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**Milne Method and Phase-Amplitude
Method**

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Abstract: Bound and quasi-bound states of one-dimensional systems play an important role in quantum physics. In this thesis we solve the Schrödinger equation numerically via the Milne method. We show the relation between the Schrödinger and the Milne equation. The quantum action and the quantum number function are defined. We find bound-state energies of chosen symmetrical and unsymmetrical potentials. Dependence of bound-state energies on the number of points and the step size is studied. We also analyze the influence of the choice of trial energies and the number of iterations. Then we modify the Milne equation and using the phase-amplitude method we illustrate the search of resonances on the example of a diatomic molecule.

Keywords: Schrödinger equation Milne equation bound states quasibound states

Contents

Introduction	2
1 Milne Method	3
1.1 Theoretical Background of the Method	3
1.1.1 Relation between the Schrödinger Equation and the Milne Equation	3
1.1.2 Quantum Number Function	4
1.2 Numerical Illustration	9
1.2.1 Predictor-Corrector Method	9
1.2.2 Integration and Iteration	11
1.2.3 Examples	13
2 Phase-Amplitude Method	29
2.1 Theoretical Background of the Method	29
2.1.1 Modification of the Milne Method	29
2.1.2 Resonance Positions and Widths	31
2.2 Numerical Illustration	31
2.2.1 Solving the Modified Milne Equations	31
2.2.2 Three Criteria for a Resonance	32
2.2.3 Examples	32
Conclusion	34
Bibliography	35
A Attachments	36
A.1 Attachment 1 - Source Code	36

Introduction

One-dimensional time-independent Schrödinger equation plays a crucial role in quantum mechanics. There exist only few systems, for which we know the analytical solution. Therefore, several numerical techniques were developed to tackle the equation.

The subject of our interest are bound states and quasibound states. Systems described by the first include, for example, a symmetrical linear harmonic oscillator or unsymmetrical Morse oscillator and Lennard-Jones potential. The last two mentioned can be used to model a diatomic molecule and can serve as testing systems for more complicated diatomic molecules. Quasibound states including resonances demonstrate themselves in nature as a tunneling rate in α decay [1]; another example is tunneling decay in the case of molecules and molecular ions being in metastable states. Generally, for one-dimensional systems there is a substantial number of applications in electronics and optoelectronics such as LEDs, diodes and photodetectors [2].

In this thesis, we find bound-state energies of chosen symmetrical and unsymmetrical potentials and resonance energies of a diatomic molecule. In the first chapter, we show the relation between the Schrödinger and the Milne equation. We explain how to solve the latter equation and define quantities for determination of bound states. Then we demonstrate the method on examples of the linear harmonic oscillator, the octic oscillator and the Morse potential.

In the second chapter, we explain the need of modification of the Milne method for the search of quasibound states. We discuss the search of resonance widths and illustrate the use of the phase-amplitude method on the example of ${}^3\text{He}{}^4\text{He}^{2+}$.

1. Milne Method

1.1 Theoretical Background of the Method

1.1.1 Relation between the Schrödinger Equation and the Milne Equation

Our goal is to find the solution of the linear differential equation

$$u''(x) + k^2(x)u(x) = 0. \quad (1.1)$$

It can be solved with the help of the non-linear equation [3]

$$w''(x) + k^2(x)w(x) = \frac{1}{w^3(x)} \quad (1.2)$$

since once $w(x)$ is known, $u(x)$ can be generated by means of [4]

$$u(x) = cw(x) \sin \left(a \int_{x_0}^x w^{-2}(x') dx' - b \right), \quad (1.3)$$

where $a, b, c \in \mathbb{R}$. For our purposes we can assume $c \neq 0$ and also $a = 1$.

Proof. Let $\alpha(x) = \int_{x_0}^x w^{-2}(x') dx'$.

$$\begin{aligned} u''(x) &= [cw'(x) \sin(\alpha(x) - b) + cw(x) \cos(\alpha(x) - b) \cdot \alpha'(x)]' = \\ &= c \sin(\alpha(x) - b) [w''(x) - w(x)(\alpha'(x))^2] + \\ &+ c \cos(\alpha(x) - b) [2w'(x)\alpha'(x) + w(x)\alpha''(x)]. \end{aligned} \quad (1.4)$$

According to the fundamental theory of calculus $\alpha'(x) = w^{-2}(x)$. Hence $\alpha''(x) = -2w'(x)w^{-3}(x)$ and we may cancel out the second term in (1.4). We get

$$u''(x) = c \sin(\alpha(x) - b) [w''(x) - w^{-3}(x)],$$

which along with (1.3) turns (1.1) into

$$c \sin(\alpha(x) - b) [w''(x) + k^2(x)w(x) - w^{-3}(x)] = 0.$$

Since the expression in the square bracket is nothing but (1.2), (1.3) is the contrived solution. \square

On the other hand [3],[5]

$$w(x) = \left(Au_1^2(x) + Bu_2^2(x) + 2Cu_1(x)u_2(x) \right)^{1/2}, \quad (1.5)$$

where $\{u_1(x), u_2(x)\}$ is a fundamental set of solutions of (1.1) and A, B and C are constants connected with $AB - C^2 = W^{-2}$, where Wronskian $W(u_1, u_2) = u_1u_2' - u_2u_1'$.

Proof. To show that (1.5) is valid, one may study [6]. \square

We have just shown the relations between $w(x)$ and $u(x)$. Back to Equations (1.1) and (1.2), respectively, we presume

$$p(x, E) = \sqrt{2m(E - V(x))} \quad (1.6)$$

$$k(x, E) = p(x, E)/\hbar. \quad (1.7)$$

Again, V represents the potential energy, m is the mass, \hbar is the so-called reduced Planck constant and E is the energy. For simplicity, let us write $p(x)$ and $k(x)$. The same dependence and simplification will appear in the following paragraphs for functions $w(x, E)$, $K(x, E)$, $\phi(x, E)$ and $u(x, E)$. With Assumptions (1.6) and (1.7) Equation (1.1) becomes the Schrödinger equation. Equation (1.2) is named after Milne, who first derived it [3], [4].

1.1.2 Quantum Number Function

Let $x \in \mathbb{R}$. Our goal is to find the bound-state energies E_n , i.e. eigenvalues of Hamiltonian from (1.1). To manage this, we define the quantum number function $N(E)$ and the density of states $D(E)$. Let $w(x)$ be an arbitrary solution of (1.2), then $u(x)$ (1.3) gives the general solution of (1.1). The energy E and $u(x)$ have real values. As $u_1(x)$, $u_2(x)$ in (1.5) are linearly independent, $w(x)$ cannot be equal to 0 on the real axis. While there are no boundary conditions on $w(x)$, at a bound-state energy $E = E_n$ we require $u \in \mathcal{L}^2(\mathbb{R})$ and consequently $\lim_{x \rightarrow \pm\infty} u(x) = 0$. Considering the argument of the sine function in (1.3), we get the quantisation condition for E_n :

$$\int_{-\infty}^{+\infty} w^{-2}(x)dx = (n + 1)\pi, \quad n \in \mathbb{N}_0, \quad (1.8)$$

where obviously n shows the number of nodes of $u(x)$. Quantum momentum defined as $P(x) = K(x)\hbar$, where $K(x)$ given by

$$K(x) = w^{-2}(x). \quad (1.9)$$

If we substitute $K(x)$ into (1.8), we get

$$N(E) = \frac{1}{\pi} \int_{-\infty}^{+\infty} K(x)dx = n + 1, \quad n \in \mathbb{N}_0. \quad (1.10)$$

This is the quantum number function, which shows us that when $E = E_n$, the area under the $K(x)$ curve is quantised. In other words, it is the function from which E_n will emerge — see the next section. The integral exists also for $E \neq E_n$. For such energies N is not unique — it depends on the choice of $w(x)$ and is only limited by the condition $n < N(E) < n + 1$ [5]. In the article [5], the authors illustrated graphically that $N(E)$ grows with energy. It is demonstrated on the example of the potential, where $V(x) = 0$ for $x \in (-d, d)$ and tends to infinity elsewhere.

Example. Such behaviour of $N(E)$ is proven for a special case of initial conditions more rigorously in [7]. In that paper the solution of the Schrödinger equation (1.1)

$$u(x) = v_1(x) + iv_2(x) \quad (1.11)$$

satisfies the initial conditions

$$v_k(x_0) = \delta_{k1} \quad v'_k(x_0) = \delta_{k2}. \quad (1.12)$$

We assume that $V(x)$ is such that at least one of the v_k 's diverges as $x \rightarrow \pm\infty$ and x_0 is the location of its minimum. Let us write one solution in the form $u(x) = w(x) \exp[i\phi(x)]$, where ϕ satisfies $\phi(x_0) = 0$. The other solution $u^*(x) = w(x) \exp[-i\phi(x)]$; $W(u^*, u) = u^*u' - (u^*)'u$. Using (1.11) and (1.12) one gets $W(u^*, u) = (v_1 - iv_2)(v'_1 + iv'_2) - (v'_1 - iv'_2)(v_1 + iv_2) = v_1v'_1 - v_1v'_1 + 2iv_1v'_2 - 2iv_2v'_1 + v_2v'_2 - v_2v'_2 = 2i(v_1v'_2 - v_2v'_1) = 2i$. Now, substituting the exponential form of u , u^* and their derivatives into the Wronskian yields $W(u^*, u) = w \exp(-i\phi)[w' \exp(i\phi) + i\phi'w \exp(i\phi)] - w \exp(i\phi)[w' \exp(-i\phi) - i\phi'w \exp(-i\phi)] = ww' - ww' + i\phi'w^2 + i\phi w^2$. Then $2iw^2\phi' = 2i$, which along with (1.9) provides the definition of the quantum action [3]

$$\phi(x) = \int_{x_0}^x K(x') dx'. \quad (1.13)$$

This quantity will also be used further on in this section. Let us calculate the first derivative of (1.13) with respect to E , employing (1.9). On the basis of the theory about differentiation under the integral sign, we may change the order of differentiation and integration. Hence

$$\frac{\partial\phi(x)}{\partial E} = \int_{x_0}^x -2w^{-3}(x') \frac{\partial w(x')}{\partial E} dx'.$$

