitable for cases where only standard double-precision is wanted (but there are

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examples where it is a competitive method). And we have not yet seriously explored the possible improvements which may be made by appropriate use of analytic continuations.

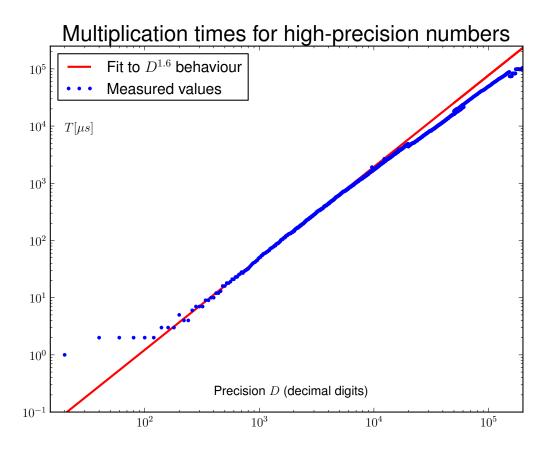


Figure 2.1.: The most time-consuming algebraic operation in our solution algorithm is the multiplication of two high-precision numbers. This figure shows a measurement of how this time varies with precision D on a standard linux workstation. The theoretical prediction is that it should grow like a power $D^{1.6}$ for low values of D. As can be seen this is followed quite accurately for precision values in the range $100 \le D \le 10^4$. Eventually the theoretical growth should reduce to a rate $D \log D \log \log D$; this does not seem to be achievable in practice on our computers. The discontinuous behavior at low D occurs because the real computational precision increased in steps of 64 bits, corresponding to 19^+ decimal digits.

It should be kept in mind that each computational step will require more time as one increases precision. In our method the multiplication of two high-precision numbers is the most time-consuming operation. We have based all high-precision numerical computations on the CLN Class Library for Numbers [12], compiled with the GNU Multiple Precision

Arithmetic Library [13]. These libraries use the Schönhage-Strassen algorithm [14] for multiplying numbers. With this algorithm the time T of multiplying two high precision numbers scale theoretically at a rate between $D^{1.6}$ and $D \log D \log \log D$ with precision D. Hence the total time requirement of our high-precision method increases somewhat faster than D^2 with the precision D. In practical computations one finds $T \sim D^{1.6}$ for $D \leq 2000$, cf. figure 2.1.

Although it is of limited practical interest to compute physical quantities like eigenenergies to much more than 20 decimals precision, it may be the case that computation of the wave-functions in some regions of interest require very precise knowledge of the eigenenergy — otherwise it would be impossible to find solutions with the correct behavior. This is one practical motivation for developing methods to solve eigenvalue problems to otherwise ridiculously high precision.

In paper II [36] it was demonstrated, and analyzed, that the very-high-precision wavefunctions can be inserted into straightforward numerical integration routines to compute normalization integrals to comparable precision within acceptable time.

We believe that these algorithms also can be used to compute functional determinants of one-dimensional differential operators to comparable precision. Since the functional determinant of a separated sum of differential operators is the product of the individual determinants, the algorithms can also be used to compute functional determinants of higher-dimensional separable differential operators [15]. The algorithms can also be used to compute the resolvent of one-dimensional differential operators, but in this case an extension to higher-dimensional separable operators becomes more complicated since one must first compute the partition functions of the individual one-dimensional operators.

2.2. Method for solving the differential equation

Our method of solution is (perhaps disappointingly) simple: We just expand the solution $\psi(x)$ in a power series,

$$\psi(x) = x^{\sigma} \sum_{m>0} a_m x^m, \tag{2.1}$$

where $\sigma = 0$ for the even parity solutions, and $\sigma = 1$ for the odd parity solutions. For a given x the quantities $A_m(x) \equiv a_m x^{2m+\sigma}$ can be generated recursively from equation (1.3),

$$A_{m+1}(x) = \frac{1}{(2m+2+\sigma)(2m+1+\sigma)} \sum_{n=0}^{N} V_n(x) A_{m-n}(x),$$
 (2.2)

where

$$V_n(x) = \begin{cases} v_0 - \varepsilon, & \text{for } n = 0, \\ v_n x^{2n}, & \text{for } 1 \le n < N, \\ x^{2N}, & \text{for } n = N. \end{cases}$$
 (2.3)

This recursion is initialized with $A_{-n}(x) = \delta_{n0} x^{\sigma}$ $(n \ge 0)$. As is seen from equation (2.2) only the last N+1 coefficients $A_m(x)$ need to be considered at any time while the sum is accumulated. This means that one only needs to store N+1 coefficients A_m and at

most N+1 coefficients V_n , together with the accumulated sums for $\psi(x)$ and optionally $\psi'(x)$. Hence the total memory requirement is 2N+4 high precision numbers, which is quite modest when the potential is a low order polynomial.

In principle the sum in equation (2.1) runs over infinitely many terms. But since equation (1.3) has no singular points in the finite plane the sum will eventually converge very fast, and can be cut off at some finite value \mathcal{N} . The value of \mathcal{N} depends on the desired accuracy of the sum, the value of x, and of course the parameters in equation (2.1).

The energy eigen-function $\psi(x)$ should become very small when |x| becomes very large. Hence there will be large cancellations in the sum, and associated accumulation of round-off errors. Therefore, the interesting aspects of this method is not to code the recursion algorithm (2.2), but f.i. to estimate the proper choice of \mathcal{N} and the numerical precision which must be employed in the computation. We have found that the WKB approximation combined with a Legendre transformation can be used for this analysis, see article IV(a) [38].

2.3. Eigenvalue conditions

The standard eigenvalue condition is that $\psi(x) \to 0$ as $x \to \pm \infty$. With parity symmetry $(x \to -x)$ it is sufficient to consider only one of these limits. I.e., we may start with solutions $\psi_{\sigma}(x;\varepsilon)$ of desired parity, and use the single condition

$$\lim_{x \to \infty} \psi_{\sigma}(x, \varepsilon) = 0, \tag{2.4}$$

to determine the allowed eigenvalues ε .

The assumption that the potential V should be even is not necessarily physical, and not really necessary. In the general case one can expand the general solution in two linearly independent solutions $\varphi_a(x;\varepsilon)$ and $\varphi_b(x;\varepsilon)$,

$$\psi(x;\varepsilon) = C_a \varphi_a(x;\varepsilon) + C_b \varphi_b(x;\varepsilon),$$

where C_a and C_b are coefficients to be determined. The eigenvalue condition is then that there should be a nontrivial solution of the equation

$$\lim_{x \to \infty} \begin{pmatrix} \varphi_a(x; \varepsilon) & \varphi_b(x; \varepsilon) \\ \varphi_a(-x; \varepsilon) & \varphi_b(-x; \varepsilon) \end{pmatrix} \begin{pmatrix} C_a \\ C_b \end{pmatrix} = 0.$$

The condition for this is that the system determinant must vanish,

$$\lim_{x \to \infty} \det \begin{pmatrix} \varphi_a(x; \varepsilon) & \varphi_b(x; \varepsilon) \\ \varphi_a(-x; \varepsilon) & \varphi_b(-x; \varepsilon) \end{pmatrix} = \lim_{x \to \infty} \left[\varphi_a(x; \varepsilon) \varphi_b(-x; \varepsilon) - \varphi_a(-x; \varepsilon) \varphi_b(x; \varepsilon) \right] = 0.$$
(2.5)

This is in principle not different from the condition that a single function must vanish, but is in practice a nontrivial extension. The numerical implementation becomes more

complex, since we must solve an eigenvalue problem, and the program execution will be more demanding since one must compute and store four functions at each step instead of one. The assumption that the polynomial V should be of low order, i.e. that N should be small, is mostly motivated by storage requirement.

With our method of solution it is not possible to evaluate the wave-functions at, or very close to, $x = \infty$. We must therefore replace the condition (2.4) or (2.5) with boundary conditions at finite, but sufficiently large, x_0 . For each eigenvalue ε there exist a Robin boundary condition at x_0 ,

$$-\frac{\psi'(x_0)}{\psi(x_0)} = R(x_0) \tag{2.6}$$

which is equivalent to (2.4). We do not know $R(x_0)$ exactly (it even depends weakly on the eigenvalue ε), but it can be estimated from asymptotic analysis of equation (1.3) as $x_0 \to \infty$. Define

$$Q(x) \equiv x^{2N} + \sum_{n=0}^{N-1} v_n x^{2n} - \varepsilon,$$

and let \bar{x} be the largest solution of Q(x) = 0 (i.e., the largest classical turning point). Since Q(x) becomes large when $x \gg \bar{x}$ we may choose

$$R(x_0) = \sqrt{Q(x_0)} + \text{ higher-order corrections}$$
 (2.7)

for a sufficiently large $x_0 \gg \bar{x}$. This may often be further approximated by $R(x_0) = \infty$. I.e., a Dirichlet boundary condition, $\psi(x_0) = 0$, at x_0 . The most important property is that the eigenvalue is not very sensitive to the precise choice of $R(x_0)$. For $x > \bar{x}$ the solution can be approximated as

$$\psi(x) \approx K_{+}(\varepsilon) Q(x)^{-1/4} \exp\left(\int_{\bar{x}}^{x} dt \sqrt{Q(t)}\right) +$$

$$K_{-}(\varepsilon) Q(x)^{-1/4} \exp\left(-\int_{\bar{x}}^{x} dt \sqrt{Q(t)}\right),$$
(2.8)

where the coefficients K_{\pm} are expected to be of the same magnitude in general (both of order unity and slowly varying with ε).

The exact quantization condition, the Dirichlet boundary condition at x_0 , and the Robin boundary condition at x_0 become respectively, with $Q_0 \equiv Q(x_0)$ and $Q'_0 \equiv Q'(x_0)$,

$$K_{+}(\varepsilon) = 0, (2.9a)$$

$$K_{+}(\varepsilon) + K_{-}(\varepsilon) \exp\left(-2\int_{\bar{\tau}}^{x_0} dt \sqrt{Q(t)}\right) = 0,$$
 (2.9b)

$$K_{+}(\varepsilon) - \frac{1}{8}K_{-}(\varepsilon)Q_{0}^{-3/2}Q_{0}'\exp\left(-2\int_{\bar{\varepsilon}}^{x_{0}}dt\sqrt{Q(t)}\right) = 0.$$
 (2.9c)

To compare solutions let $\varepsilon_{\text{exact}}$ be the solution of equation (2.9a), and expand

$$K_{+}(\varepsilon) = K'_{+}(\varepsilon_{\text{exact}}) (\varepsilon - \varepsilon_{\text{exact}}) + \dots$$

Then the solutions of equations (2.9b) and (2.9c) become respectively

$$\varepsilon_{\text{Dirichlet}} = \varepsilon_{\text{exact}} - \frac{K_{-}(\varepsilon_{\text{exact}})}{K'_{+}(\varepsilon_{\text{exact}})} \exp\left(-2\int_{\bar{x}}^{x_0} dt \sqrt{Q(t)}\right),$$
(2.10a)

$$\varepsilon_{\text{Robin}} = \varepsilon_{\text{exact}} + \frac{K_{-}(\varepsilon_{\text{exact}})}{8 K'_{+}(\varepsilon_{\text{exact}})} Q_0^{-3/2} Q'_0 \exp\left(-2 \int_{\bar{x}}^{x_0} dt \sqrt{Q(t)}\right). \tag{2.10b}$$

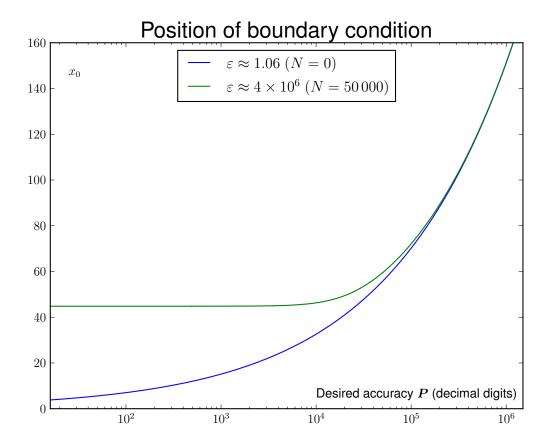


Figure 2.2.: The exact boundary condition, that $|\psi(x)| \to 0$ as $|x| \to \infty$, cannot be realized in a numerical computation, but must be replaced by a Robin or Dirichlet boundary condition at some finite (large) value x_0 . This figure illustrates how x_0 must be chosen to maintain a described accuracy 10^{-P} of the computed eigenvalues, for the pure anharmonic oscillator, $V(x) = x^4$, for the lowest eigenvalue and eigenvalue number $N = 50\,000$. Large values of x_0 is computationally challenging, but possible, even if one evaluates the wave-function directly by a series expansion around x=0.