Since $uu^* = w^2$, its derivative w.r.t. E yields

$$\frac{\partial u}{\partial E} u^* + u \frac{\partial u^*}{\partial E} = 2w \frac{\partial w}{\partial E},$$

$$\frac{\partial\phi(x)}{\partial E} = - \int_{x_0}^x \left[\frac{\partial u}{\partial E} u^* + u \frac{\partial u^*}{\partial E} \right] \cdot w^{-4} dx'. \quad (1.14)$$

On the other hand, we have the Schrödinger equation (1.1), which after substitution of k using (1.7) and (1.6) and rearranging the terms yields

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) - E \right] u(x) = 0.$$

Then applying $\frac{\partial}{\partial E}$ this yields

$$\left[\frac{\partial^2}{\partial x^2} - \frac{2m}{\hbar^2} (V(x) - E) \right] \frac{\partial u(x)}{\partial E} = -u(x). \quad (1.15)$$

Now we solve Equation (1.15) using the variation of constants, i.e. we search the general solution of (1.15) in the form

$$\frac{\partial u(x)}{\partial E} = A(x)u_1(x) + B(x)u_2(x),$$

where

$$A(x) = - \int_{x_0}^x \frac{1}{W(u_1, u_2)} u_2(x') f(x') dx',$$

$$B(x) = \int_{x_0}^x \frac{1}{W(u_1, u_2)} u_1(x') f(x') dx',$$

where $f(x')$ is the right hand-side of Equation (1.15). Let $u_1 \rightarrow u^*$ and $u_2 \rightarrow u$. Then

$$A(x) = \frac{1}{2i} \int_{x_0}^x u^2(x') dx',$$

$$B(x) = -\frac{1}{2i} \int_{x_0}^x |u(x')|^2 dx',$$

$$\frac{\partial u(x)}{\partial E} = \frac{1}{2i} \left[u^*(x) \int_{x_0}^x u^2(x') dx' - u(x) \int_{x_0}^x |u(x')|^2 dx' \right], \quad (1.16)$$

$$\frac{\partial u^*(x)}{\partial E} = -\frac{1}{2i} \left[u(x) \int_{x_0}^x u^{*2}(x') dx' - u^*(x) \int_{x_0}^x |u(x')|^2 dx' \right]. \quad (1.17)$$

Now we can substitute (1.16) and (1.17) into (1.14).

$$\begin{aligned} \frac{\partial \phi(x)}{\partial E} &= \frac{1}{2i} \int_{x_0}^x \left[\left(|u(x')|^2 \int_{x_0}^{x'} |u(x'')|^2 dx'' - u^{*2}(x') \int_{x_0}^{x'} u^2(x'') dx'' \right) \right. \\ &\quad \left. - \left(|u(x')|^2 \int_{x_0}^{x'} |u(x'')|^2 dx'' - u^2(x') \int_{x_0}^{x'} u^{*2}(x'') dx'' \right) \right] w^{-4}(x') dx' = \\ &= \frac{1}{2i} \int_{x_0}^x \left[w^2(x') \exp[i2\phi(x')] \int_{x_0}^{x'} w^2(x'') \exp[-i2\phi(x'')] dx'' - \right. \\ &\quad \left. - w^2(x') \exp[-i2\phi(x')] \int_{x_0}^{x'} w^2(x'') \exp[i2\phi(x'')] dx'' \right] w^{-4}(x') dx' = \\ &= \left| \phi(x_0) = 0 \right| = \frac{1}{2i} \int_{x_0}^x w^2(x'') \int_{\phi(x'')}^{\phi(x')} \exp[i2(\phi(x') - \phi(x''))] dx'' - \\ &\quad - \exp[-2i(\phi(x') - \phi(x''))] d\phi(x') dx''. \end{aligned}$$

Setting $\alpha = \phi(x') - \phi(x'')$ (i.e. $d\alpha = d\phi(x')$) and knowing $\frac{\exp(i2\alpha) - \exp(-i2\alpha)}{2i} = \sin(2\alpha) = 2 \sin \alpha \cos \alpha = \partial_\alpha \sin^2 \alpha$, we finally get

$$\frac{\partial \phi(x)}{\partial E} = \int_{x_0}^x w^2(x'') \sin^2 [\phi(x) - \phi(x'')] dx''. \quad (1.18)$$

Let $\beta(x) = \int_{x_0}^x w^2(x'') \sin^2 [\phi(x) - \phi(x'')] dx''$. Using the definition of $N(E)$ (1.10) and (1.13) we get

$$\frac{dN(E)}{dE} = \frac{1}{\pi} (\beta(x)|_{x=+\infty} - \beta(x)|_{x=-\infty}). \quad (1.19)$$

Because of the positivity of the function β , the difference of the integrals is always positive. Hence N grows with E .

Back to Equation (1.3), unlike $K(x)$, $u(x)$ does not hinge on the particular choice of $w(x)$, i.e. on the initial conditions $w(x_0)$, $w'(x_0)$, $x_0 \in \mathbb{R}$. In order to have a smooth $w(x)$, we choose classical initial conditions [3]

$$\begin{aligned} w(x_0) &= K^{-1/2}(x_0) = k^{-1/2}(x_0) \\ w'(x_0) &= -\frac{1}{2}K^{-3/2}(x_0)K'(x_0) = 0. \end{aligned} \quad (1.20)$$

Moreover, let us assume that $V(x)$ has a single minimum $V(x_0)$. The case of double-well potentials is discussed in the Section 1.3.1. Equations (1.20) were arrived at via the WKB theory.

Similarly to (1.13), we define the right-hand and the left-hand action integrals

$$N_{\pm}(E) = \frac{1}{\pi} \int_{x_0}^{\pm\infty} K(x') dx'. \quad (1.21)$$

Therefore, (1.10) yields

$$N(E) = N_+(E) - N_-(E) = n + 1 \quad n \in \mathbb{N}_0. \quad (1.22)$$

The wavefunction (1.3) with (1.9)

$$u(x) = \frac{c}{\sqrt{K(x)}} \sin \left(\int_{x_0}^x K(x') dx' - b \right) \quad (1.23)$$

and the bound-state wavefunction [3]

$$u_n(x) = \frac{c_n}{\sqrt{K(x)}} \sin \int_{-\infty}^x K(x') dx', \quad (1.24)$$

where we require $u_n(x)$ to be square integrable and normalised with $c_n > 0$, that is

$$1 = \int_{-\infty}^{\infty} |u_n^2(x)| dx.$$

Now we will subtract the mathematical identities [8]:

$$\begin{aligned} u \frac{\partial u''}{\partial E} &= \frac{\partial}{\partial x} \left[u \frac{\partial u'}{\partial E} \right] - u' \frac{\partial u'}{\partial E} \\ u'' \frac{\partial u}{\partial E} &= \frac{\partial}{\partial x} \left[u' \frac{\partial u}{\partial E} \right] - u' \frac{\partial u'}{\partial E}. \end{aligned}$$

$$\frac{\partial}{\partial x} \left[u' \frac{\partial u}{\partial E} - u \frac{\partial u'}{\partial E} \right] = u'' \frac{\partial u}{\partial E} - u \frac{\partial u''}{\partial E} = u^2 \frac{\partial k}{\partial E}. \quad (1.25)$$

The last equality emerges from the Schrödinger equation (1.1). Now we can substitute (1.23) into (1.25). Let γ denote $(\int_{x_0}^x K(x') dx' - b)$ or $(\phi - b)$ (1.13),

respectively. Then

$$\begin{aligned}\frac{\partial u'}{\partial E}u &= \frac{\partial}{\partial E} \left((K^{-1/2})' \sin \gamma + K^{1/2} \cos \gamma \right) K^{-1/2} \sin \gamma = \\ &= \frac{\partial(K^{-1/2})'}{\partial E} \sin^2 \gamma + (K^{-1/2})' K^{-1/2} \sin \gamma \cos \gamma \frac{\partial \gamma}{\partial E} + \\ &+ \frac{1}{2} K^{-1} \sin \gamma \cos \gamma \frac{\partial K}{\partial E} - \sin^2 \gamma \frac{\partial \gamma}{\partial E},\end{aligned}$$

$$\begin{aligned}u' \frac{\partial u}{\partial E} &= \left[(K^{-1/2})' \sin \gamma + K^{1/2} \cos \gamma \right] \cdot \left[\frac{\partial(K^{-1/2})}{\partial E} \sin \gamma + K^{-1/2} \cos \gamma \frac{\partial \gamma}{\partial E} \right] = \\ &= \frac{\partial(K^{-1/2})}{\partial E} (K^{-1/2})' \sin^2 \gamma + (K^{-1/2})' K^{-1/2} \sin \gamma \cos \gamma \frac{\partial \gamma}{\partial E} - \\ &- \frac{1}{2} K^{-1} \sin \gamma \cos \gamma \frac{\partial K}{\partial E} + \cos^2 \gamma \frac{\partial \gamma}{\partial E}.\end{aligned}$$