We note that the Robin boundary condition improves the accuracy by a relative amount $\frac{1}{8}Q_0^{-3/2}Q_0'$, which may correspond to a few decimal digits. This may be further improved by

systematically adding correction terms to the parameter $R(x_0)$, cf. equation (2.7). Each order of correction will provide a few extra decimals of accuracy. This may be a good approach if one wants the eigenvalue to standard precision (i.e. 15-16 decimal digits) only, but it makes little difference if one wants hundreds of decimals or more. Then one must make use of the fact that the factor¹

$$\exp\left(-2\int_{\bar{x}}^{x_0} dt \sqrt{Q(t)}\right) \sim \exp\left(-\frac{2x_0 Q_0^{1/2}}{N+1}\right)$$
 (2.11)

vanishes exponentially fast with increasing x_0 . As an example consider the case that $Q(x) = x^4 - \varepsilon$. Then the quantization condition (2.9b) or (2.9c) leads to an error in the eigenvalue of order

$$\Delta \varepsilon \sim e^{-\frac{2}{3}x_0\sqrt{x_0^4-\varepsilon}},$$
 (2.12)

which clearly vanishes exponentially fast as x_0 increases. Figure 2.2 displays how large one must select x_0 to obtain a desired accuracy of eigenvalue number N. As can be seen, this value is quite large for large N, even at moderate accuracy. This may not be a serious obstacle if $\psi(x)$ is evaluated by analytic continuation, but it is quite time-consuming if one evaluates it by a direct power series expansion around the origin.

¹For this crude estimate of the integral we make a partial integration, using $Q(\bar{x}) = 0$, and the approximation $t \frac{d}{dt} Q(t) \approx 2N Q(t)$.

Part II. Mathematical background

3. Linear Ordinary Differential Equations

In this part the mathematical background used for the thesis projects is discussed. Some of the more technical parts is placed in the Appendices.

A linear differential equation is any differential equation that can be written in the following form,

$$\left[p_n(z)\frac{d^n}{dz^n} + p_{n-1}(z)\frac{d^{n-1}}{dz^{n-1}} + \dots + p_0(z)\right]f(z) = g(z),\tag{3.1}$$

or more symbolically,

$$\mathcal{L}f = g. \tag{3.2}$$

Equation (3.1) is said to be of order n, it is called linear because \mathcal{L} is a linear operator,

$$\mathcal{L}(c_1 f_1 + c_2 f_2) = c_1 \mathcal{L} f_1 + c_2 \mathcal{L} f_2 \tag{3.3}$$

when c_1 and c_2 do not depend on z, and ordinary because it only involves one independent variable as opposed to a partial differential equation. If g = 0 the equation is said to be homogeneous, otherwise it is inhomogeneous.

3.1. Expansions around ordinary and regular singular points

We will assume the coefficients $p_k(z)$ to be analytic (usually polynomials) in the region of interest. The homogeneous version of equation (3.1) is said to have a regular singular point at z_0 if some of the functions $p_k(z)/p_n(z)$ has a (perhaps higher order) pole singularity at z_0 , but such that each

$$\alpha_k \equiv \lim_{z \to z_0} (z - z_0)^{n-k} p_k(z) / p_n(z)$$
 (3.4)

is finite. In generic cases the solutions can be expanded in Frobenius series around z_0 ,

$$f(z) = (z - z_0)^{\sigma} \sum_{m \ge 0} f_m (z - z_0)^m,$$
(3.5)

provided σ is a solution of the *indicial equation*

$$\sum_{k=0}^{n} \alpha_k \, \sigma^k = 0. \tag{3.6}$$

However, there are exceptional cases when equation (3.6) has multiple roots, or when some roots differ by integers, for which one must modify the series (3.5) with logarithmic factors.

The general analysis becomes rather complicated, with many special cases to consider. For this reason the published code in Paper III [37] excludes all exceptional cases.

For second order equations the exceptional cases can be reduced to only two possibilities. Since it was difficult to find the general recursion formulas for even these cases in the literature, in an explicit form suitable for coding, we have derived and published them in Paper IV(b) [39].

3.2. Second-order equations as first-order systems

Many ordinary differential equations originate by separation of variables from partial differential equations involving the Laplace operator, and will therefore be of second order. They can often be transformed to the form

$$\[p(z) \frac{d^2}{dz^2} + q(z) \frac{d}{dz} + r(z) \] f(z) = 0, \tag{3.7}$$

where p(z), q(z), and r(z) are low-order polynomials in z, or the inhomogeneous version of such equations. This equation is well suited for expansion in a Frobenius series (cf. equation (2.1),

$$\psi(z) = z^{\sigma} \sum_{m>0} a_m z^m,$$

since only a few coefficients a_{m-k} are required for computation of each next coefficient a_{m+1} . Although the series is assured to converge up to the nearest singular point of equation (3.7), it may be convenient to evaluate f(z) indirectly through one or more points z_i by analytic continuation. Analytic continuation of functions which satisfy a second-order differential equation is rather simple to implement, since the function is fully specified by just two complex numbers, $f(z_i)$ and $f'(z_i)$, together with the differential equation.

Hence we want to make coordinate transformations of equations like (3.7), and to implement robust algorithms for such transformations. This is simple as long as we limit ourselves to translations, since a translation of the independent variable, $z = z_0 + u$, only transforms equation (3.7) to

$$\left[\tilde{p}(u)\,\frac{d^2}{du^2}+\tilde{q}(u)\,\frac{d}{du}+\tilde{r}(u)\right]\tilde{f}(u)=0,$$

where $\tilde{p}(u) = p(z_0 + u)$, $\tilde{q}(u) = q(z_0 + u)$, $\tilde{r}(u) = r(z_0 + u)$ are polynomials of the same order as the original ones. However, we would like to include the full group of Möbius transformations,

$$z = \frac{\alpha u + \beta}{\gamma u + \delta}, \text{ with } \alpha \delta - \beta \gamma = 1.$$
 (3.8)

These are the most general transformations of the Riemann sphere which do not introduce new singularities. It is not straightforward to describe a class of equations of the form (3.7) which are invariant under Möbius transformations, in particular to computers. For this reason it seems preferable to reformulate (3.7) as a system of first-order equations. This should be done with some care. The perhaps most obvious choice

$$y_0(z) = f(z), \quad y_1(z) = f'(z),$$

introduces an irregular singular point $z = \infty$, since (with u = 1/z)

$$\frac{d}{du}y_0(u^{-1}) = -\frac{1}{u^2}y_1(u^{-1}).$$

This is unwanted unless $z = \infty$ already is an irregular singular point. Instead, if equation (3.7) has singular points at $z = z_0$ and $z = z_1 \neq \infty$, the choice

$$y_0(z) = f(z), \quad y_1(z) = C(z - z_0)(z - z_1)f'(z),$$

will not introduce new singularities. One may choose the constant $C \neq 0$ freely. By setting $C = -z_1^{-1}$ and taking the limit $z_1 \to \infty$ one obtains

$$y_0(z) = f(z), \quad y_1(z) = (z - z_0)f'(z).$$

3.2.1. Example: Reformulation of the hypergeometric equation

Consider the hypergeometric equation

$$z(1-z)f''(z) + [c - (a+b+1)z]f'(z) - abf(z) = 0.$$
(3.9)

This is known to have regular singular points at $z = 0, 1, \infty$, and no other singular points. Hence, there are three possible pairs of singular points which may be used to define $y_1(z)$. We choose z = 0 and ∞ , and a vector y with components

$$y_0 = f, \quad y_1 = zf',$$
 (3.10)

and obtain the system of first-order equations

$$z(1-z)\frac{d}{dz}\begin{pmatrix} y_0 \\ y_1 \end{pmatrix} = \begin{pmatrix} 0 & 1-z \\ abz & 1-c+(a+b)z \end{pmatrix} \begin{pmatrix} y_0 \\ y_1 \end{pmatrix}. \tag{3.11}$$

The regular singular points of this equation, with the corresponding indices, can be arranged according to the tableau

$$\begin{cases} 0 & 1 & \infty \\ 0 & 0 & a \\ 1 - c & c - a - b - 1 & b \end{cases}.$$

The first line of this pattern lists the positions of the regular singularities (here z=0, z=1, and $z=\infty$), and the two entries below each position are the indices ν_k at that position. Here $\nu_1=0$, $\nu_2=1-c$ at z=0, $\nu_1=0$, $\nu_2=c-a-b-1$ at z=1, and $\nu_1=a$,

 $\nu_2 = b$ at $z = \infty$. Note that the sum of all indices at all singular points is zero, not equal to one as in the 2nd order formulation.

The general equation with regular singular points at $0, 1, \infty$ is obtained by considering $f(z) = z^{\mu}(1-z)^{\nu}y(z)$. Since

$$z(1-z)\frac{d}{dz}z^{\mu}(1-z)^{\nu} = -z^{\mu}(1-z)^{\nu} \left[\mu(z-1) + \nu z\right],$$

one finds

$$z(1-z)\frac{d}{dz}\mathbf{f}(z) = \begin{pmatrix} \mu - (\mu+\nu)z & 1-z \\ abz & (1+\mu-c) + (a+b-\mu-\nu)z \end{pmatrix} \mathbf{f}(z).$$
 (3.12)

The right-hand side is still a first-order matrix polynomial, in contrast to the second-order formulation where the polynomials increase in order when one generalizes the hypergeometric equation in the same manner.

Finally, a Möbius transformation (3.8) which transforms the points $0, 1, \infty$ to u_0, u_1, u_∞ leads to the equation

$$R_{1}(u-u_{0})(u-u_{1})(u-u_{\infty})\frac{d}{du}\tilde{\mathbf{f}}(u)$$

$$= \begin{pmatrix} -\nu R_{2}(u-u_{0}) + \mu(u_{1}-u) & u_{1}-u \\ abR_{2}(u-u_{0}) & (1+\mu-c)R_{3}(u-u_{\infty}) + (a+b-\mu-\nu)R_{2}(u-u_{0}) \end{pmatrix}\tilde{\mathbf{f}}(u),$$
(3.13)

with

$$R_1 = \left(\frac{1}{u_{\infty} - u_0}\right), \quad R_2 = \left(\frac{u_1 - u_{\infty}}{u_0 - u_{\infty}}\right), \quad R_3 = \left(\frac{u_1 - u_0}{u_0 - u_{\infty}}\right).$$
 (3.14)

The important feature here is that the factor multiplying $\frac{d}{du}$ is a third-order polynomial in u, and that right-hand side involves a first-order matrix polynomial in u. This structure is stable under Möbius transformations, and transformations

$$f(u) \to (u - u_0)^{\mu} (u - u_1)^{\nu} (u - u_{\infty})^{-\mu - \nu} f(u).$$

3.3. System of first-order equations

Consider a system of first-order equations,

$$p(z)\frac{d}{dz}\boldsymbol{y}(z) = \boldsymbol{A}(z)\,\boldsymbol{y}(z), \tag{3.15}$$

where y(z) is a K-component vector, p(z) is an ordinary polynomial of order N, and A(z) is a $K \times K$ matrix polynomial,

$$p(z) = \sum_{k=0}^{N} p_k z^k \equiv C \prod_{k=0}^{N-1} (z - z_k),$$
 (3.16)

$$\mathbf{A}(z) = \sum_{k \ge 0} \mathbf{A}_k \, z^k. \tag{3.17}$$

3.3.1. Expansion around an ordinary point

If $p_0 \neq 0$ the solution can be expanded in an ordinary power series,

$$\mathbf{y}(z) = \sum_{m \ge 0} \mathbf{a}_m \, z^m. \tag{3.18}$$

We insert the series into equation (3.15) and introduce matrices

$$\mathcal{M}_k(\mu) \equiv (\mu - k) \, p_{k+1} - \mathbf{A}_k. \tag{3.19}$$

In terms of these one finds the recursion formula

$$\mathbf{a}_{m+1} = -\frac{1}{(m+1)p_0} \sum_{k>0} \mathcal{M}_k(m) \, \mathbf{a}_{m-k}, \tag{3.20}$$

where a_0 can be chosen freely, and $a_{-n} = 0$ for $n = 1, 2, \cdots$. According to general theory the series (3.18) will converge at least to the closest zero of p(z). I.e., the radius R of convergence satisfies

$$R \ge \min_{k} |z_k|. \tag{3.21}$$

3.3.2. Expansion around a regular singular point

If $p_0 = 0$ but $p_1 \neq 0$ the point z = 0 is a regular singular point for equation (3.15). The solution can be found by use of the Frobenius method. We assume a solution of the form

$$y(z;\nu) = \sum_{m>0} a_m z^{m+\nu},$$
 (3.22)

and find that equation (3.15) implies

$$\left(p(z)\frac{d}{dz} - \mathbf{A}\right)\mathbf{y}(z;\nu) = \sum_{m\geq 0} \left(\sum_{k\geq 0} \mathcal{M}_k(m+\nu)\mathbf{a}_{m-k}\right) z^{m+\nu} = 0, \quad (3.23)$$

where the coefficients $\mathbf{a}_{-n} = 0$ for $n = 1, 2, \cdots$. The coefficient of each power $z^{m+\nu}$ must vanish. For m = 0 this implies

$$\mathcal{M}_0(\nu)\boldsymbol{a}_0 = 0, \tag{3.24}$$

which has a nontrivial solution only when the indicial equation,

$$\det \mathcal{M}_0(\nu) = 0, \tag{3.25}$$

is fulfilled. This K^{th} -order algebraic equation has K solutions ν_s (counting multiplicities). There is at least one right eigenvector $\mathbf{a}_0(\nu_s)$ for each distinct index ν_s , and equally many left eigenvectors $\bar{\mathbf{a}}_0(\nu_s)$. Each index ν_s corresponds to an eigenvalue $\lambda_s = \nu_s p_1$ of the matrix \mathbf{A}_0 .