What the integration of (1.25) yields is then

$$\begin{aligned}\left[\left\{ \left(K^{-1/2} \right)' \frac{\partial(K^{-1/2})}{\partial E} - K^{-1/2} \frac{\partial(K^{-1/2})'}{\partial E} \right\} \sin^2(\phi - b) + \frac{\partial(\phi - b)}{\partial E} - \right. \\ \left. - \frac{1}{K} \frac{\partial K}{\partial E} \frac{\sin[2(\phi - b)]}{2} \right]_{x_0}^x = \int_{x_0}^x \frac{1}{K} \sin^2(\phi - b) \frac{\partial k^2}{\partial E} dx'. \quad (1.26)\end{aligned}$$

Since $b \in \mathbb{R}$, we may choose $b = \phi(x)$, which means that concerning the left hand-side of (1.26), there is no contribution of the “ x -term”.

$$\frac{\partial k^2}{\partial E} = \frac{2m}{\hbar^2};$$

$$(K^{-1/2})'(x_0) = 0, \quad \frac{\partial(K^{-1/2})'(x_0)}{\partial E} = 0, \quad \phi(x_0) = 0.$$

Therefore,

$$\begin{aligned}\frac{\partial \phi(x)}{\partial E} &= \frac{2m}{\hbar^2} \int_{x_0}^x \frac{dx'}{K(x')} \sin^2(\phi(x') - \phi(x)) + \\ &+ \frac{1}{2K(x_0)} \frac{\partial K(x_0)}{\partial E} \sin[2\phi(x)].\end{aligned} \quad (1.27)$$

This result corresponds with (1.18) from [7] since their initial conditions $\frac{\partial K(x_0)}{\partial E} = 0$. In our case, i.e. for the classical initial conditions

$$\begin{aligned}\frac{\partial N_{\pm}}{\partial E} &= \frac{2m}{\pi \hbar^2} \int_{x_0}^{\pm\infty} \frac{dx'}{K(x')} \sin^2(\phi(x') - \pi N_{\pm}) + \frac{m}{2\pi p^2(x_0)} \sin(2\pi N_{\pm}) = \\ &= \frac{2m}{\pi \hbar^2} \int_{x_0}^{\pm\infty} \frac{dx'}{K(x')} \sin^2 \left(\int_{\pm\infty}^{x'} K(x'') dx'' \right) + \frac{m}{2\pi p^2(x_0)} \sin(2\pi N_{\pm}).\end{aligned} \quad (1.28)$$

The density of states is equal to

$$D(E) = \frac{\partial N}{\partial E} = \frac{\partial N_+}{\partial E} - \frac{\partial N_-}{\partial E}. \quad (1.29)$$

When $E = E_n$, $\sin(2\pi N_+) - \sin(2\pi N_-) = 2 \sin[\pi(N_+ - N_-)] \cos[\pi(N_+ + N_-)] = 2 \sin[\pi(n + 1)] \cos[\pi(N_+ + N_-)] = 0$, i.e.

$$D(E_n) = \frac{2m}{\pi\hbar^2} \left[\int_{x_0}^{+\infty} \frac{dx'}{K(x')} \sin^2 \left(\int_{+\infty}^{x'} K(x'') dx'' \right) - \int_{x_0}^{-\infty} \frac{dx'}{K(x')} \sin^2 \left(\int_{-\infty}^{x'} K(x'') dx'' \right) \right] = \frac{2m}{\pi\hbar^2} \frac{1}{c_n^2}, \quad (1.30)$$

which means that the normalisation constant of the wavefunction (1.24)

$$c_n = \sqrt{\frac{2m}{\hbar^2\pi} \frac{1}{D(E_n)}}. \quad (1.31)$$

1.2 Numerical Illustration

Using FORTRAN 77 programming language and GNU compiler, we conducted numerical calculations. The code is attached to this work – see the Attachment 1. In it we specify the potential function. As the output we get the set of bound-state energies $\{E_0, \dots, E_M\}$ and the wavefunction connected to one of the energies belonging to $\{E_0, \dots, E_M\}$.

The input consists of the potential function already mentioned, number of bound states $M + 1$ (*NUE* in notation of the program) that we aim to find, step and number of points, by which the grid is constructed, plus three trial energies $E1$, $E2$ and $E3$. With such an input we call subroutine “Quant” for $E1$, $E2$ and $E3$. After we generate the grid (field $X(N)$), potential function $V(N)$ and $K2(k(x))$ in terms of the naming in the previous section), we draw our attention to the Milne equation (1.2).

1.2.1 Predictor-Corrector Method

For solving Equation (1.2) we use the “predictor-corrector” method, which was suggested in 1933 by Milne [3], [5]. Generally, the method deals numerically with the second-order differential equation

$$\frac{d^2y}{dx^2} = f(x, y).$$

In our case

$$f(x, y) = y^{-3} - k^2(x)y. \quad (1.32)$$

From this point we stick to the original notation, i.e. we set y equal to w . Corrector-predictor method is specified by the equidistant set of points $\{x_i\}$. We start the integration at the potential minimum x_0 . Four initial points are needed to be calculated first. To manage this, we have to expand the solution $w(x)$ of (1.2) in the neighborhood of x_0 :

$$w = \sum_{\nu=0}^5 \lambda_\nu (x - x_0)^\nu = \lambda_0 + \lambda_1(x - x_0) + \lambda_2(x - x_0)^2 + \dots \quad (1.33)$$

For proceeding calculations we multiply Equation (1.2) by $w^3(x)$. We obtain

$$w^3(x)w''(x) + k^2(x)w^4(x) = 1. \quad (1.34)$$

Our goal is to find $\{\lambda_i\}$ for $i = 0, 1, \dots, 5$. We substitute (1.33) into (1.34) and expand $k^2(x)$ about x_0 :

$$\begin{aligned} k^2(x) &= \frac{2m[E - V(x_0)]}{\hbar^2} - \frac{2m}{\hbar^2}V'(x_0)(x - x_0) - \frac{m}{\hbar^2}V''(x_0)(x - x_0)^2 \\ &\quad - \frac{m}{3\hbar^2}V'''(x_0)(x - x_0)^3 - \frac{m}{12\hbar^2}V^{IV}(x_0)(x - x_0)^4 - \frac{m}{60\hbar^2}V^V(x_0)(x - x_0)^5. \end{aligned}$$

From the initial conditions (1.20) we know that $w(x_0) = k^{-1/2}(x_0)$. Therefore, from (1.33) obviously $\lambda_0 = k^{-1/2}(x_0)$. Now we inspect the coefficients λ_i in front of the $(x - x_0)^0$ power of (1.34). We get

$$\begin{aligned} 2\lambda_0^3\lambda_2 + \frac{2m[E - V(x_0)]}{\hbar^2}\lambda_0^4 &= 1 \\ 2k^{-3/2}(x_0)\lambda_2 + \frac{2m[E - V(x_0)]}{\hbar^2}k^{-2}(x_0) &= 1. \end{aligned}$$

The second term on the left hand-side of this equation is equal to 1. Hence $\lambda_2 = 0$. From the second initial condition (1.20) we know that $w'(x_0) = 0$. On the other hand

$$w'(x) = \lambda_1 + 2\lambda_2(x - x_0) + \dots,$$

therefore $w'(x_0) = \lambda_1$ and necessarily $\lambda_1 = 0$. Now we look at the $(x - x_0)$ power:

$$6\lambda_0^3\lambda_3 + 2\lambda_2 3\lambda_0^2\lambda_1 + \frac{2m[E - V(x_0)]}{\hbar^2} \cdot 4\lambda_0^3\lambda_1 - \frac{2m}{\hbar^2}V'(x_0) = 0.$$

Substituting $\lambda_1, \lambda_2 = 0$ and $V'(x_0) = 0$ (potential minimum), we gain $\lambda_3 = 0$. Let us inspect coefficients of $(x - x_0)^2$:

$$\begin{aligned} 12\lambda_4\lambda_0^3 + \underbrace{18\lambda_0\lambda_1\lambda_3}_{=0} + \underbrace{6\lambda_0^2\lambda_2}_{=0} + \frac{2m[E - V(x_0)]}{\hbar^2} \cdot (\underbrace{6\lambda_0^2\lambda_1^2}_{=0} + \underbrace{4\lambda_0^3\lambda_2}_{=0}) + \\ + 0 - \lambda_0^4 \frac{m}{\hbar^2}V''(x_0) = 0. \end{aligned}$$

Then $\lambda_4 = \frac{m}{12\hbar^2}V''(x_0)\lambda_0 = \frac{m}{12\hbar^2}V''(x_0)w(x_0)$. Last but not least, let us inspect the $(x - x_0)^3$ power:

$$\begin{aligned} 20\lambda_5\lambda_0^3 + \underbrace{36\lambda_0^2\lambda_1\lambda_4}_{=0} + \underbrace{6\lambda_0^2\lambda_3\lambda_2}_{=0} + \frac{2m[E - V(x_0)]}{\hbar^2} \cdot (\underbrace{4\lambda_0\lambda_1^3}_{=0} + \underbrace{12\lambda_0^2\lambda_1\lambda_2}_{=0} + \underbrace{4\lambda_0^3\lambda_3}_{=0}) + \\ + 0 - \underbrace{\frac{4m}{\hbar^2}V''(x_0)\lambda_0^3\lambda_2}_{=0} - \frac{m}{3\hbar^2}V'''(x_0)\lambda_0^4 = 0. \end{aligned}$$

As a result $\lambda_5 = \frac{m}{60\hbar^2}V'''(x_0)w(x_0)$.