3.3.3. Distinct indices with non-integer differences

Assume first that all indices ν_s are distinct, and that the difference between any two of them is non-integer. Then higher-order (vector) coefficients can be computed recursively as

$$\mathbf{a}_{m+1}(\nu) = -\mathcal{M}_0(m+1+\nu)^{-1} \sum_{k\geq 1} \mathcal{M}_k(m+1+\nu) \, \mathbf{a}_{m+1-k}(\nu), \tag{3.26}$$

for $m = 1, 2, \dots$, where the coefficients $\mathbf{a}_{-n} = 0$ for $n = 1, 2, \dots$. The recursion is solvable at each step since all matrices $\mathcal{M}_0(m+1+\nu)$ are invertible by assumption. (If one of them were not, the corresponding $m+1+\nu$ would also be a solution of (3.25), contrary to the assumption.)

3.3.4. Distinct indices; one pair with integer difference

Assume next that all indices ν_s are distinct, that the difference between two of them is integer, $\nu_2 = \nu_1 + \ell$ with $\ell > 0$, and that all other possible differences are non-integer. We must then make a more general solution ansatz for the ν_1 -solution,

$$\mathbf{y}(z;\nu_1) = \sum_{m\geq 0} \mathbf{a}_m z^{m+\nu_1} + \sum_{m\geq \ell} \mathbf{b}_m z^{m+\nu_1} \log(z).$$
 (3.27)

Now equation (3.15) implies

$$\left(p(z)\frac{d}{dz} - \mathbf{A}\right)\mathbf{y}(z;\nu_1) = \sum_{m\geq 0} \sum_{k\geq 0} \mathcal{M}_k(m+\nu_1) \, \mathbf{a}_{m-k} \, z^{m+\nu_1}
+ \sum_{m\geq \ell} \sum_{k\geq 0} p_{k+1} \mathbf{b}_{m-k} \, z^{m+\nu_1} + \mathcal{M}_k(m+\nu_1) \, \mathbf{b}_{m-k} \, z^{m+\nu_1} \, \log(z) = 0.$$
(3.28)

The coefficients of each of the terms $z^{m+\nu}$ and $z^{m+\nu}\log(z)$ must vanish. For m=0 this implies

$$\mathcal{M}_0(\nu_1)\boldsymbol{a}_0 = 0, \tag{3.29}$$

as before. For $m = \ell$ this implies

$$\mathcal{M}_0(\ell + \nu_1)\boldsymbol{b}_{\ell} = 0, \tag{3.30}$$

which has a nontrivial solution since $\ell + \nu_1 = \nu_2$ is also an index by assumption. Hence \boldsymbol{b}_{ℓ} must be chosen as a right eigenvector corresponding to the index ν_2 . There is a corresponding left eigenvector $\bar{\boldsymbol{b}}_{\ell}$. For $m = \ell$ we must further have

$$\mathcal{M}_0(\ell + \nu_1) \, \boldsymbol{a}_{\ell} = -p_1 \, \boldsymbol{b}_{\ell} - \sum_{k \ge 1} \mathcal{M}_k(\ell + \nu_1) \, \boldsymbol{b}_{\ell - k}. \tag{3.31}$$

This is not solvable for \mathbf{a}_{ℓ} in general, since $\det \mathcal{M}_0(\ell + \nu_1) = 0$. The solution criterion is that the right-hand side must be orthogonal to the left eigenvector $\bar{\mathbf{b}}_{\ell}$, i.e. that

$$p_1 \, \bar{\boldsymbol{b}}_{\ell} \cdot \boldsymbol{b}_{\ell} + \sum_{k \ge 1} \bar{\boldsymbol{b}}_{\ell} \cdot \mathcal{M}_k(\ell + \nu_1) \, \boldsymbol{b}_{\ell - k} = 0. \tag{3.32}$$

We can always choose the length of b_{ℓ} such that this equation is fulfilled. Then (3.31) can be solved for a_{ℓ} . The solution is not unique. We can add a right eigenvector b_{ℓ} of arbitrary length to a_{ℓ} , and still have a solution. This corresponds to adding a solution proportional to

$$y(z, \nu_2) = \sum_{m>0} a_m(\nu_2) z^{m+\nu_2}.$$

The remaining coefficients can then calculated by the recursion formulas

$$\mathbf{a}_{m+1}(\nu_1) = -\mathcal{M}_0(m+1+\nu_1)^{-1} \sum_{k\geq 1} \mathcal{M}_k(m+1+\nu_1) \, \mathbf{a}_{m+1-k}(\nu_1), \tag{3.33}$$

for $m + 1 = 1, 2, \dots, \ell - 1$, and

$$\mathbf{b}_{m+1}(\nu_1) = -\mathcal{M}_0(m+1+\nu_1)^{-1} \sum_{k\geq 1} \mathcal{M}_k(m+1+\nu_1) \, \mathbf{b}_{m+1-k}(\nu_1),$$

$$\mathbf{a}_{m+1}(\nu_1) = -\mathcal{M}_0(m+1+\nu_1)^{-1} \sum_{k\geq 1} \mathcal{M}_k(m+1+\nu_1) \, \mathbf{a}_{m+1-k}(\nu_1) + p_{k+1} \, \mathbf{b}_{m+1-k}(\nu_1),$$
(3.34)

for $m + 1 = \ell + 1, \ell + 2, \cdots$.

3.3.5. One double degenerate index

Assume next that an index ν_1 is doubly degenerate, that all the others are distinct, and that all index differences are non-integer. If there are two linearly independent right eigenvectors $\mathbf{a}_m(\nu_1, r)$ corresponding to the index ν_1 , then the solution ansatz (3.22) still works:

$$\mathbf{y}(z;\nu_1) = \sum_{m>0} \sum_{r=1}^{2} \mathbf{a}_m(\nu_1, r) z^{m+\nu_1}.$$
 (3.35)

If there is only one eigenvector one again makes an ansatz with a logarithmic term

$$\mathbf{y}(z;\nu_1) = \sum_{m>0} \mathbf{a}_m(\nu_1) z^{m+\nu_1} + \mathbf{b}_m(\nu_1) z^{m+\nu_1} \log(z).$$
 (3.36)

Equation (3.15) implies that

$$\mathcal{M}_0(m+\nu_1) \, \boldsymbol{b}_m + \sum_{k\geq 1} \mathcal{M}_k(m+\nu_1) \, \boldsymbol{b}_{m-k} = 0,$$
(3.37)

$$\mathcal{M}_0(m+\nu_1) \, \boldsymbol{a}_m + p_1 \, \boldsymbol{b}_m + \sum_{k>1} \mathcal{M}_k(m+\nu_1) \, \boldsymbol{a}_{m-k} + p_{k+1} \, \boldsymbol{b}_{m-k} = 0,$$

for $m=0,1,\cdots$, with $\boldsymbol{b}_{-n}=\boldsymbol{a}_{-n}=0$ for $n=1,2,\cdots$. For m=0 this implies that

$$\mathcal{M}_0(\nu_1)\,\boldsymbol{b}_0 = 0,\tag{3.38}$$

i.e. that b_0 must be a right eigenvector corresponding to the index ν_1 , and

$$\mathcal{M}_0(\nu_1) \, \boldsymbol{a}_0 = -p_1 \, b_0. \tag{3.39}$$

Even though det $\mathcal{M}_0(\nu_1) = 0$, this equation does have a solution as explained in subsection 5.1. It is not a unique solution, because we may add a right eigenvector \boldsymbol{b}_0 of arbitrary length to \boldsymbol{a}_0 , and still have a solution.

3.4. Construction of the resolvent

For a real independent variable x an integral expression for a solution of the inhomogenous equation can be written down if n independent solutions $\{y_k(x) \mid k = 1, \dots n\}$ of the homogeneous equation are known. We first find a solution G(x, x') of

$$\left[p_n(x)\frac{d^n}{dx^n} + p_{n-1}(x)\frac{d^{n-1}}{dx^{n-1}} + \dots + p_0(x)\right]G(x, x') = \delta(x - x'). \tag{3.40}$$

A solution of equation (3.1) can then be expressed as

$$f(x) = \int G(x, x')g(x')dx'. \tag{3.41}$$

Since G(x, x') is a solution of the homogeneous equation when $x \neq x'$ we must have

$$G(x, x') = \sum_{k=1}^{n} c_k y_k(x), \tag{3.42}$$

where the coefficients c_k depend on x', and is different for x > x' (denoted $c_k^>$) and x < x' (denoted $c_k^>$). Only the difference $\Delta c_k = c_k^> - c_k^<$ contributes to the inhomogeneous solution. The function G(x,x') and its first n-2 derivatives with respect to x (denoted $G^{(k)}(x,x')$) must be continuous at x=x'. Further, by dividing equation (3.40) by $p_n(x)$, and integrating it from $x=x'-\epsilon$ to $x=x'+\epsilon$ we obtain one more condition. Altogether

$$\lim_{\epsilon \to 0^{+}} \left[G^{(k)}(x' + \epsilon, x') - G^{(k)}(x' - \epsilon, x') \right] = 0, \quad \text{for } k = 0, \dots, n - 2,$$
and
$$\lim_{\epsilon \to 0^{+}} \left[G^{(n-1)}(x' + \epsilon, x') - G^{(n-1)}(x' - \epsilon, x') \right] = p_{n}(x')^{-1}.$$
(3.43)

This can be written in matrix form,

$$\begin{pmatrix} y_1 & y_2 & \cdots & y_n \\ y_1^{(1)} & y_2^{(1)} & \cdots & y_n^{(1)} \\ \vdots & \vdots & & \vdots \\ y_1^{(n-1)} & y_2^{(n-1)} & \cdots & y_n^{(n-1)} \end{pmatrix} \begin{pmatrix} \Delta c_1 \\ \Delta c_2 \\ \vdots \\ \Delta c_n \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ p_n^{-1} \end{pmatrix},$$
(3.44)

where all quantities are evaluated at the point x'. According to Cramer's rule the solution of this equation can be expressed in terms of determinants. For n=2 one finds

$$\begin{pmatrix} \Delta c_1 \\ \Delta c_2 \end{pmatrix} = \frac{1}{W(y_1, y_2)(x') p_2(x')} \begin{pmatrix} -y_2(x') \\ y_1(x') \end{pmatrix}, \tag{3.45}$$

where $W(y_1, y_2)(x') \equiv [y_1(x')y_2'(x') - y_1'(x')y_2(x')]$ is the Wronski determinant. By choosing $c_1^> = c_2^< = 0$ this gives for n = 2,

$$G(x,x') = \frac{y_1(x_{<}) y_2(x_{>})}{W(y_1, y_2)(x') p_2(x')},$$
(3.46)

where $x \le \min(x, x')$ and $x \ge \max(x, x')$.

G(x, x') is the kernel of the integral operator \mathcal{L}^{-1} . This method is often referred to as variation of parameters. It can be extended from equations formulated on the real line to equations formulated on well-behaved curves in the complex plane.

For equations formulated in regions of the complex plane one should instead search for a solution to the problem

$$\mathcal{L}\,\tilde{G}(z,z') = \frac{1}{(z'-z)},\tag{3.47}$$

in terms of which

$$f(z) = \int_{\mathcal{C}} \frac{dz'}{2\pi i} \, \tilde{G}(z, z') g(z'), \tag{3.48}$$

will solve $\mathcal{L}f(z) = g(z)$ when \mathcal{C} is a suitable curve in the z'-plane, encircling the point z once in the positive (anticlockwise) direction.

4. The WKB approximation

It is almost 100 years since Niels Bohr made his first formulations of a quantum theory of matter [17, 18]. Subsequent developments by him and others, including William Wilson [19] and Arnold Sommerfelt [20], completed the "old quantum theory", and led to the formulation of the Bohr-Sommerfelt or Sommerfelt-Wilson or Bohr-Sommerfelt-Wilson quantization rules. With the advent of quantum mechanics and the Schrödinger equation these rules can be derived by the WKB approximation [21–24] to some extent.

In this thesis we have used the WKB method for many purposes: (i) To make a priori estimates of the wave-functions before computing normalization integrals, as done in Paper II [36], (ii) to estimate the magnitude of coefficients in the Frobenius series by use of the leading order WKB approximation, as done in Paper III [37], Paper IV(a) [38] and Paper IV(b) [39] and (iii) to compare the very-high-precision numerical solutions against higher order WKB results, as done in Paper V [40].

The time-independent Schrödinger equation usually has the form

$$\epsilon^2 \psi''(x) = Q(x)\psi(x),\tag{4.1}$$

with Q(x) = V(x) - E. We will mostly consider cases with the boundary condition $\lim_{x\to\pm\infty} \psi(x) = 0$, and where V(x) is a polynomial in x.

The standard WKB formulas can be found in most textbooks on Quantum Mechanics, f.i. [25, 26]. A more thorough discussion is given by Bender and Orszag [27]. Then two leading order WKB solutions of equation (4.1) are

$$\psi_{\pm}(x) = Q(x)^{-1/4} \exp\left(\pm \frac{1}{\epsilon} \int_{-\infty}^{x} \sqrt{Q(t)} \, \mathrm{d}t\right). \tag{4.2}$$

To satisfy the boundary conditions to this order the quantization condition

$$\frac{1}{\epsilon} \int_{x}^{x_{+}} \sqrt{-Q(x)} \, \mathrm{d}x = \left(N + \frac{1}{2}\right) \pi,\tag{4.3}$$

must be fulfilled in the case of a situation with two turning points x_{\pm} at which $Q(x_{\pm}) = 0$, so that $Q(x) \leq 0$ for $x_{-} \leq x \leq x_{+}$. Here $N = 0, 1, \cdots$.