Altogether

$$\begin{aligned} w &= k^{-1/2}(x_0) + \frac{m}{12\hbar^2}V''(x_0)w(x_0)(x-x_0)^4 + \frac{m}{60\hbar^2}V'''(x_0)w(x_0)(x-x_0)^5 = \\ &= k^{-1/2}(x_0) \left[1 + \frac{m}{12\hbar^2}V''(x_0)(x-x_0)^4 + \frac{m}{60\hbar^2}V'''(x_0)(x-x_0)^5 \right]. \end{aligned} \quad (1.35)$$

As we may observe, it was fully sufficient to take into account the powers i of $(x-x_i)^i$ corresponding with λ_i and omit the rest. We use formula (1.35) to calculate first four initial points $x_i = x_0 + ih$ of $w(x)$, where step $h = x_{i+1} - x_i$. If we integrate to the right hand-side, then $i = -1, 0, 1, 2$; integration to the left inverts the sign of i . In the next step we calculate points $f(x_i)$ using (1.32) for the values of i already mentioned and we get $w(x_3)$, $w(x_4)$ or $w(x_{-3})$, $w(x_{-4})$, respectively, with the use of the equations

$$\begin{aligned} w_{i+1} &= w_i + w_{i-2} - w_{i-3} + \frac{\hbar^2}{4}(5f_i + 2f_{i-1} + 5f_{i-2}), \\ f_{i+1} &= f(x_{i+1}, w_{i+1}), \\ w_{i+1} &= 2w_i - w_{i-1} + \frac{\hbar^2}{12}(f_{i+1} + 10f_i + f_{i-1}). \end{aligned}$$

For other points the following formulas are needed:

$$\begin{aligned} w_{i+1} &= w_i + w_{i-4} - w_{i-5} + \frac{\hbar^2}{48}(67f_i - 8f_{i-1} + 122f_{i-2} - 8f_{i-3} + 67f_{i-4}), \\ w_{i+1} &= w_i + w_{i-2} - w_{i-3} + \frac{\hbar^2}{240}(17f_{i+1} + 232f_i + 222f_{i-1} + 232f_{i-2} + 17f_{i-3}). \end{aligned}$$

In the program we set the lower limit of the magnitude of the calculated function $w(x)$ equal to 10^{-15} . This corresponds with the fact that we work in double precision. Precision is discussed further in the thesis. The lower limit concretely concerns the end points, where from our calculations we find out that $w(x) \rightarrow 0$.

In the case of symmetrical potentials, it is fully sufficient to integrate to one of the hand-sides and set the unknown values of $w(x)$ equal to the ones on the other hand-side.

1.2.2 Integration and Iteration

In the following step we demand that the number of points $NMIN$ and $NMAX$ is divisible by four, so that in all proceeding calculations the condition for the number of integration points is correct.

According to the formula (1.9), we calculate “ $KK(N)$ ”. Then we integrate it in the way as written in (1.21) and get the right-hand and the left-hand action integrals NQR and NQL . We use Composite Simpson’s rule, which we have tested before on simpler functions. Using (1.22) we finally get the quantum number function NQ , which is the output of the subroutine “Quant”. Now we can

proceed to the calculation of bound states E_n .

Back to the main program, now with the three known values of NQ — let us label them $N1$, $N2$ and $N3$ — we calculate coefficients α_1 , α_2 and α_3 via solving the linear equations

$$E_\nu(N_\nu) = \alpha_1 N_\nu + \alpha_2 N_\nu^2 + \alpha_3 N_\nu^3, \quad (1.36)$$

where E_ν , $\nu = 1, 2, 3$, stands for $E1$, $E2$ and $E3$, and analogically we substitute $N1$, $N2$ and $N3$ for N_ν . We use Cramer's rule. The known coefficients α_1 , α_2 and α_3 can be now substituted back into Equation (1.36) and what we obtain is a “trial energy”, for which we call another subroutine called “DensG”.

In the first part of this subroutine, we call “Quant”. In it we do some technical work with fields $X(N)$ and $KK(N)$ (the reason is explained further in this section): we shift the fields so that they start at $N = 0$. This rearrangement is needed for the functions “spline” and “splint”, which follow.

In “spline” one calculates the second derivative of KK in the defined points. Then new “x-values” of KK are constructed: our goal is to divide each interval $x_{i+1} - x_i$ into two pieces or in other words add to the “x-field” the points in the middle of each interval $x_{i+1} - x_i$. After that, using the values from “spline”, we proceed to the function “splint” to gain “y-values” of KK .

Now we have a new field KK with a double number of points compared to the original field. At this point we find the density of states (1.29). We calculate (1.28). The inner integral is summed using the already mentioned Composite Simpson's rule, the outer integral is counted with the use of Trapezoidal rule, which have been again tested on simpler functions first. Because of the division of the intervals of KK , we get values for all original points. This is the reason, why we used functions “spline” and “splint” — to keep the original input. Trapezoidal rule is accurate enough - there is no need to use more precise methods of integration such as Simpson's rule or Boole's rule. On the basis of our calculations we found out that it would have no effect on the precision of the calculation.

Back to the main program, we use the calculated values of quantum number function NQ along with the density of states DD and calculate another energy E using

$$E = E + [(M + 1) - NQ]/DD,$$

where E on the right hand-side represents the “trial energy” and $(M + 1)$ is connected to the M -th eigenvalue. We iterate until we receive the M -th eigenvalue. This procedure is repeated for other values of M corresponding with NUE . As a final result we obtain the set of bound-state energies $\{E_0, \dots, E_M\}$. The number of iterations needed is discussed further in this section.

Now let us find eigenstates. In the main program we choose an eigenvalue for which we seek the wavefunction. Again, we call subroutine “DensG”, now with an additional part consisting of the calculation of a normalisation constant via

(1.31) to calculate the integral in (1.23) with the help of Composite Simpson's rule.

In the case of symmetrical potentials, it is sufficient to integrate to one of the sides and set the unknown values of $w(x)$ equal to the other side (Side contains the interval starting at the potential minimum and ending at $NMIN$ or $NMAX$).

1.2.3 Examples

LHO

As an illustrative example we take the **1D linear harmonic oscillator**, where $m, \hbar, \omega = 1$ and the potential function is $V(x) = \frac{1}{2}x^2$. Our goal is to solve the Schrödinger equation 1.1. We use the standard abbreviation LHO. Since we know the analytic solution $u_n(x) = \frac{1}{\sqrt{2^n n!}} \pi^{-1/4} \exp(-x^2/2) H_n(x)$ and $E_n = (n + \frac{1}{2})$ from theory, where H_n represents the Hermite polynomials and n is the $(n+1)$ -th bound state, we use this system as a test example.

We will be interested in how many times it is needed to iterate before we obtain bound-state energies with desired accuracy. Also, we will investigate how the calculated energies E_n depend on the choice of trial energies $E1, E2, E3$ and on the number of integration points and the magnitude of the step h for fixed values of $E1, E2, E3$ and the number of iterations it .

We will also demonstrate the behaviour of the functions $K(x, E)$, which play a major role in the method. We will plot several wavefunctions for chosen energies, by which we will show that the calculation of a wavefunction is correct. Consequently, this will allow us to calculate wavefunctions of other symmetrical potentials. Also, we will illustrate the $N(E)$ and $D(E)$ -dependence for this particular system.

At this place we could also discuss the general accuracy of the program, however, we will leave this onto a separate section, where we will also investigate the behaviour at the end points.

We choose $E1 = 45, E2 = 20$ and $E3 = 0.5$. In Table 1.1 we present the dependence of calculated bound-state energies E_n on the number of iterations it . $NMIN$ and $NMAX$ is connected with the step h in a way that both $X(NMIN)$ and $X(NMAX)$ have always the same value. In this case we take the step $h = 0.01$ and the number of points $NMIN = -1000$ and $NMAX = 1000$. Tables 1.2 and 1.3 illustrate the same dependence with a different step and a number of points. In the first case, we take $h = 0.0025, NMIN = -4000$ and $NMAX = 4000$, while in the other case, we set $h = 0.025, NMIN = -400$ and $NMAX = 400$. Let us focus on each table separately and then compare them with each other.

As for Table 1.1, it can be observed that comparing the resulting energies after two iterations with the ones after three iterations, the resulting energies are more precise in the second case. Mostly by 2 digits. In the case of E_0 the differ-

ence counts 0 digits; on the contrary in the cases of E_2 and E_3 , the difference is 5 digits. We may assume that the iteration invariance of E_0 corresponds with the exact solution taken as E_3 .

We will take a closer look at the choice of trial energies in the following paragraphs. As for more iterations, there is almost no difference in accuracy between $it = 3$, $it = 4$ and $it = 5$. Therefore, we naturally expect higher values of it to demonstrate the same phenomenon, which is indeed confirmed with $it = 10$.

From Table 1.2 we can see that in the case of a smaller step h , i.e. higher number of integration points, we receive similar results. If we opt for a lower number of integration points — see Table 1.3, we find out that for $it > 3$ we obtain the same accuracy as for $it = 3$ with no exception. Comparing Table 1.1 with Table 1.2, we see, that we generally get the results of the same accuracy even for $it = 2$, however, if we decide to count with a higher number of integration points, the comparison of results for different it gives us the condition to use $it > 2$. To keep the time of calculations the lowest, we choose $it = 3$.

To sum it up, in the case of symmetrical potentials (asymmetrical potentials will be studied later) it is sufficient and needed to iterate three times in order to get satisfying accuracy, which is also a matter of convenience because it of such a low value speeds up the calculation.

Now let us inspect the choice of trial energies E_1 , E_2 and E_3 . On the basis of previous results, we set $it = 3$. From Table 1.4 it is obvious that we can choose E_1 , E_2 and E_3 , which are further from E_n .

Table 1.1: Dependence of the calculated bound-state energies E_n of LHO on the number of iterations it for the step $h = 0.01$ and the number of points $NMIN = -1000$, $NMAX = 1000$. We list the first 11 energies.

n	$E_n, it = 2$	$E_n, it = 3$	$E_n, it = 4$
0	0.50000000004460	0.50000000004462	0.50000000004459
1	1.50000000507697	1.50000000000914	1.50000000000915
2	2.49999886500916	2.50000000009996	2.50000000009996
3	3.50000026660797	3.50000000000584	3.50000000000584
4	4.4999998397862	4.50000000013407	4.50000000013406
5	5.50000000069406	5.50000000000653	5.50000000000649
6	6.4999999735715	6.50000000016159	6.50000000016164
7	7.50000000213856	7.50000000000569	7.50000000000570
8	8.4999999916786	8.50000000018131	8.50000000018130
9	9.50000000047519	9.50000000000792	9.50000000000792
10	10.5000000002764	10.50000000020212	10.50000000020210
n	$E_n, it = 5$	$E_n, it = 10$	
0	0.50000000004461	0.50000000004462	
1	1.50000000000916	1.50000000000915	
2	2.50000000009995	2.50000000009993	
3	3.50000000000582	3.50000000000583	
4	4.50000000013403	4.50000000013406	
5	5.50000000000652	5.50000000000653	
6	6.50000000016162	6.50000000016163	
7	7.50000000000571	7.50000000000571	
8	8.50000000018129	8.50000000018129	
9	9.50000000000793	9.50000000000793	
10	10.50000000020212	10.50000000020210	

Table 1.5 shows the dependence of bound-state energies of LHO on the number of integration points and the step. It can be observed that in the case of /a/ and /b/ odd energies are by 1-3 digits more precise. This phenomenon ceases with a higher number of integration points /c/ and /d/. The accuracy of E_n depends on the number of integration points and the step. We can reach the accuracy 10^{-12} .

Figure 1.1 shows how the quantum number function N and the density of states D depend on energy. Figure 1.2 illustrates the function $K(x)$ for certain bound-state energies E_n . Corresponding wavefunctions u_n are plotted in Figure 1.3.

Table 1.2: Dependence of the calculated bound-state energies E_n of LHO on the number of iterations it for the step $h = 0.0025$ and the number of points $NMIN = -4000$, $NMAX = 4000$. We list the first 11 energies.

n	$E_n, it = 2$	$E_n, it = 3$	$E_n, it = 4$
0	0.50000000000562	0.50000000000549	0.50000000000552
1	1.500000000516774	1.50000000000665	1.50000000000640
2	2.49999886898550	2.50000000000566	2.50000000000587
3	3.50000026318464	3.50000000000589	3.50000000000578
4	4.49999998433134	4.50000000000606	4.50000000000590
5	5.50000000068621	5.50000000000563	5.50000000000587
6	6.49999999736013	6.50000000000586	6.50000000000584
7	7.50000000195649	7.50000000000583	7.50000000000590
8	8.49999999912288	8.50000000000581	8.50000000000577
9	9.50000000039703	9.50000000000561	9.50000000000539
10	10.49999999986822	10.50000000000594	10.50000000000592
n	$E_n, it = 5$	$E_n, it = 10$	
0	0.50000000000545	0.50000000000543	
1	1.50000000000637	1.50000000000640	
2	2.50000000000582	2.50000000000597	
3	3.50000000000571	3.50000000000557	
4	4.50000000000625	4.50000000000621	
5	5.50000000000563	5.50000000000558	
6	6.50000000000585	6.50000000000585	
7	7.50000000000563	7.50000000000589	
8	8.50000000000582	8.50000000000574	
9	9.50000000000564	9.50000000000544	
10	10.50000000000594	10.50000000000594	

Table 1.3: Dependence of the calculated bound-state energies E_n of LHO on the number of iterations it for the step $h = 0.025$ and the number of points $NMIN = -400$, $NMAX = 400$. We list the first 11 energies.

n	$E_n, it = 2$	$E_n, it = 3$	$E_n, it = 4$
0	0.50000000370057	0.50000000370057	0.50000000370058
1	1.50000000459684	1.50000000003827	1.50000000003828
2	2.49999885153179	2.50000000924097	2.50000000924098
3	3.50000028588758	3.50000000005840	3.50000000005840
4	4.49999999356111	4.50000001250217	4.50000001250217
5	5.50000000076970	5.50000000006826	5.50000000006827
6	6.50000001145418	6.50000001507693	6.50000001507694
7	7.50000000315859	7.50000000007129	7.50000000007129
8	8.50000001560191	8.50000001730162	8.50000001730162
9	9.50000000091168	9.50000000005690	9.50000000005690
10	10.50000001894249	10.50000001929450	10.50000001929451
n	$E_n, it = 5$	$E_n, it = 10$	
0	0.50000000370057	0.50000000370057	
1	1.50000000003828	1.50000000003827	
2	2.50000000924099	2.50000000924099	
3	3.50000000005840	3.50000000005840	
4	4.50000001250217	4.50000001250216	
5	5.50000000006827	5.50000000006827	
6	6.50000001507694	6.50000001507693	
7	7.50000000007129	7.50000000007129	
8	8.50000001730162	8.50000001730162	
9	9.50000000005690	9.50000000005690	
10	10.50000001929450	10.50000001929451	

Table 1.4: Dependence of the calculated bound-state energies E_n of LHO on the choice of trial energies $E1$, $E2$ and $E3$ for $h = 0.0025$, no. of points 8001, /1/ $E1 = 12$, $E2 = 5$, $E3 = 0.3$, /2/ $E1 = 90$, $E2 = 5$, $E3 = 0.6$, /3/ $E1 = 50$, $E2 = 20$, $E3 = 0.6$.

n	/1/	/2/	/3/
0	0.50000000000546	0.50000000000527	0.50000000000566
1	1.50000000000663	1.50000000000668	1.50000000000634
2	2.50000000000591	2.50000000000568	2.50000000000583
3	3.50000000000580	3.50000000000581	3.50000000000593
4	4.50000000000620	4.50000000000616	4.50000000000611
5	5.50000000000558	5.50000000000554	5.50000000000554
6	6.50000000000616	6.50000000000601	6.50000000000602
7	7.50000000000569	7.50000000000576	7.50000000000553
8	8.50000000000577	8.50000000000576	8.50000000000570
9	9.50000000000547	9.50000000000569	9.50000000000557
10	10.50000000000591	10.50000000000601	10.50000000000574

Table 1.5: Computed bound-state energies of LHO using the Milne method: [a] $h = 0.025$, no. of points 801, [b] $h = 0.01$, no. of points 2001, [c] $h = 0.0025$, no. of points 8001, [d] $h = 0.001$, no. of points 20001.

n	[a]	[b]	[c]
0	0.50000000370057	0.50000000004462	0.50000000000549
1	1.50000000003827	1.50000000000914	1.50000000000665
2	2.50000000924099	2.50000000009996	2.50000000000566
3	3.50000000005840	3.50000000000584	3.50000000000589
4	4.50000001250216	4.50000000013407	4.50000000000606
5	5.50000000006827	5.50000000000653	5.50000000000563
6	6.50000001507693	6.50000000016159	6.50000000000586
7	7.50000000007129	7.50000000000569	7.50000000000583
8	8.50000001730162	8.50000000018131	8.50000000000581
9	9.50000000005690	9.50000000000792	9.50000000000561
10	10.50000001929451	10.50000000020212	10.50000000000594
n	[d]		
0		0.50000000000598	
1		1.50000000000577	
2		2.50000000000481	
3		3.50000000000543	
4		4.50000000000544	
5		5.50000000000555	
6		6.50000000000483	
7		7.50000000000627	
8		8.50000000000485	
9		9.50000000000554	
10		10.50000000000484	

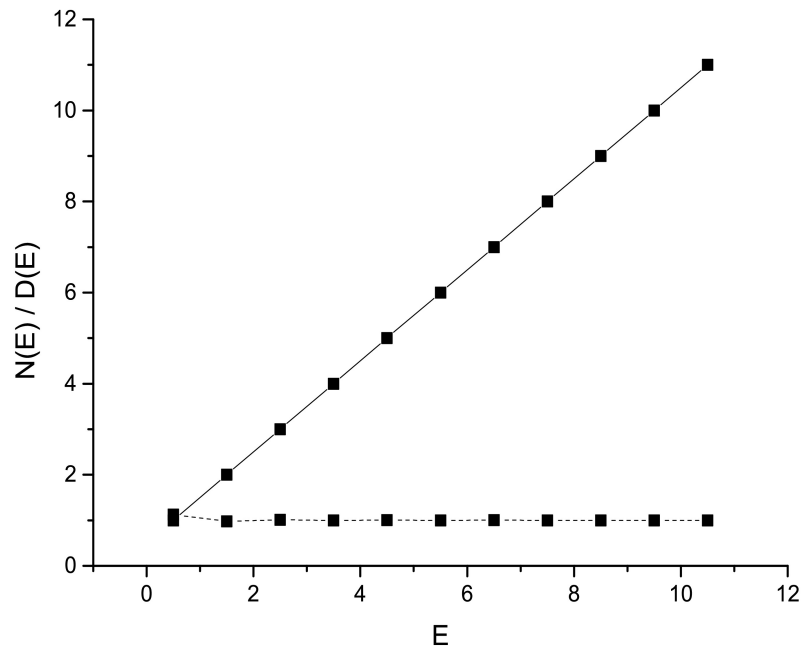


Figure 1.1: Quantum number function $N(E)$ (full-line) and density of states $D(E)$ (dashed-line) of LHO. First 11 bound-state energies are marked.