There are two extensions of these formulas which may be less known. These are (i) the Langer correction to (4.2) and (4.3) near a (regular) singular point, and (ii) a more general quantization condition derived by Dunham [28] which makes higher order WKB corrections to (4.3) quite straightforward to compute. These extensions are discussed in this chapter.

¹Note that this notation differs from the corresponding one in paper III [37], paper IV(a) [38], and paper IV(b) [39].

4.1. The Langer correction

Consider a generalization of equation (4.1),

$$\epsilon^2 \left(\frac{d^2}{dx^2} + \frac{1 - \nu_+ - \nu_-}{x} \frac{d}{dx} + \frac{\nu_+ \nu_-}{x^2} \right) \psi(x) = Q(x) \, \psi(x). \tag{4.4}$$

Such equations may f.i. arise as radial equations of rotation symmetric problems. The difference is that we now have a boundary condition at x=0. By writing $x=\mathrm{e}^u$ the point x=0 is transformed to $u=-\infty$. Equation (4.4) becomes, with $\psi(x)=\mathrm{e}^{\frac{1}{2}(\nu_++\nu_-)u}\,\Psi(u)$,

$$\epsilon^2 \left[\frac{d^2}{du^2} - \frac{1}{4} (\nu_+ - \nu_-)^2 \right] \Psi(u) = e^{2u} Q(e^u) \Psi(u).$$
 (4.5)

This equation can now be solved by the WKB method, and transformed back to the x-variable. The results are that

$$\psi_{\pm}(x) \approx x^{\nu_{\pm}} \left(\tilde{Q}(0) / \tilde{Q}(x) \right)^{1/4} \exp\left(\pm \frac{1}{\epsilon} \int_0^x \left[\sqrt{\tilde{Q}(t)} - \sqrt{\tilde{Q}(0)} \right] \frac{\mathrm{d}t}{t} \right).$$
 (4.6)

Here $\tilde{Q}(x) = \frac{1}{4}\epsilon^2(\nu_+ - \nu_-)^2 + x^2 Q(x)$. The normalization has been chosen so that

$$\psi_{\pm}(x) \sim x^{\nu_{\pm}} \text{ as } x \to 0^{+}.$$

The Langer corrected quantization condition becomes

$$\frac{1}{\epsilon} \int_{\tau}^{x_{+}} \sqrt{-\tilde{Q}(t)} \, \frac{\mathrm{d}t}{t} = \left(N + \frac{1}{2}\right) \pi,\tag{4.7}$$

where $\tilde{Q}(x_{\pm}) = 0$ and $\tilde{Q}(x_{\pm}) \leq 0$ for $x_{-} \leq x \leq x_{+}$. This corresponds to the classically allowed region, with x_{\pm} being the classical turning points. For the radial Schrödinger equation in 3 dimensions,

$$-\epsilon^{2} \left(\frac{d^{2}}{dr^{2}} + \frac{2}{r} \frac{d}{dr} - \frac{\ell(\ell+1)}{r^{2}} \right) \psi(r) + V(r) \psi(r) = E \psi(r), \tag{4.8}$$

with $\epsilon^2 = \hbar^2/2m$, we have $\nu_+ = \ell$, $\nu_- = -(\ell+1)$. The quantization condition becomes

$$\frac{1}{\epsilon} \int_{r_{-}}^{r_{+}} \sqrt{E - V(r) - \epsilon^{2} \left(\ell + \frac{1}{2}\right)^{2} r^{-2}} \, dr = \left(N + \frac{1}{2}\right) \pi. \tag{4.9}$$

In this case the Langer correction is a modification of the "centrifugal potential",

$$\frac{\ell(\ell+1)}{r^2} \longrightarrow \frac{\left(\ell+\frac{1}{2}\right)^2}{r^2}.$$

With this correction the WKB quantization formulas for the hydrogen atom and the 3-dimensional rotation symmetric harmonic oscillator turns out to be exact.

4.2. Higher order WKB quantization condition

4.2.1. Recursive calculation of higher order corrections

Higher order corrections to the WKB approximated wave-function,

$$\psi(x) = \exp\left[\frac{1}{\epsilon} \sum_{n=0}^{\infty} \epsilon^n S_n(x)\right]. \tag{4.10}$$

can be found by substituting (4.10) into (4.1), and comparing terms order-by-order in ϵ . We have the equations

$$S_0'^2 = Q, (4.11a)$$

$$S_{n-1}'' + \sum_{j=0}^{n} S_j' S_{n-j}' = 0, \quad \text{for } n = 1, 2, \dots$$
 (4.11b)

We find recursively,

$$S_0' = -\sqrt{Q},\tag{4.12a}$$

$$S'_{n} = \frac{1}{2\sqrt{Q}} \left(S''_{n-1} + \sum_{j=1}^{n-1} S'_{j} S'_{n-j} \right). \tag{4.12b}$$

The first terms of the recursion (4.12b) are

$$S_1'(x) = -\frac{1}{4} \frac{Q'(x)}{Q(x)} = -\frac{1}{2} \frac{d}{dx} \log S_0(x), \tag{4.13a}$$

$$S_2'(x) = \frac{5}{32} \frac{Q'(x)^2}{[Q(x)]^{5/2}} - \frac{1}{8} \frac{Q''(x)}{[Q(x)]^{3/2}},$$
(4.13b)

$$S_3'(x) = -\frac{15}{64} \frac{Q'(x)^3}{Q(x)^4} + \frac{9}{32} \frac{Q'(x)Q''(x)}{Q(x)^3} - \frac{1}{16} \frac{Q'''(x)}{Q(x)^2} = -\frac{1}{2} \frac{d}{dx} \frac{S_2'(x)}{S_0'(x)}.$$
 (4.13c)

There is another solution obtained by changing the sign of all even terms S'_{2m} .

The solutions can also be expressed in terms of multivariate polynomials. Define the infinite-dimensional vector

$$Q = (Q_0, Q_1, \dots, Q_k, \dots) \equiv (Q(x), Q'(x), \dots, Q^{(k)}(x), \dots).$$
(4.14)

Then the general term can be written as

$$S'_{n} = \frac{1}{2} \left[4Q_{0} \right]^{(1-3n)/2} \mathcal{T}_{n}(\mathbf{Q}), \tag{4.15}$$

where $\mathcal{T}_n(\mathbf{Q})$ is a homogeneous n'th order polynomial in the components of \mathbf{Q} , with integer coefficients, and also homogeneous of n'th order in derivatives. I.e., it consists of all monomials of the form

$$Q_0^{n_0}Q_1^{n_1}\cdots Q_k^{n_k}\cdots$$
, with all $n_k\geq 0$, $\sum_k n_k=n$, $\sum_k kn_k=n$.

This means that number of terms in \mathcal{T}_n is equal to the number of partitions of n. The first terms are

$$\mathcal{T}_0 = -1, \tag{4.16a}$$

$$\mathcal{T}_1 = -2Q_1,\tag{4.16b}$$

$$\mathcal{T}_2 = 10 Q_1^2 - 8 Q_0 Q_2, \tag{4.16c}$$

$$\mathcal{T}_3 = -120 Q_1^3 + 144 Q_0 Q_1 Q_2 - 32 Q_0^2 Q_3, \tag{4.16d}$$

$$\mathcal{T}_4 = 2210 Q_1^4 - 3536 Q_0 Q_1^2 Q_2 + 608 Q_0^2 Q_2^2 + 896 Q_0^2 Q_1 Q_3 - 128 Q_0^3 Q_4. \tag{4.16e}$$

Equation (4.13) indicate that each of the odd terms can be written as the derivative of expressions involving the even terms, and hence can be integrated explicitly. This is the case in general. In the classically allowed region, $E \geq V(x)$ or $Q(x) \geq 0$, all even terms S'_{2m} are imaginary and all odd terms S'_{2m+1} are real. I.e, one can write the sum $S' = \sum_{n=0}^{\infty} \epsilon^n S'_n$ as $S' = S'_R + iS'_I$, with $S'_R = \sum_{m=0} \epsilon^{2m+1} S'_{2m+1}$ and $S'_I = \sum_{m=0}^{\infty} \epsilon^{2m} S'_{2m}$ both real. They satisfy the equation

$$(S'_{R} + iS'_{I})^{2} + \epsilon (S''_{R} + iS''_{I}) = -Q.$$
(4.17)

From the imaginary part of this equation we find

$$S_{R}' = -\frac{\epsilon}{2} \frac{d}{dx} \log S_{I}' = -\frac{\epsilon}{2} \frac{d}{dx} \log S_{0}' - \frac{\epsilon}{2} \frac{d}{dx} \log \left(1 + \sum_{m=1}^{\infty} \epsilon^{2m} \frac{S_{2m}'}{S_{0}'} \right), \tag{4.18}$$

which implies that (for m > 0)

$$S'_{2m+1} = -\frac{1}{2} \frac{d}{dx} \log \left(1 + \sum_{k=1}^{\infty} \epsilon^{2k} \frac{S'_{2k}}{S'_0} \right) \bigg|_{\text{Order } \epsilon^{2m} \text{ coefficient}}.$$
 (4.19)

Hence S'_{2m+1} is the derivative of a single-valued function when m > 0. The next example beyond equation (4.13c) is

$$S_5' = -\frac{1}{2} \frac{d}{dx} \left(\frac{S_4'}{S_0'} - \frac{1}{2} \frac{S_2'^2}{S_0'^2} \right). \tag{4.20}$$

This relation is straightforward to verify with a computer algebra program, but the explicit expressions in terms of Q are too lengthy to write down.

One should be aware that the expansion (4.10) will not converge towards the exact result in general. Consider a case with a non-constant Q < 0 everywhere, so that the WKB solution describes a wave moving to (say) the right. The higher order corrections will modify the shape of this right-moving wave, but never generate a left-moving wave. However, the exact solution for a quantum particle moving over a potential barrier will usually contain an exponentially small back-scattered wave. Hence one should expect exponentially small corrections to the WKB-series considered above.

4.2.2. The Dunham formula

We now return to the two-turning point eigenvalue problem (4.1), with a potential V(x) which is assumed to be analytic in x. The two-turning point quantization condition (4.3) has been generalized to arbitrary order in ϵ by Dunham [28] (apparently as part of a Ph.D thesis at Harvard, after which no published research by the author seems to exist),

$$\frac{1}{2i\epsilon} \oint \sum_{n=0}^{\infty} \epsilon^n S_n'(z) dz = N\pi.$$
 (4.21)

The above integral is a complex contour integral which encircles a branch cut between the two classical turning points x_{\pm} on the real axis. The WKB expansion breaks down near the turning points, but by extending the expansion into the complex plane the turning points can be avoided. The quantization condition is obtained by requiring the wave-function to be single valued. The integral in (4.21) is finite because the contour *encircles* the turning points instead of passing through them. The quantization condition (4.3) is recovered by considering the first two terms of the expansion. The contribution from S_0 becomes

$$\frac{1}{2\mathrm{i}\epsilon} \oint S_0'(z) \mathrm{d}z = -\frac{1}{2\mathrm{i}\epsilon} \oint \sqrt{Q(z)} \mathrm{d}z = \frac{1}{\epsilon} \int_{x_1}^{x_2} \sqrt{-Q(x)} \mathrm{d}x,$$

and the contribution from S_1 becomes

$$\frac{1}{2\mathbf{i}} \oint S_1'(z) dz = -\frac{1}{8\mathbf{i}} \oint \frac{d}{dz} \log Q(z) dz = -\frac{1}{8\mathbf{i}} 4\pi \mathbf{i} = -\frac{\pi}{2},$$

since the logarithmic integral encircles two simple zeros. Hence the Dunham quantization condition becomes

$$\frac{1}{\epsilon} \int_{x_1}^{x_2} \sqrt{-Q(x)} dx + \frac{1}{2i\epsilon} \oint \sum_{m=1}^{\infty} \epsilon^{2m} S'_{2m}(z) dz = \left(N + \frac{1}{2}\right) \pi. \tag{4.22}$$

4.2.3. Exactly solved cases

The quantization condition (4.22) seems to depend only on Q(z) in the region near the branch cut from x_1 to x_2 , and therefore obviously cannot always be correct. We could modify the potential in a far-away region, thereby changing the exact eigenvalues, without changing the value of Q(z) in the region of integration. However, this is only possible with a non-analytic potential. The interesting question is whether (4.22) is exact or not for analytic potentials. To our knowledge this had proven to be true for all cases where the expansion in (4.22) can be carried out to all orders, and a comparison with exactly known solutions can be made [28-31].

This is known to be the case for

1. the harmonic oscillator,

$$Q(z) = z^2 - E,$$

where the integration contour of all correction terms in (4.22) can be deformed to infinity, leading to the conclusion that all correction terms vanish. Hence, the condition (4.22) reduces to the standard first order WKB results, which is known to reproduce the correct result.

2. the Morse potential [32],

$$Q(z) = e^{-2z} - e^{-z} - E$$

where the same procedure can be carried out after a change integration variable, $u = e^{-z}$, in (4.22).

3. the radial equation of the hydrogen atom,

$$Q(z) = a z^{-1} + b z^{-2} - E,$$

where the same procedure can also be carried out after a change of integration variable, $u = z^{-1}$, in (4.22).