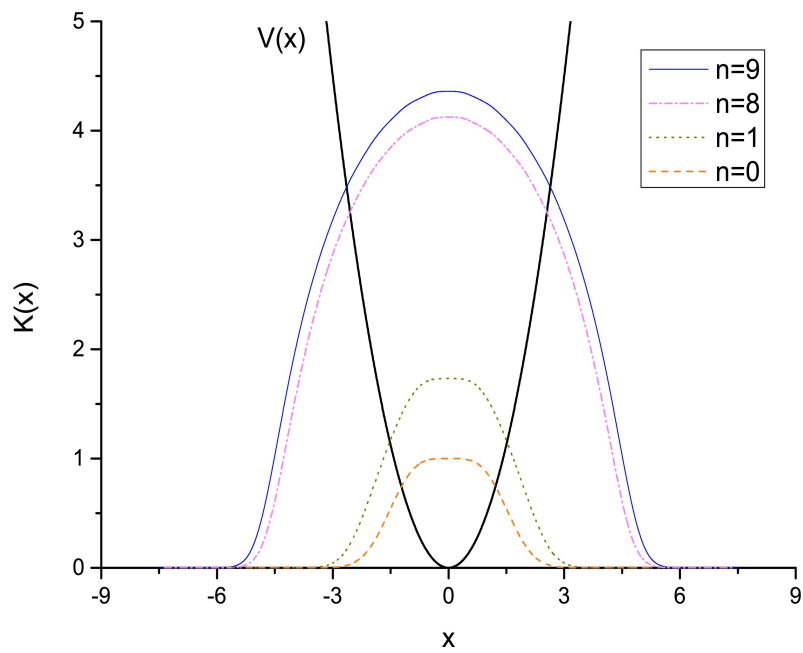


Figure 1.2: Function $K(x)$ of LHO for $n = 0$, $n = 1$, $n = 8$ and $n = 9$.

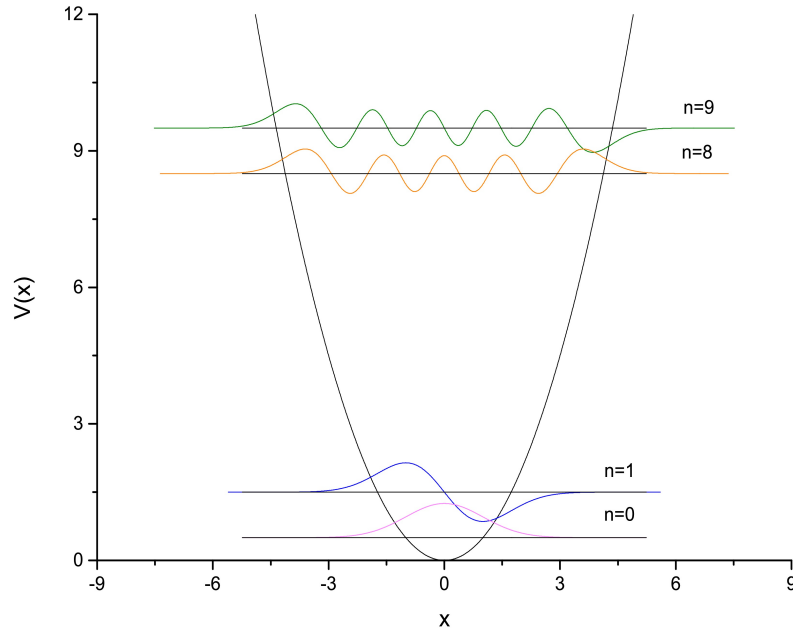


Figure 1.3: Calculated wavefunctions $u_n(x)$ of LHO for chosen bound-state energies E_n marked by n .

Other Symmetrical Potentials

Let us test the method on another symmetrical potential — the **octic oscillator** $V(x) = x^8/2$ with the parameters $m, \hbar, \omega = 1$ and $x_0 = 0$ [3]. On the basis of previous results we use $it = 3$. In Table 1.6 we can see the dependence of E_n on h and the number of integration points with $E1 = 50$, $E2 = 20$ and $E3 = 0.5$.

Figure 1.5 depicts the $N(E)$ - and $D(E)$ -dependence. Calculated bound-state energies (with parameters from Table 1.6, /II/) are marked. We plotted $K(x)$ and $u(x)$ for $n = 0, 1, 6, 7$ — see Figure 1.5 and 1.6, respectively.

One may also be interested in the case of symmetrical **double-well potentials**. For some of these, the analytical solution exists, but this is just a small number [3]. The standard Milne method can be applied to double-well potentials, however, we are able to gain energies only above the central maximum of the potential. As for the energies below the central maximum, one cannot obtain the function $K(x)$, since when we start calculating $w(x)$ in one of the wells (one of the minima), it diverges in the other. Consequently, $N(E)$ has some irregularities and does not behave so elegantly as it does in the cases of single-well potentials.

We may choose a higher number of integration points – with a reasonably smaller h . One gets energies even below the level of the central maximum then. Nonetheless, it prolongs the time of the calculation, which means that the method loses its efficiency. Even if one decides to start the integration from the central maxi-

Table 1.6: Computed bound-state energies of the octic oscillator using the Milne method: /I/ $h = 0.025$, $NMIN = -400$, $NMAX = 400$ /II/ $h = 0.01$, $NMIN = -1000$, $NMAX = 1000$, /III/ $h = 0.0025$, $NMIN = -4000$, $NMAX = 4000$. The first 11 bound-state energies are listed.

n	/I/	/II/	/III/
0	0.61291007867788	0.61291005699677	0.61291005690205
1	2.37793729561293	2.37793720737761	2.37793720698397
2	5.12247369710752	5.12247348953308	5.12247348862261
3	8.67154438085891	8.67154398704025	8.67154398529727
4	12.90450404316453	12.90450337863008	12.90450337565740
5	17.74895043982706	17.74894940717804	17.74894940259340
6	23.15638677248602	23.15638525431555	23.15638524752610
7	29.08982711996058	29.08982498438697	29.08982497485493
8	35.51963175193474	35.51962885095933	35.51962883794862
9	42.42131614451011	42.42131231343459	42.42131229615888
10	49.77418139421832	49.77417645111993	49.77417642884164

mum of the potential, the energies can be obtained only above the central maximum. Hence, one must search for another approach to the problem.

F. Robicheaux et al. [9] and S. Y. Lee and J. C. Light [10] tackle this issue by dividing of the domain of $V(x)$ into intervals. In each interval the wavefunction is calculated and these wavefunctions are matched, so that one obtains a C_1 solution.

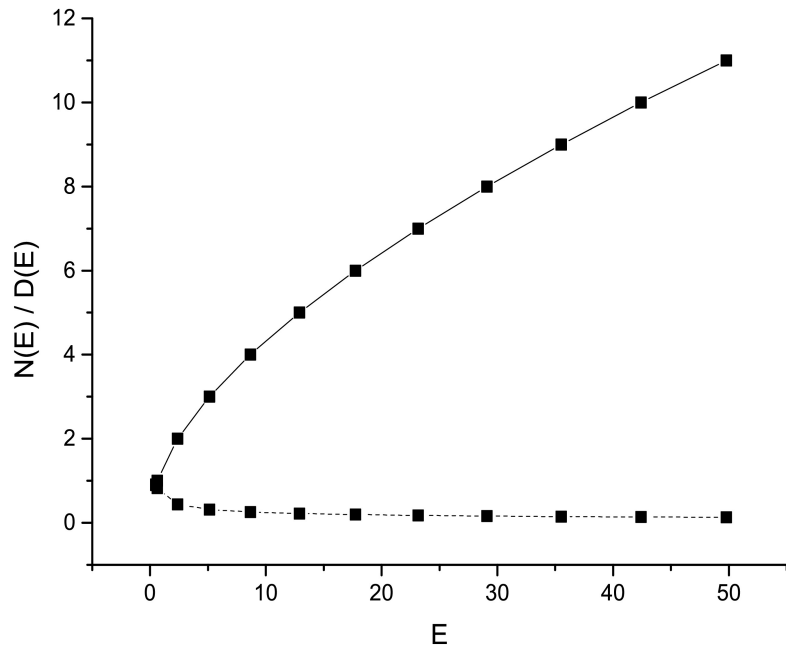


Figure 1.4: Quantum number function $N(E)$ (full-line) and density of states $D(E)$ (dashed-line) of the octic oscillator. Bound-state energies are marked.