4. the radial equation of the rotation symmetric harmonic oscillator,

$$Q(z) = a z^2 + b z^{-2} - E.$$

One may show that only a subset of the terms in the WKB expansion have a non-zero integral. These terms can be computed explicitly.

5. the Pöschl-Teller potential [33],

$$Q(z) = a \operatorname{sech}^2 z - E.$$

By introducing the parameter $u = \sinh z$ one may show that only a subset of the terms in the WKB expansion have a non-zero integral. These terms can be computed explicity [29].

All cases have the common property that they have only a single branch cut in the full complex plane of the final integration variable.

4.2.4. Polynomial potentials

Now restrict to the case that Q(x) is a polynomial of order K. We observe from (4.13a-4.13c) that S_n' has the form

$$S'_{n}(x) = \frac{1}{[Q(x)]^{(3n-1)/2}} P_{n}(x), \tag{4.23}$$

where P_n is a polynomial of order (K-1)n. By substituting this ansatz into (4.12b) we verify that it is correct, and find the recursion relation

$$P_{n+1} = \frac{1}{4}(3n-1)Q'P_n - \frac{1}{2}QP'_n + \frac{1}{2}\sum_{j=1}^n P_jP_{n+1-j},$$
(4.24)

with $P_0 = -1$. This gives

$$P_1 = \frac{1}{4}Q',\tag{4.25}$$

$$P_2 = \frac{5}{32}Q'^2 - \frac{1}{8}QQ'', \tag{4.26}$$

$$P_3 = \frac{15}{64}Q'^3 - \frac{9}{32}QQ'Q'' + \frac{1}{16}Q^2Q''', \tag{4.27}$$

and so on. Since every odd S'_{2m+1} , $(m = 1, 2, \cdots)$ is the derivative of a single-valued function it does not contribute to the quantization condition (4.21). Thus, (4.21) simplifies to a sum over even-numbered terms only,

$$\frac{1}{2i\epsilon} \oint \sum_{m=0}^{\infty} \epsilon^{2m} S'_{2m}(z) dz = (N + \frac{1}{2})\pi.$$
 (4.28)

Further, we may subtract any total derivative of the form

$$\frac{d}{dx} \frac{R_{2m}(x)}{[Q(x)]^{\alpha_m}} = \frac{1}{[Q(x)]^{\alpha_m+1}} \left[Q(x) R'_{2m}(x) - \alpha_m Q'(x) R_{2m}(x) \right]$$
(4.29)

(with R_{2m} a single-valued function) from S_{2m} without changing the value of the contour integral. By choosing $\alpha_m = 3m - \frac{3}{2}$, and R_{2m} a polynomial of order (K-1)(2m-1), this can be used to replace P_{2m} , of order (K-1)2m, by a polynomial \tilde{P}_{2m} of order (K-2) or less.

Part III.

Appendices

5. Differential Equations

In this appendix we provide a fairly complete analysis of the general expansion of solutions to a general first order homogeneous linear matrix differential equations at a regular singular point, for the cases when higher order logarithmic terms occur. The derivations are done for the purpose of later numerical implementations, but we have not yet done such implementations.

5.1. Matrices with fewer eigenvectors than eigenvalues

An arbitrary $D \times D$ matrix K cannot be completely diagonalized in general. Although the polynomial eigenvalue equation,

$$\det\left(\mathcal{K} - \mu\right) = 0,\tag{5.1}$$

always has D solutions $\{\mu_d \mid d=1,\ldots,D\}$ counting multiplicities, a d-fold degenerate distinct root μ may have $d_{\mu} < d$ linearly independent eigenvectors (with $d_{\mu} \geq 1$). I.e., the geometric multiplicity d_{μ} of an eigenvalue μ may be lower than its algebraic multiplicity d.

However, any $D \times D$ matrix \mathcal{K} can be brought to *Jordan normal form* [34]. I.e., if \mathcal{K} has d linearly independent eigenvectors it can be similarity transformed to a block diagonal form,

$$\mathcal{J} = \mathcal{S}^{-1} \mathcal{K} \mathcal{S} = \begin{pmatrix} \mathbf{J}_1 & \cdots & \mathbf{0} \\ \vdots & \ddots & \vdots \\ \mathbf{0} & \cdots & \mathbf{J}_d \end{pmatrix}, \tag{5.2}$$

where each block J_n is a $d_n \times d_n$ bidiagonal matrix of form

$$J_n = \begin{pmatrix} \mu_n & 1 & \cdots & 0 \\ 0 & \mu_n & \ddots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mu_n \end{pmatrix}. \tag{5.3}$$

There may be more than one block for each distinct eigenvalue. Now observe that there is a sequence of column vectors,

$$e^{(k)} = (0, \dots, \underbrace{1}_{\text{position } k}, \dots, 0)^T, \quad k = 1, \dots, d_n,$$

(where ^T stands for transposition) such that

$$(J_n - \mu_n) e^{(k)} = e^{(k-1)}, \text{ for } k = 2, \dots, d_n$$
 (5.4)

$$(J_n - \mu_n) e^{(1)} = 0. (5.5)$$

There is also a corresponding sequence of row vectors,

$$\bar{e}^{(k)} = (0, \dots, \underbrace{1}_{\text{position } d_n + 1 - k}, \dots, 0), \quad k = 1, \dots, d_n,$$

such that

$$\bar{\boldsymbol{e}}^{(k)} \left(\boldsymbol{J}_n - \mu_n \right) = \bar{\boldsymbol{e}}^{(k-1)}, \quad \text{for } k = 2, \cdots, d_n$$
(5.6)

$$\bar{\boldsymbol{e}}^{(1)}\left(\boldsymbol{J}_{n}-\boldsymbol{\mu}_{n}\right)=0. \tag{5.7}$$

Equation (5.5) means that $e^{(1)}$ is a right eigenvector of J_n , while equation (5.7) means that $\bar{e}^{(1)}$ is a left eigenvector of J_n , both with eigenvalue μ_n . There is a (perhaps unusual) orthonormality relation for these vectors. Define the "backward identity matrix" E as

$$\boldsymbol{E} = \begin{pmatrix} 0 & 1 \\ & \ddots & \\ 1 & 0 \end{pmatrix}. \tag{5.8}$$

Then we have the relation

$$\bar{\boldsymbol{e}}^{(k)} \boldsymbol{E} \boldsymbol{e}^{(\ell)} = \delta_{k\ell}. \tag{5.9}$$

One may extend the column vectors $\boldsymbol{e}^{(k)}$ to *D*-dimensional column vectors $\boldsymbol{\varepsilon}^{(k,n)}$, and the row vectors $\boldsymbol{\bar{e}}^{(k)}$ to *D*-dimensional row vectors $\boldsymbol{\bar{e}}^{(k,n)}$ by inserting them into the *n*'th block, with zeros in all other blocks. They satisfy the relations

$$(\mathcal{J} - \mu_n) \ \boldsymbol{\varepsilon}^{(k,n)} = \boldsymbol{\varepsilon}^{(k-1,n)}, \quad \text{for } k = 2, \dots, d_n$$
 (5.10)

$$(\mathcal{J} - \mu_n) \, \boldsymbol{\varepsilon}^{(1,n)} = 0, \tag{5.11}$$

for $n = 1, 2, \dots d$. These relations, combined with equation (5.2), means that we can find a solution to the equations

$$(\mathcal{K} - \mu_n) \ \boldsymbol{x}^{(1)} = 0,$$

$$(\mathcal{K} - \mu_n) \ \boldsymbol{x}^{(2)} = c_2 \ \boldsymbol{x}^{(1)}$$

$$\vdots$$

$$(\mathcal{K} - \mu_n) \ \boldsymbol{x}^{(d_n)} = c_{d_n} \ \boldsymbol{x}^{(d_n - 1)},$$

$$(5.12)$$

in terms of the vectors $\mathcal{S}_{\varepsilon}^{(k,n)}$. We make the ansatz $\boldsymbol{x}^{(k)} = N_k \mathcal{S}_{\varepsilon}^{(k,n)} + P_k \mathcal{S}_{\varepsilon}^{(1,n)}$, and find

$$\boldsymbol{x}^{(1)} = N_1 \, \mathcal{S}\boldsymbol{\varepsilon}^{(1,n)},$$

$$\boldsymbol{x}^{(k)} = N_1 \, \prod_{j=2}^k \, c_j \, \mathcal{S}\boldsymbol{\varepsilon}^{(k,n)}, \quad \text{for } k = 2, \dots, d_n,$$

$$(5.13)$$

where N_1 is a free parameter.

5.2. General case

In the general case the initialization step constitutes of finding a complete set of solutions to the equation

$$\left(p_1 z \frac{d}{dz} - \mathbf{A}_0\right) \mathbf{a}(z) = 0. \tag{5.14}$$

5.2.1. The Jordan normal form

 A_0 can be brought to Jordan normal form by a similarity transform [34],

$$\mathbf{A}_0 = \mathcal{S}\mathcal{J}\mathcal{S}^{-1},\tag{5.15}$$

with \mathcal{J} block diagonal

$$\mathcal{J} = \begin{pmatrix} \boldsymbol{J}_1 & \cdots & \boldsymbol{0} \\ \vdots & \ddots & \vdots \\ \boldsymbol{0} & \cdots & \boldsymbol{J}_d \end{pmatrix}. \tag{5.16}$$

Here each block \boldsymbol{J}_n is a $d_n \times d_n$ bidiagonal matrix of form

$$J_{n} = \begin{pmatrix} \lambda_{n} & 1 & \cdots & 0 \\ 0 & \lambda_{n} & \ddots & 0 \\ \vdots & \vdots & \ddots & 1 \\ 0 & 0 & \cdots & \lambda_{n} \end{pmatrix}. \tag{5.17}$$

This representation is unique up to permutation of the blocks. There may be more than one block for each distinct eigenvalue. Introduce $K_n \equiv J_n - \lambda_n$, and observe that (we let T denote transposition)

$$\boldsymbol{K}_{n}^{T} \begin{pmatrix} \alpha_{1} \\ \alpha_{2} \\ \vdots \\ \alpha_{d_{n}} \end{pmatrix} = \begin{pmatrix} 0 \\ \alpha_{1} \\ \vdots \\ \alpha_{d_{n}-1} \end{pmatrix}, \quad \boldsymbol{K}_{n} \begin{pmatrix} \alpha_{1} \\ \alpha_{2} \\ \vdots \\ \alpha_{d_{n}} \end{pmatrix} = \begin{pmatrix} \alpha_{2} \\ \vdots \\ \alpha_{d_{n}} \\ 0 \end{pmatrix}$$
(5.18)

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This means that the matrix

$$\boldsymbol{K}_{n}\boldsymbol{K}_{n}^{T} = \operatorname{diag}(1, 1, \dots, 1, 0) \tag{5.19}$$

is a projection onto the subspace orthogonal to the left eigenvector $\bar{e}_n = (0, \dots, 0, 1)$ of K_n . For a coordinate invariant description, one notes by taking the scalar product of the equation

$$\mathbf{K}_n \mathbf{f} = \mathbf{g} \tag{5.20}$$

with the left eigenvector \bar{e}_n , that

$$\bar{\boldsymbol{e}}_n \boldsymbol{K}_n \boldsymbol{f} = 0 = \bar{\boldsymbol{e}}_n \cdot \boldsymbol{g},$$

since $\bar{e}_n K_n = 0$. Hence, equation (5.20) has a solution only if the solubility condition

$$\bar{\boldsymbol{e}}_n \cdot \boldsymbol{g} = 0 \tag{5.21}$$

is fulfilled. Further, when there is a solution f it cannot be unique; we may always add a term αe_n to f, since $K_n e_n = 0$. When equation (5.21) holds the general solution is

$$\mathbf{f} = \mathbf{K}_n^T \mathbf{g} + \alpha \, \mathbf{e}_n, \tag{5.22}$$

where the coefficient α can be chosen freely.

5.2.2. Solution of a homogeneous block equation

The initialization step consists of finding the general solution of the homogeneous equation

$$\left(p_1 z \frac{d}{dz} - \boldsymbol{J}_n\right) \boldsymbol{\varphi}(z) = 0. \tag{5.23}$$

We make the ansatz

$$\varphi(z) = \sum_{k=0}^{d_n - 1} \varphi_k z^{\nu} \log(z)^{d_n - 1 - k}, \tag{5.24}$$

where $p_1\nu = \lambda_n$ is the eigenvalue of A_0 corresponding to the n'th block. Inserted into equation (5.23) this leads to the conditions

$$K_n \varphi_k = p_1 (d_n - k) \varphi_{k-1}, \text{ for } k = 0, \dots, d_n - 1,$$
 (5.25)

where $\varphi_{-1} \equiv \mathbf{0}$. This means that φ_0 must be an eigenvector of K_n ,

$$\varphi_0 = \alpha_0 \, \boldsymbol{e}_n \equiv \alpha_0 \, \boldsymbol{e}_n^{(0)}$$

The next d_n-1 equations can be solved iteratively,

$$\boldsymbol{\varphi}_k = p_1(d_n - k)\boldsymbol{K}_n^T \boldsymbol{\varphi}_{k-1} + \alpha_k \, \boldsymbol{e}_n = \sum_{j=0}^k \alpha_j \, P_j^k \, \boldsymbol{e}_n^{(k-j)},$$

for $k = 1, \dots, d_n - 1$. Here

$$e_n^{(\ell)} \equiv (\boldsymbol{K}_n^T)^{\ell} \boldsymbol{e}_n$$
, and $P_j^k \equiv \prod_{\ell=j+1}^k p_1 (d_n - \ell)$ with $P_k^k \equiv 1$. (5.26)

Hence we have found a d_n -dimensional space of solutions to equation (5.23),

$$\varphi(z) = \sum_{j=0}^{d_n-1} \alpha_j \sum_{k=j}^{d_n-1} P_j^k e_n^{(k-j)} z^{\nu} \log(z)^{d_n-1-k} \equiv \sum_{j=0}^{d_n-1} \alpha_j \varphi^{(j)}(z),$$
 (5.27)

when $p_1\nu$ is an eigenvalue of J_n with algebraic multiplicity d_n and geometric multiplicity 1.

5.2.3. Solution of an inhomogeneous block equation (regular case)

The recursion step essentially consists of solving an inhomogeneous equation like

$$\left(p_1 z \frac{d}{dz} - J_n\right) \varphi(z) = \sum_{k=0}^{\ell} \chi_k z^{\mu} \log(z)^{\ell-k}.$$
 (5.28)

Assume that $p_1\mu$ is not an eigenvalue of J_n , so that $p_1\mu - J_n$ is invertible. We make the solution ansatz

$$\varphi(z) = \sum_{k=0}^{\ell} \varphi_k z^{\mu} \log(z)^{\ell-k}.$$
 (5.29)

Inserted into equation (5.28) this leads to the conditions

$$(p_1\mu - \boldsymbol{J}_n)\boldsymbol{\varphi}_k = \boldsymbol{\chi}_k - p_1 (\ell + 1 - k) \boldsymbol{\varphi}_{k-1} \quad \text{with } \boldsymbol{\varphi}_{-1} = \boldsymbol{0}.$$
 (5.30)

These can be solved recursively as

$$\varphi_k = (p_1 \mu - J_n)^{-1} \left[\chi_k - p_1 (\ell + 1 - k) \varphi_{k-1} \right]. \tag{5.31}$$

5.2.4. Solution of an inhomogeneous block equation (singular case)

Assume that $p_1\nu = \lambda_n$ is the unique eigenvalue of J_n , i.e. $(p_1\nu - J_n) = -K_n$. To solve equation (5.28) we make the ansatz

$$\varphi(z) = \sum_{k=0}^{d_n+\ell} \varphi_k z^{\nu} \log(z)^{d_n+\ell-k}, \tag{5.32}$$

which inserted leads to the condition

$$K_n \varphi_{k+1} = -\chi_{k+1} + p_1 (d_n + \ell - k) \varphi_k. \tag{5.33}$$

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Here one should interpret $\varphi_{-1} = \mathbf{0}$, and $\chi_k = \mathbf{0}$ for $k = 0, 1 \cdots, d_n - 1$. Since $\bar{e}_n K_n = 0$, equation (5.33) can only have a solution if the right-hand side is orthogonal to \bar{e}_n . I.e.,

$$\bar{\mathbf{e}}_n \cdot \mathbf{\chi}_{k+1} = p_1 \left(d_n + \ell - k \right) \, \bar{\mathbf{e}}_n \cdot \mathbf{\varphi}_k. \tag{5.34}$$

This determines the last component of all but one of the φ_k 's,

$$\varphi_k = C_k^{(d_n - 1)} e_n^{(d_n - 1)} + \tilde{\varphi}_k^{(1)}, \quad \text{for } k = 0, 1, \dots, d_n + \ell - 1.$$
 (5.35)

Here

$$C_k^{(d_n-1)} = \frac{(\bar{\boldsymbol{e}}_n \cdot \boldsymbol{\chi}_{k+1})}{p_1(d_n + \ell - k)} = \frac{(\bar{\boldsymbol{e}}_n^{(0)} \cdot \boldsymbol{\chi}_{k+1})}{p_1(d_n + \ell - k)},$$
(5.36)

and $\tilde{\boldsymbol{\varphi}}_k^{(1)}$ denotes the restriction of $\boldsymbol{\varphi}_k$ to the space orthogonal to $\bar{\boldsymbol{e}}_n$. I.e. the first d_n-1 components of $\boldsymbol{\varphi}_k$. We define $\tilde{\boldsymbol{\chi}}_k^{(1)}$ in the same manner. Insert the partial solution (5.35) into equation (5.33), and use that $\boldsymbol{K}_n\boldsymbol{e}_n^{(d_n-1)}=\boldsymbol{e}_n^{(d_n-2)}$. Since $\boldsymbol{K}_n\tilde{\boldsymbol{\varphi}}_k^{(1)}$ is also orthogonal to the space spanned by $\boldsymbol{e}_n^{(d_n-2)}$, we can use this to determine the last component of all but two of the $\tilde{\boldsymbol{\varphi}}_k^{(1)}$'s,

$$\tilde{\varphi}_k^{(1)} = C_k^{(d_n - 2)} e_n^{(d_n - 2)} + \tilde{\varphi}_k^{(2)}, \quad \text{for } k = 0, 1, \dots, d_n + \ell - 2.$$
(5.37)

Here

$$C_k^{(d_n-2)} = \frac{1}{p_1(d_n+\ell-k)} \left[(\bar{\boldsymbol{e}}_n^{(1)} \cdot \tilde{\boldsymbol{\chi}}_{k+1}^{(1)}) + C_{k+1}^{(d_n-1)} \right], \tag{5.38}$$

and $\tilde{\boldsymbol{\varphi}}_k^{(2)}$ denotes the restriction of $\boldsymbol{\varphi}_k$ to the space orthogonal to $\bar{\boldsymbol{e}}_n^{(0)}$ and $\bar{\boldsymbol{e}}_n^{(1)}$. I.e., the first d_n-2 components of $\boldsymbol{\varphi}_k$. We define $\tilde{\boldsymbol{\chi}}_k^{(2)}$ in the same manner. Note that we cannot determine $C_{d_n+\ell-1}^{(d_n-2)}$ yet, because we do not know $C_{d_n+\ell}^{(d_n-1)}$. The solution process thus far is illustrated by the first two frames of figure 5.1, for the case that $\ell=2$ and $d_n=4$,

Figure 5.1.: This figure give a schematic description of how one can solve the recursion equations at a step m, when $m + \nu_1$ is a multiple root of the indicial equation, and where one already have logarithmic terms in the expansion.

This process can be continued. At step r the vector $\mathbf{K}_n \tilde{\boldsymbol{\varphi}}_k^{(r-1)}$ is orthogonal to $\bar{\boldsymbol{e}}_n^{(0)}, \bar{\boldsymbol{e}}_n^{(1)}, \dots, \bar{\boldsymbol{e}}_n^{(r)}$, leading to

$$\tilde{\varphi}_k^{(r-1)} = C_k^{(d_n-r)} e_n^{(d_n-r)} + \tilde{\varphi}_k^{(r)}, \quad \text{for } k = 0, 1, \dots, d_n + \ell - r,$$
 (5.39)

with

$$C_k^{(d_n-r)} = \frac{1}{p_1(d_n+\ell-k)} \left[(\bar{\boldsymbol{e}}_n^{(r-1)} \cdot \tilde{\boldsymbol{\chi}}_{k+1}^{(r-1)}) + C_{k+1}^{(d_n-r+1)} \right]. \tag{5.40}$$

After d_n steps all consequences of the solubility condition (5.35) have been deduced, as indicated by the third frame of figure 5.1. The first $\ell + 1$ vectors $\varphi_0, \ldots, \varphi_\ell$ are completely determined at this stage. To determine the last d_n vectors completely we solve equation (5.33) in the forward direction,

$$\varphi_k = -\mathbf{K}_n^T \chi_k + p_1(d_n + \ell + 1 - k) \mathbf{K}_n^T \varphi_{k-1} + \alpha_k \mathbf{e}_n,$$
 (5.41)

for $k = \ell + 1, \dots, \ell + d_n$. Each solution involves an arbitrary constant α_k . This process is indicated by the last three frames in figure 5.1.

WKB Quantization of the Quartic **Potential**

The contents of this appendix started out as a small example of the WKB quantization method to high orders. It soon grew in magnitude and resulted in Paper V [40] — and delayed the completion of my thesis with several weeks. It provides more details of the computations reported in Paper V, for the high order WKB analysis of the problem

$$\left[-\epsilon^2 \frac{d^2}{dx^2} + x^4 \right] \psi(x) = E\psi(x). \tag{6.1}$$

One can set the parameter $\epsilon = 1$ without loss of generality, but it is useful for initial organization of the WKB expansion.

6.1. High order WKB expansion

As an example consider the case $V(x) = x^4$. The first few polynomials P_{2m} and \tilde{P}_{2m} become

n	$P_n(x)$	$\tilde{P}_n(x)$
2	$x^6 + \frac{3}{2}Ex^2$	$\frac{1}{2}Ex^2$
4	$14x^{12} + \frac{333}{4}Ex^8 + \frac{321}{8}E^2x^4 + \frac{3}{4}E^3$	$-\frac{77}{1768}E^3$
6	$671x^{18} + \frac{3223}{4}Ex^{14} + \frac{104595}{8}E^2x^{10} + \frac{63075}{16}E^3x^6 + \frac{279}{2}E^4x^2$	$-\frac{61\ 061}{62\ 928}E^4\ x^2$

The general pattern is that

$$\tilde{P}_{4\ell}(x) = (-1)^{\ell} E^{3\ell} p_{\ell}^{(e)},$$
(6.2)

$$\tilde{P}_{4\ell+2}(x) = (-1)^{\ell} E^{3\ell+1} x^2 p_{\ell}^{(o)}, \tag{6.3}$$

where the coefficients $p_\ell^{(e)}$ and $p_\ell^{(o)}$ are positive rational numbers. F.i., as can be seen from the table above, $p_0^{(o)}=\frac{1}{2},\ p_1^{(e)}=\frac{77}{1768},\ p_1^{(o)}=\frac{61\,061}{62\,928}$. Thus we have to do two types of

$$I_k^{(e)} = \frac{1}{2i} \oint \frac{1}{(z^4 - E)^{k+1/2}} dz, \quad \text{for } k = 6\ell - 1,$$

$$I_k^{(o)} = \frac{1}{2i} \oint \frac{z^2}{(z^4 - E)^{k+1/2}} dz, \quad \text{for } k = 6\ell + 2.$$

$$I_k^{(o)} = \frac{1}{2i} \oint \frac{z^2}{(z^4 - E)^{k+1/2}} dz$$
, for $k = 6\ell + 2$

We find, by writing $z = E^{1/4}u$, and deforming the integral along the real axis,

$$I_{-1}^{(e)} = \frac{1}{2i} \oint (z^4 - E)^{1/2} dz = E^{3/4} \int_{-1}^1 du \sqrt{1 - u^4}$$
$$= \frac{1}{2} B(\frac{1}{4}, \frac{3}{2}) E^{3/4} = \frac{1}{3} B(\frac{1}{4}, \frac{1}{2}) E^{3/4}, \tag{6.4}$$

where $B(a,b) = \Gamma(a)\Gamma(b)/\Gamma(a+b)$ is the Beta function. The remaining integrals of interest cannot be deformed to convergent integrals along the real axis, but they are *E*-derivatives of integrals which can be deformed. For k=0 we find, by writing $z=E^{1/4}u$, and deforming the integral along the real axis,

$$\begin{split} I_0^{(\mathrm{e})} &= \frac{1}{2\mathrm{i}} \oint \frac{1}{(z^4 - E)^{1/2}} \, dz = 2 E^{-1/4} \int_0^1 \frac{1}{\sqrt{1 - u^4}} \, du = \frac{1}{2} \mathrm{B}(\frac{1}{4}, \frac{1}{2}) \, E^{-1/4}, \\ I_0^{(\mathrm{o})} &= \frac{1}{2\mathrm{i}} \oint \frac{z^2}{(z^4 - E)^{1/2}} \, dz = 2 E^{1/4} \int_0^1 \frac{u^2}{\sqrt{1 - u^4}} \, du = \frac{1}{2} \mathrm{B}(\frac{3}{4}, \frac{1}{2}) \, E^{1/4}, \end{split}$$