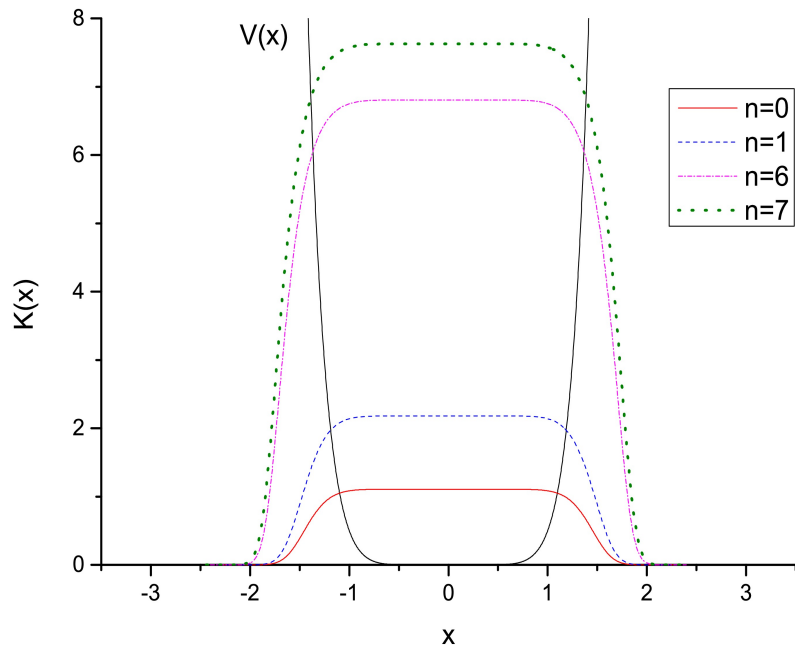


Figure 1.5: Function $K(x)$ of the octic oscillator for $n = 0$, $n = 1$, $n = 6$ and $n = 7$.

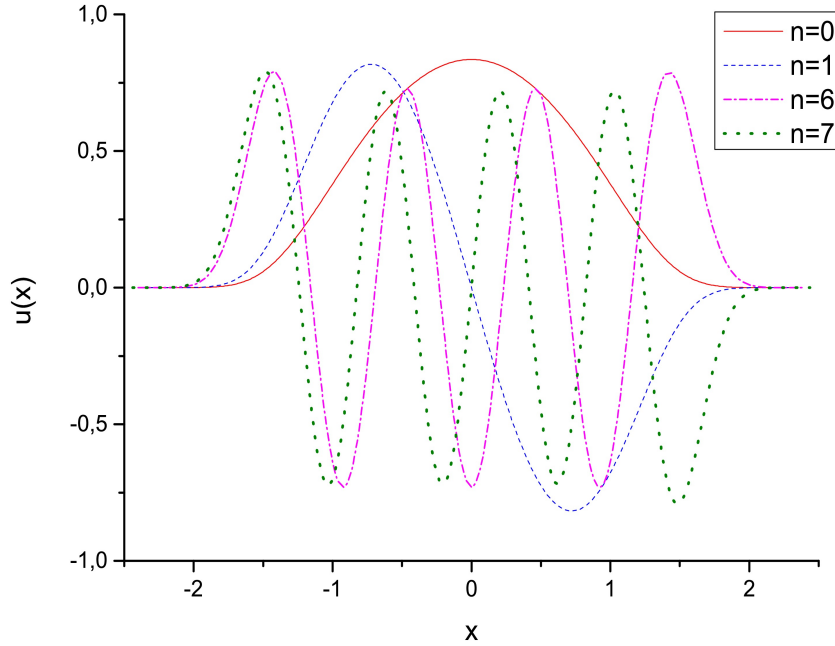


Figure 1.6: Calculated wavefunctions $u_n(x)$ of the octic oscillator for chosen bound-state energies E_n , $n = 0, 1, 6, 7$.

Morse Potential

Let us inspect one case of asymmetrical potentials. We consider the **Morse potential** from [3] given by $V(x) = D[\exp(-\alpha x) - 1]^2$, where $D = 5$ and $\alpha = 1/\sqrt{10}$. We assume $m, \hbar, \omega = 1$ and $x_0 = 0$. We know that $E_n = (n + \frac{1}{2}) - 0,05(n + \frac{1}{2})^2$ [3]. We derive the potential function and as (1.35) we obtain

$$w(x) = k^{-1/2}(x_0) \left\{ 1 + \frac{1}{12}x^4 + \frac{1}{60} \left(\frac{-2\sqrt{2}}{\sqrt{5}} + \frac{1}{\sqrt{10}} \right) x^5 \right\}. \quad (1.37)$$

Table 1.7 shows the dependence of E_n on h and the number of integration points with $E1 = 0.5$, $E2 = 3$, $E3 = 4.8$ and $it = 5$. The second column shows the exact energies. From the next columns we can see that we are able to reach the accuracy up to 10^{-11} .

Again, we ought to inspect the dependence of the calculated E_n on $E1$, $E2$ and $E3$ along with it . We choose $h = 0.01$, $NMIN = -500$ and $NMAX = 1500$. We find out that in this case, we should iterate at least five times to get satisfactory results. As for the choice of the trial energies, there is, again, a wider range of possible choices. The results are illustrated in Table 1.8. We list E_n for $n = 0, 1, \dots, 7$.

Figure 1.7 depicts the $N(E)$ - and $D(E)$ -dependence. Exact bound-state energies are marked. Figure 1.8 shows the computed bound-state energies of the

Table 1.7: Computed bound-state energies of the Morse oscillator using the Milne method: [a] exact, [b1] $h = 0.025$, $NMIN = -200$, $NMAX = 600$, [b2] $h = 0.01$, $NMIN = -500$, $NMAX = 1500$, [b3] $h = 0.001$, $NMIN = -5000$, $NMAX = 15000$

n	[a]	[b1]	[b2]	[b3]
0	0.48750	0.48750000282430	0.48750000003735	0.48750000000651
1	1.38750	1.38750000160551	1.38750000002389	1.38750000000681
2	2.18750	2.18750000087238	2.18750000001660	2.18750000000659
3	2.88750	2.887500000525415	2.88750000006003	2.88750000000691
4	3.48750	3.487500000567683	3.48750000006493	3.48750000000586
5	3.98750	3.987500000288674	3.98750000003559	3.98750000000635
6	4.38750	4.387500000076720	4.38750000001372	4.38750000000588
7	4.68750	4.68750000009700	4.68750000000624	4.68750000000576

Morse potential. We can observe the gradually decreasing spacing between the neighbouring energy levels when the energy increases.

We choose four E_n , for which we plot the values of $K(x)$ and $u(x)$ — see Figure 1.9 and 1.10, respectively.

General Remarks

At this place, before we move onto the next chapter, a few comments on the number of grid points given by $NMIN$ and $NMAX$ should be noted. As it is mentioned at the very beginning of the chapter Numerical Illustration, we choose them as input parameters. Later (see the section Predictor-Corrector Method), they are cut by the condition limiting $w(x)$ to the magnitude of 10^{-15} .

There is no reason to set a lower boundary to the limit, since we use double precision. In fact, we find out that the accuracy of the method has its boundary in the end points. We have tested the program also in quad precision and changed the condition limiting $w(x)$ to the magnitude of 10^{-34} . The results show that from a certain point, wavefunctions start to change their behaviour, they can even diverge. We can observe it on the example of LHO in Figure 1.11. This result does not correspond with theory, which requires $u(x) \rightarrow 0$ for $x \rightarrow \pm\infty$. It is fully sufficient to use double precision in the program.

Table 1.8: Computed lowest eight bound-state energies E_n of the Morse potential using the Milne method. For /1/-/3/ $it = 3$, for /4/-/6/ $it = 5$ and for /7/-/9/ $it = 10$. For the first column $E1 = 0.5$, $E2 = 3$ and $E3 = 5$, for the second column $E1 = 0.5$, $E2 = 6$ and $E3 = 10$ and for the last column $E1 = 0.5$, $E2 = 10$ and $E3 = 20$.

/1/	/2/	/3/
0.48750000003734	0.48750000003731	0.48750000003735
1.38750000002440	1.38750000004564	1.38750000004800
2.18750000001661	2.18750000015046	2.18750000020205
2.88750000006001	2.88750000490285	2.88750000692754
3.48750000006836	3.48750001040841	3.48750001785018
3.98750005952636	3.98750000185422	3.98750000705012
4.38756960115965	4.38750000004452	4.38750000001370
4.69351822632350	4.68750001971269	4.68751384353718
/4/	/5/	/6/
0.48750000003735	0.48750000003735	0.48750000003735
1.38750000002389	1.38750000002388	1.38750000002390
2.18750000001660	2.18750000001659	2.18750000001659
2.88750000006002	2.88750000006003	2.88750000006002
3.48750000006493	3.48750000006492	3.48750000006492
3.98750000003559	3.98750000003559	3.98750000003558
4.38750000001372	4.38750000001373	4.38750000001371
4.68750000091284	4.68750000000622	4.68750000000624
/7/	/8/	/9/
0.48750000003735	0.48750000003735	0.48750000003736
1.38750000002389	1.38750000002390	1.38750000002388
2.18750000001661	2.18750000001660	2.18750000001661
2.88750000006002	2.88750000006002	2.88750000006002
3.48750000006493	3.48750000006492	3.48750000006492
3.98750000003559	3.98750000003558	3.98750000003558
4.38750000001371	4.38750000001371	4.38750000001370
4.68750000000623	4.68750000000624	4.68750000000624

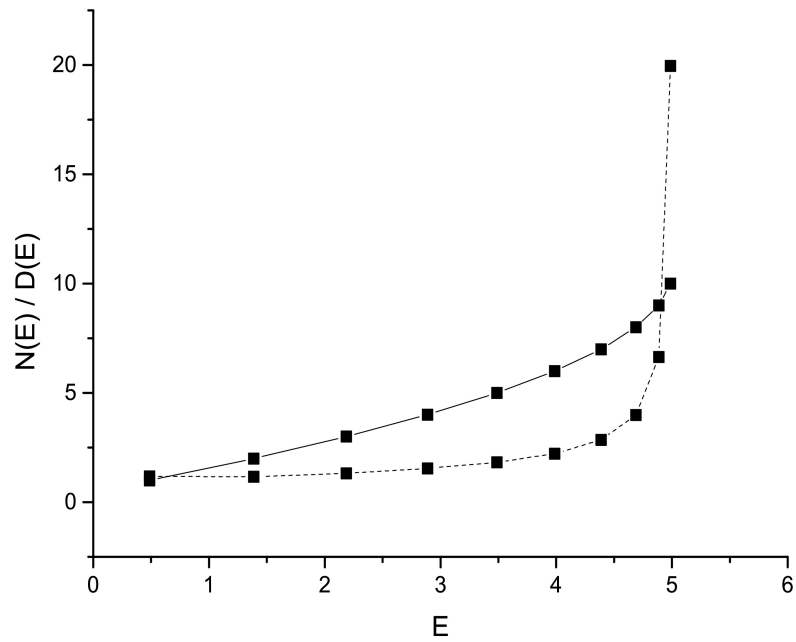


Figure 1.7: Quantum number function $N(E)$ (full-line) and density of states $D(E)$ (dashed-line) of the Morse oscillator. Bound-state energies are marked.