By differentiating these relations k times with respect to E we find

$$I_{k}^{(e)} = (-1)^{k} \frac{1}{2} \frac{\left(\frac{1}{4}\right)\left(\frac{1}{4}+1\right) \cdots \left(\frac{1}{4}+k-1\right)}{\left(\frac{1}{2}\right)\left(\frac{1}{2}+1\right) \cdots \left(\frac{1}{2}+k-1\right)} B\left(\frac{1}{4},\frac{1}{2}\right) E^{-1/4-k}$$

$$= (-1)^{k} \frac{1}{2} B\left(\frac{1}{4},\frac{1}{2}-k\right) E^{-1/4-k},$$

$$I_{k}^{(o)} = (-1)^{k} \frac{1}{2} \frac{\left(-\frac{1}{4}\right)\left(-\frac{1}{4}+1\right) \cdots \left(-\frac{1}{4}+k-1\right)}{\left(\frac{1}{2}\right)\left(\frac{1}{2}+1\right) \cdots \left(\frac{1}{2}+k-1\right)} B\left(\frac{3}{4},\frac{1}{2}\right) E^{1/4-k}$$

$$= (-1)^{k} \frac{1}{2} B\left(\frac{3}{4},\frac{1}{2}-k\right) E^{1/4-k}.$$

$$(6.6)$$

We introduce the quantity

$$\rho = \frac{1}{\pi^4} B(\frac{1}{4}, \frac{1}{2})^4 = \frac{1}{\pi^2} \frac{\Gamma(\frac{1}{4})^4}{\Gamma(\frac{3}{4})^4} \approx 7.764\,068\,784\dots,\tag{6.7}$$

in terms of which $B(\frac{1}{4}, \frac{1}{2}) = \pi \rho^{1/4}$ and $B(\frac{3}{4}, \frac{1}{2}) = 4 \rho^{-1/4}$. Inserting (6.2-6.3) and (6.5-6.6) into (4.21) gives the quantization condition

$$\frac{\pi}{3\epsilon} \rho^{1/4} E^{3/4} - \frac{\epsilon}{4} \rho^{-1/4} E^{-3/4} + \sum_{\ell=1}^{\infty} q_{\ell}^{(e)} \epsilon^{4\ell-1} E^{-(12\ell-3)/4} + \sum_{\ell=1}^{\infty} q_{\ell}^{(o)} \epsilon^{4\ell+1} E^{-(12\ell+3)/4} = \left(N + \frac{1}{2}\right) \pi.$$
(6.8)

Here

$$q_{\ell}^{(e)} = (-1)^{\ell} \frac{1}{2} p_{\ell}^{(e)} \frac{\left(\frac{1}{4}\right)\left(\frac{1}{4} + 1\right) \cdots \left(\frac{1}{4} + 6\ell - 2\right)}{\left(\frac{1}{2}\right)\left(\frac{1}{2} + 1\right) \cdots \left(\frac{1}{2} + 6\ell - 2\right)} \pi \rho^{1/4}, \tag{6.9}$$

$$q_{\ell}^{(o)} = (-1)^{\ell} \, 2p_{\ell}^{(o)} \, \frac{\left(-\frac{1}{4}\right)\left(-\frac{1}{4}+1\right)\cdots\left(-\frac{1}{4}+6\ell+1\right)}{\left(\frac{1}{2}\right)\left(\frac{1}{2}+1\right)\cdots\left(\frac{1}{2}+6\ell+1\right)} \, \rho^{-1/4}. \tag{6.10}$$

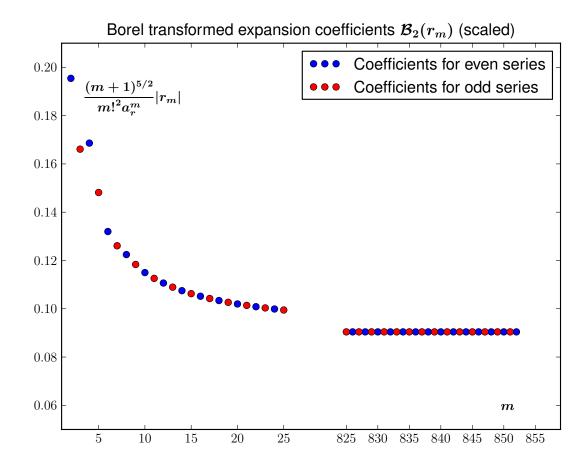


Figure 6.1.: Rescaled form of the WKB expansion coefficients r_m of equation (6.12) for $m=0,\ldots,852$. The index $\nu=\frac{5}{2}$ is chosen as the simplest rational number close to the best fit, after which we find $a_r\approx 0.202\,641\,423\,4$ as the best fit to a sequence approaching a constant absolute value for large m.

By introducing

$$\varepsilon \equiv \kappa^{-1} \epsilon^2 E^{-3/2},\tag{6.11}$$

with $\kappa = \frac{1}{9} \rho^{1/2} \approx 0.309\,600\,873\ldots$, we can rewrite equation (6.8) as

$$\varepsilon = \frac{1}{(N + \frac{1}{2})^2} \left(1 + \sum_{m=1}^{\infty} r_m \, \varepsilon^m \right)^2 \tag{6.12}$$

with new coefficients $r_{2\ell} = \kappa^{2\ell} q_\ell^{(e)}$ and $r_{2\ell+1} = \kappa^{2\ell+1} q_\ell^{(o)}$. The first few terms are

$$r_1 = -\frac{1}{12\pi}, \quad r_2 = \frac{11}{41472}\rho, \quad r_3 = \frac{4697}{7464960}\frac{\rho}{\pi}, \quad r_4 = -\frac{390065}{8026324992}\rho^2.$$

The further coefficients have the form

$$r_{2\ell} = (-1)^{\ell+1} \, \bar{r}_{2\ell} \, \rho^{\ell}, \quad r_{2\ell+1} = (-1)^{\ell+1} \, \bar{r}_{2\ell+1} \, \rho^{\ell}/\pi,$$

where \bar{r}_m are positive rational numbers. The coefficients r_m grow like $m!^2 a_r^m/(m+1)^{\nu}$ in magnitude for large m. We have computed these coefficients up to m=852 (corresponding to the $1\,704^{\rm th}$ order of the WKB expansion). Empirically they fit the cited behaviour quite well, with $a_r \approx 0.202\,641\,423\,4$ and $\nu = \frac{5}{2}$, see figure 6.1.

Obviously the sum $r(\varepsilon) \equiv \sum_{m=0}^{\infty} r_m \varepsilon^{\bar{m}}$ in equation (6.12) has zero radius of convergence. However, if one uses the integral formula

$$m!^{2} = \alpha^{2(m+1)} \int_{0}^{\infty} dx \, x^{m} e^{-\alpha x} \int_{0}^{\infty} dy \, y^{m} e^{-\alpha y}$$

$$= 2\alpha^{2(m+1)} \int_{0}^{\infty} d\xi \, \xi^{m} K_{0}(2\alpha\sqrt{\xi}), \quad \text{with } \alpha = e^{i\phi} \left(-\frac{\pi}{2} < \phi < \frac{\pi}{2}\right), \tag{6.13}$$

and interchange summation and integration, one obtains an integral expression (Borel resummation),

$$r(\varepsilon) = \int_0^\infty dx \, e^{-\alpha x} \int_0^\infty dy \, e^{-\alpha y} \sum_{m=0}^\infty \tilde{r}_m \left(xy a_r \varepsilon \right)^m, \tag{6.14}$$

with

$$\tilde{r}_m = \frac{\alpha^{2(m+1)}}{m!^2 a_r^m} r_m. \tag{6.15}$$

Now the sum

$$\tilde{r}(z) \equiv \sum_{m=0}^{\infty} \tilde{r}_m z^m \tag{6.16}$$

converges for |z| < 1. For $\alpha = 1$ the function $\tilde{r}(z)$ has singularities where $z^2 = -1$, with the singular parts behaving like $(1+z^2)^{3/2}$ near the singularities. In terms of the variable $z^2/(1+z^2)$ this singularity is mapped to ∞ , and the full integration range is mapped to the interval [0,1]. However, when one tries this substitution, in the hope that the (rewritten) sums for $\tilde{r}(z)$ will converge over the full integration range, one discovers that there are additional singularites where $z^2 \approx 4$. Hence, to avoid integrating through a singularity, one must introduce the phase α (or equivalently integrate along a different direction in the complex plane). A convenient choice is $\alpha = \mathrm{e}^{\mathrm{i}\pi/8}$, or its complex conjugate. Actually, to assure a real result after analytic continuation of $\tilde{r}(z)$ beyond the radius of convergence of the sum (6.16), one must take the average of these two choices. This amounts to taking the real part of the integral (6.14).

After this choice we separate $\tilde{r}(z)$ into four (infinite) sums,

$$\tilde{r}(z) = \sum_{p=0}^{3} z^{p} \sum_{\ell=0}^{\infty} \tilde{r}_{4\ell+p} z^{4\ell}.$$

The function defined by each infinite sum is singular at $z^4 = -1$, $z^4 \approx -16$, and probably at infinitely many more points on the negative real z^4 -axis. Now rewrite

$$\sum_{\ell>0} \tilde{r}_{4\ell+p} z^{4\ell} = \sum_{\ell>0} \hat{r}_{4\ell+p} \left(\frac{z^4}{1+z^4}\right)^{\ell}, \tag{6.17}$$

and use the computed coefficients $\tilde{r}_{4\ell+p}$ to find equally many coefficients $\hat{r}_{4\ell+p}$. By computing the sequence of coefficient ratios

$$\rho_{\ell}^{(p)} \equiv \frac{\hat{r}_{4(\ell-1)+p}}{\hat{r}_{4\ell+p}} \tag{6.18}$$

we find empirically (by the ratio test) that the right hand sum of equation (6.17) converges for $|z^4/(1+z^4)| < 1$, see figure 6.2. This completes the construction of a function

$$r(\varepsilon) = \int_0^\infty dx \, e^{-\alpha x} \int_0^\infty dy \, e^{-\alpha y} \, \tilde{r}(xya_r\varepsilon)$$
$$= 2 \int_0^\infty d\xi \, K_0(2\alpha\sqrt{\xi}) \, \tilde{r}(\xi a_r\varepsilon)$$
(6.19)

which has the same asymptotic expansion as the sum in (6.12), and where the integrand, notably $\tilde{r}(z)$, is computable to high precision over the full integration range.

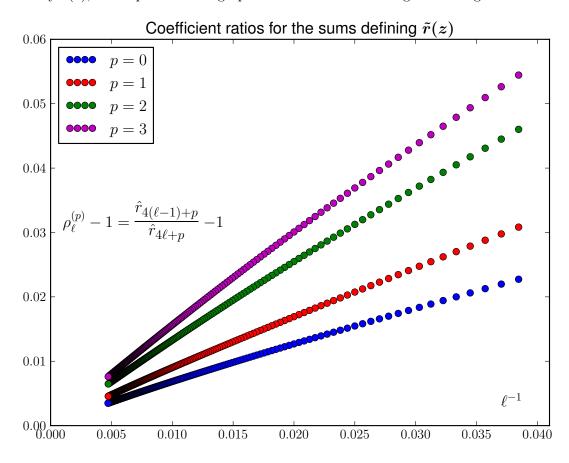


Figure 6.2.: The convergence radius of the right hand sum in equation (6.17) is, according to the ratio test, given by the inverse ratio $\rho_\ell^{(p)}$ of successive terms in this sum as $\ell \to \infty$. The computed ratios give convincing evidence that the convergence radius is unity.

6.2. Series solution of the quantization condition

The quantization condition (6.8) can now be solved numerically by first initializing $\varepsilon = \left(N + \frac{1}{2}\right)^{-2}$, next iterating the recursion

$$\varepsilon \leftarrow \left(N + \frac{1}{2}\right)^{-2} r(\varepsilon)^2 \tag{6.20}$$

until convergence, and finally applying the relation (6.11).

One may also proceed analytically by expressing ε as a series in the (small) quantity $\delta \equiv (N + \frac{1}{2})^{-2}$,

$$\varepsilon = \delta + \sum_{m=2}^{\infty} s_m \, \delta^m. \tag{6.21}$$

The coefficients s_m can be computed recursively. The first terms are

$$s_2 = 2r_1 = -\frac{1}{6\pi}, \quad s_3 = 2r_2 + 5r_1^2 = \frac{11}{20736}\rho + \frac{5}{144\pi^2}.$$
 (6.22)

Computation of the exact s_m , which are polynomials in ρ and π^{-1} with rational coefficients, becomes too memory- and time-consuming beyond the first few tens. We have computed the sequence exactly up to s_{56} , and higher s_m with about 3 800 decimals accuracy.

When the sequence of s_m is known one may use (6.11) to express E as a series in δ ,

$$E \equiv E_N = \kappa^{-2/3} \, \epsilon^{4/3} \, \delta^{-2/3} \, \left(1 + \sum_{m \ge 1} s_{m+1} \delta^m \right)^{-2/3}$$
$$= \kappa^{-2/3} \, \epsilon^{4/3} \, \delta^{-2/3} \, \left(1 + \sum_{m \ge 1} t_m \, \delta^m \right)$$
$$\equiv \kappa^{-2/3} \, \epsilon^{4/3} \, \delta^{-2/3} \, t(\delta). \tag{6.23}$$

The first few terms are

$$t_{1} = \frac{1}{9\pi},$$

$$t_{2} = -\frac{5}{648\pi^{2}} - \frac{11}{31104}\rho,$$

$$t_{3} = \frac{11}{8748\pi^{3}} - \frac{341}{466560}\frac{\rho}{\pi},$$

$$t_{4} = -\frac{1309}{5038848\pi^{4}} + \frac{9163}{25194240}\frac{\rho}{\pi^{2}} + \frac{1748093}{27088846848}\rho^{2}.$$

$$(6.25)$$

In this way an expansion of the WKB-solution (4.10) to order $2\mathcal{N}$ in the quantity ϵ can be used to compute the expansion (6.23) to order \mathcal{N} in the quantity $(N + \frac{1}{2})^{-2}$.

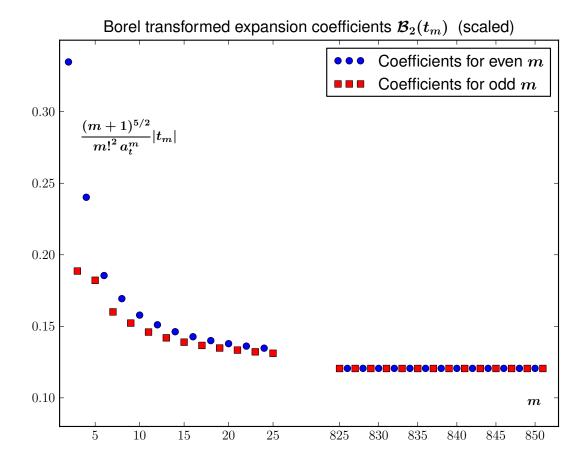


Figure 6.3.: Rescaled form of the expansion coefficients t_m in equation (6.23) for $m=0,\dots,852$. The index $\nu=\frac{5}{2}$ is chosen as the simplest rational number close to the best fit, after which we find $a_t\approx 0.202\,641\,423\,4$ as the best fit to a sequence approaching a constant absolute value for large m. Note the similarity with the r_m -sequence.

6.3. Extended Borel summation of the asymptotic series

The sequence of t_m looks very similar to the sequence of r_m , cf. figure 6.3. Hence one may use the same method to construct a convergent expression which reproduces the series expansion of $t(\delta)$.

We define

$$\tilde{t}_m = \frac{\alpha^{2(m+1)}}{m!^2 a_t^m} t_m, \tag{6.26}$$

and coefficients \hat{t}_m such that

$$\tilde{t}(z) \equiv \sum_{m \ge 0} \tilde{t}_m z^m = \sum_{p=0}^3 z^p \sum_{\ell \ge 0} \hat{t}_{4\ell+p} \left(\frac{z^4}{1+z^4}\right)^{\ell}.$$
 (6.27)

One can use the previously computed coefficients \tilde{t}_m to compute equally many coefficients \hat{t}_m . With the chosen value of $\alpha = e^{i\pi/8}$ the sums over ℓ in equation (6.27) converge for $0 \le z \le \infty$, see figure 6.4.

Then, the expansion of the integral expression

$$t(\delta) = \operatorname{Re}\left\{ \int_0^\infty dx \, e^{-\alpha x} \int_0^\infty dy \, e^{-\alpha y} \, \tilde{t}(xya_t\delta) \right\}$$
 (6.28)

as a series in δ reproduces the sum in equation (6.23). However, this particular integral may not be the best way to use the series expansion.

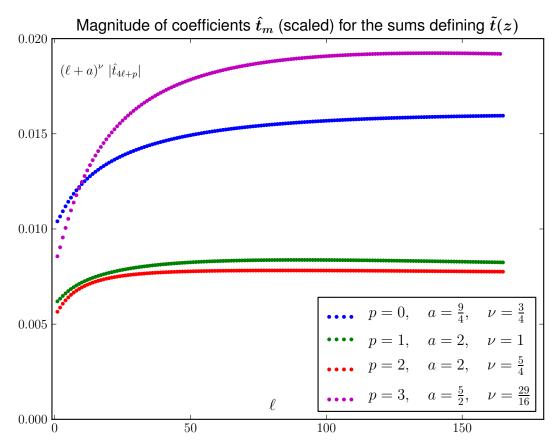


Figure 6.4.: Scaled versions of the expansion coefficients in equation (6.27). They provide convincing evidence for convergence of the sums over the full integration range, $0 \le z \le \infty$.

A better approach is to regenerate the series expansion with an integral expression for the remainder. To this end write

$$e^{-\alpha x} = -\alpha^* \frac{d}{dx} e^{-\alpha x}$$

in equation (6.28), and perform a partial integration,

$$\int_0^\infty dx \, \mathrm{e}^{-\alpha x} \, \int_0^\infty dy \, \mathrm{e}^{-\alpha y} \, \tilde{t}(xya_t\delta) = t_0 + \alpha^* a_t \delta \, \int_0^\infty dx \, \mathrm{e}^{-\alpha x} \, \int_0^\infty dy \, y \, \mathrm{e}^{-\alpha y} \, \tilde{t}^{(1)}(xya_t\delta).$$

By repeating this process M times, and taking the real part, one finds

$$t(\delta) = \sum_{m=0}^{M-1} t_m \, \delta^m + t_{\text{corr}}^{(M)}(\delta), \tag{6.29}$$

with

$$t_{\text{corr}}^{(M)}(\delta) = \text{Re}\left\{ (\alpha^* a_t \delta)^M \int_0^\infty dx \, e^{-\alpha x} \int_0^\infty dy \, y^M \, e^{-\alpha y} \, \tilde{t}^{(M)}(xya_t \delta) \right\}. \tag{6.30}$$

Here

$$\tilde{t}^{(M)}(z) = \frac{d^M}{dz^M} \tilde{t}(z) = \sum_{m \ge 0} (m+M)(m+M-1) \cdots (m+1) \tilde{t}_{m+M} z^m$$

$$\equiv \sum_{m \ge 0} \tilde{t}_m^{(M)} z^m. \tag{6.31}$$

From \mathcal{M} known coefficients \tilde{t}_m one finds $\mathcal{M} - M$ coefficients $\tilde{t}_m^{(M)}$. Again rewrite, cf. equation (6.27),

$$\tilde{t}^{(M)}(z) = \sum_{m \ge 0} \tilde{t}_m^{(M)} z^m = \sum_{p=0}^3 z^p \sum_{\ell \ge 0} \hat{t}_{4\ell+p}^{(M)} \left(\frac{z^4}{1+z^4}\right)^{\ell}, \tag{6.32}$$

and use the known coefficients $\tilde{t}_m^{(M)}$ to compute equally many coefficients $\hat{t}_m^{(M)}$.

We finally insert the expansion (6.32) into (6.30) and perform the integral numerically. This gives $t_{\text{corr}}^{(M)}(\delta)$ to a relative accuracy of about 10^{-10} . As a consistency check we verify that $t(\delta)$ is independent of M, at least for M-values around the point where $\left|t_{\text{corr}}^{(M)}(\delta)\right|$ is minimum. As can be seen qualitatively from figure 6.5 this works well for the lowest eigenvalues. But it also shows that the WKB-series does not reproduce the exact eigenvalues, even when the correction term (6.30) is included. The quantitative results are shown numerically for the two lowest eigenvalues in tables 6.1-6.2.

The WKB-series shows a quite stable result when the correction term from Borel resummation is added, with an uncertainty much smaller than the distance to the exact result. This can be seen for a larger range of eigenvalues in figure 6.6, where we plot $\log |E_{N,\text{exact}} - E_{N,\text{WKB}}|$ as function of N.

Qualitative behaviour of the WKB expansion

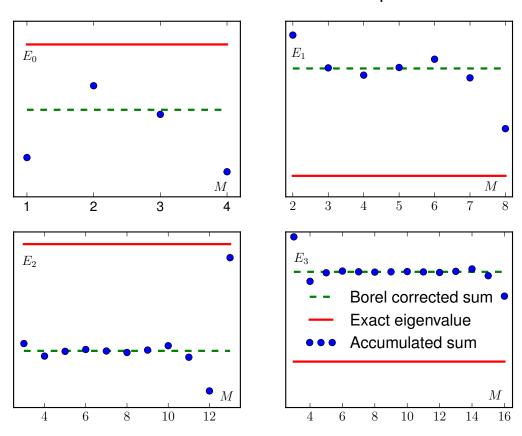


Figure 6.5.: Behaviour of the WKB expansion of the few lowest eigenvalues E_N . The blue points show the (asymptotic) sum $\sum_{m=0}^{M-1} t_m \, \delta^m$ in equation (6.29). The green line shows the full expression $t(\delta)$; it is independent of M to the expected numerical accuracy of the correction term (6.30). The red line shows the exact eigenvalue, evaluated numerically by our very-high-precision routine. The Borel corrected WKB series does not converge towards the exact eigenvalue.

We find empirically that

$$E_{N,\text{exact}} > E_{N,\text{WKB}}$$
 for all even $N = 2M$,

with a difference which varies like $e^{-\pi N}$ with for $N \leq 42$, and approximately like $e^{-\pi(21+N/2)}$ for $N \geq 42$. Further

$$E_{N,\text{exact}} < E_{N,\text{WKB}}$$
 for odd $N = 2M + 1 \le 9$,

also with a difference which varies like $e^{-\pi N}$ with N, and

$$E_{N,\text{exact}} < E_{N,\text{WKB}}$$
 for odd $N = 4M + 3 \ge 11$,

$$E_{N,\text{exact}} > E_{N,\text{WKB}}$$
 for odd $N = 4M + 1 \ge 13$.

In these cases the difference behaves approximately like $e^{-\pi(8+N/4)}$.

 $E_{0,\text{WKB}}^{(M-1)}$ $E_{0,\text{WKB}}^{(M-1)} + E_{0,\text{corr}}^{(M)}$ M $E_{0,\mathrm{exact}}$ 1 $0.867\,145\,326\,484\,821$ $0.949\,048\,242\,147\,079$ $1.060\,362\,090\,484\,183$ 2 $0.989\,821\,295\,452\,906$ $0.949\,048\,242\,213\,528$ $1.060\,362\,090\,484\,183$ 3 $0.940\,878\,506\,803\,713$ $0.949\,048\,245\,949\,142$ $1.060\,362\,090\,484\,183$ 4 $0.842\,885\,181\,871\,221$ $0.949\,048\,880\,595\,005$ $1.060\,362\,090\,484\,183$

Table 6.1.: Behaviour of WKB expansion for E_0

Behaviour of the WKB series for the lowest eigenvalue E_0 . The first column shows the results of summing the first M terms of the WKB-series. The second column the result after the correction term (6.30) from Borel resummation has been added. The last column shows the eigenvalue computed numerically to very high precision.

Table 6.2.: Behaviour of WKB expansion for E_1

M	$E_{1,\mathrm{WKB}}^{(M-1)}$	$E_{1,\text{WKB}}^{(M-1)} + E_{1,\text{corr}}^{(M)}$	$E_{1,\mathrm{exact}}$
1	3.751 919 923 550 433	3.808 235 541 533 203	3.799 673 029 801 394
2	3.810 896 378 060 855	3.808 235 541 533 340	3.799 673 029 801 394
3	3.808 282 018 212 746	3.808 235 541 531 506	3.799 673 029 801 394
4	3.807 700 409 855 639	3.808 235 541 531 468	3.799 673 029 801 394
5	3.808 311 380 649 850	3.808 235 541 532 831	3.799 673 029 801 394
6	3.808 972 737 814 702	3.808 235 541 513 511	3.799 673 029 801 394
7	3.807487485686370	3.808 235 542 141 864	3.799 673 029 801 394
8	3.803 436 692 708 719	3.808 235 536 164 707	3.799 673 029 801 394

Behaviour of the WKB series for the eigenvalue E_1 . The first column shows the results of summing the first M terms of the WKB-series. The second column the result after the correction term (6.30) from Borel resummation has been added. The last column shows the eigenvalue computed numerically to very high precision.

It should be clear that the Dunham quantization formula (4.21) does not provide exact eigenvalues in this case. There are (leading) order correction terms which look intriguingly simple. They are manifestations of the fact that the WKB approximation is inexact, even when summed to arbitrarily high order. Starting with a WKB-solution which behaves like

$$Q(z)^{-1/4} \exp\left(-\frac{1}{\epsilon} \int_{z_0}^z dt \sqrt{-Q(t)} + \cdots\right),$$

no higher-order correction will provide a contribution which changes the sign of the square root, i.e., provides a solution which behave like

$$Q(z)^{-1/4} \exp\left(\frac{1}{\epsilon} \int_{z_0}^z dt \sqrt{-Q(t)} + \cdots\right).$$

However, both behaviours are usually present in the exact solution. In asymptotic analysis they are said to emerge when Stokes lines are crossed.

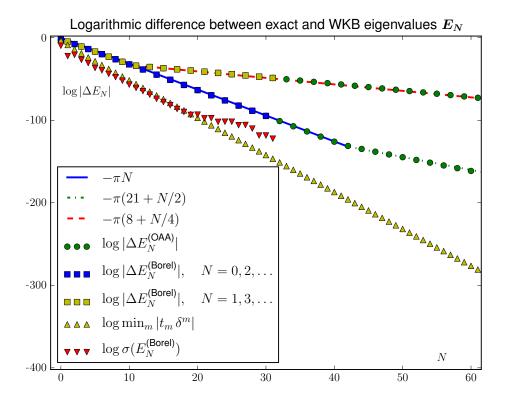


Figure 6.6.: Difference between the exact eigenvalues $E_{N, \text{exact}}$ (computed numerically to very high precision) and the WKB eigenvalues $E_{N, \text{WKB}}$, computed using either the optimal asymptotic approximation (OAA) or adding the correction integral from Borel resummation (Borel). The results of these two methods cannot be distinguished in the figure when $N \geq 1$. The later is found from equation (6.11), with $t(\delta)$ computed from equation (6.29) for a range of M-values around 2.2N. The result varies little with M, as indicated by the plotted standard deviation $\sigma(E_N)$. Hence, the difference between $E_{N,\text{exact}}$ and $E_{N,\text{WKB}}$ is much larger than the uncertainty in $E_{N,\text{WKB}}$ due to numerical evaluation of the integral (6.30), although exponentially small as function of N. The correction terms look quite simple, with an interesting difference between the even and odd eigenvalues.

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