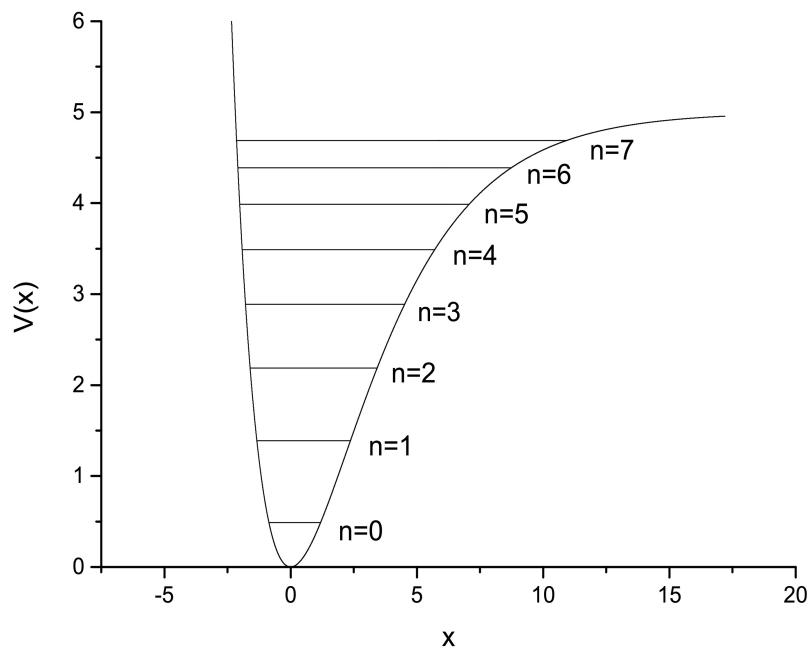


Figure 1.8: Bound-state energies E_n of the Morse oscillator for $n = 0, \dots, 7$.

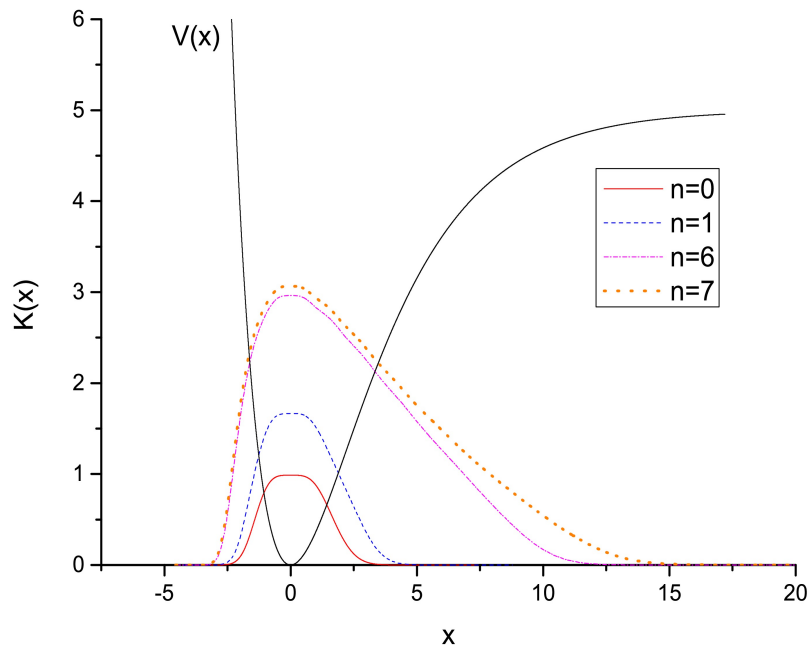


Figure 1.9: Function $K(x)$ of the Morse potential for $n = 0$, $n = 1$, $n = 6$ and $n = 7$.

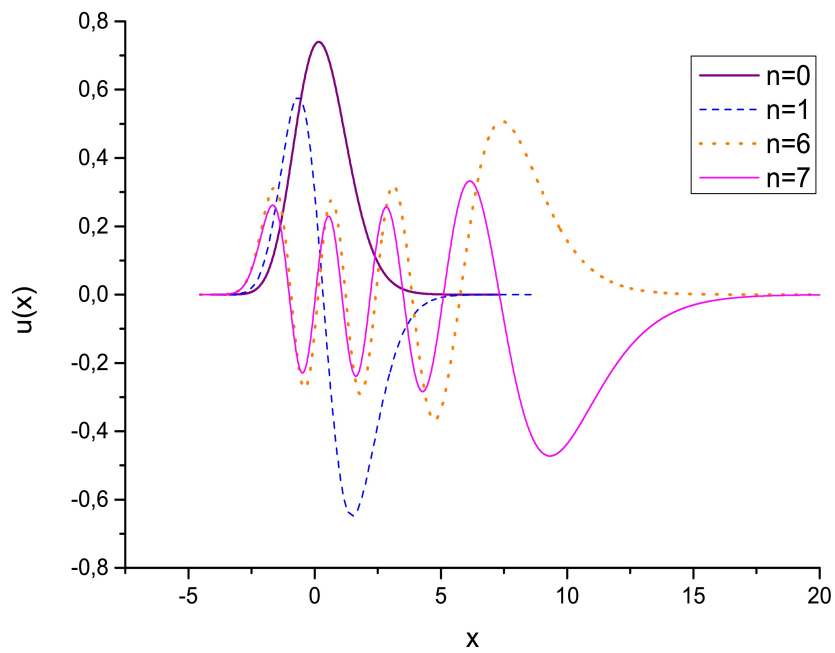


Figure 1.10: Calculated wavefunctions $u_n(x)$ of the Morse potential for chosen bound-state energies E_n , $n = 0, 1, 6, 7$.

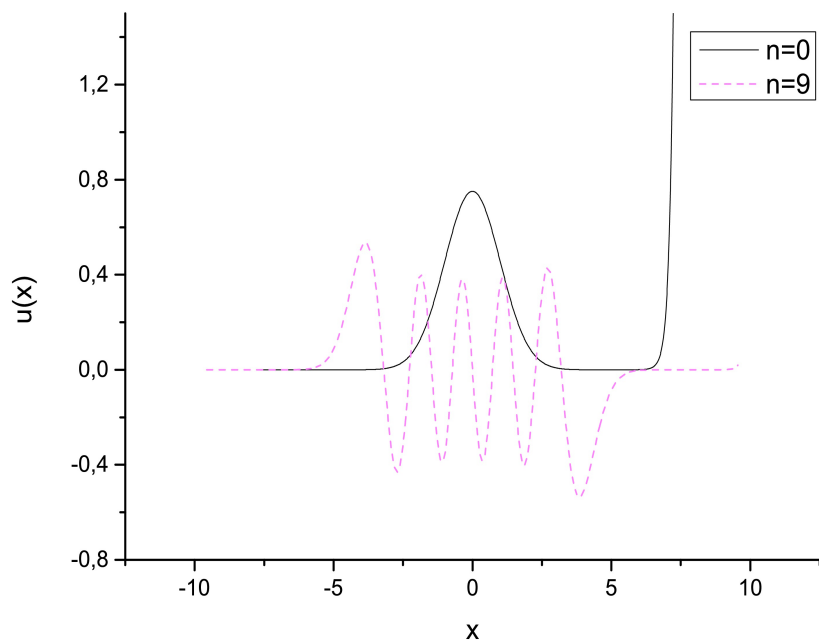


Figure 1.11: Wavefunction $u_n(x)$ of LHO for chosen bound-state energies $E_n(x)$, $n = 0$ and $n = 9$. There is a small growing tendency of $u_n(x)$ for $n = 9$ and divergence for $n = 0$ as $x \rightarrow 10$.

2. Phase-Amplitude Method

2.1 Theoretical Background of the Method

2.1.1 Modification of the Milne Method

In the first chapter, our goal was to find bound states of 1D potentials. In this chapter, we will look for quasibound states embedded in a classically trapped region. We will be interested in their resonance energies E_R and widths Γ , which can be used for determination of mean resonance lifetimes τ [1], defined as

$$\tau = \frac{\hbar}{\Gamma}.$$

Let us consider the wavefunction in the form (1.3). Let us assume that $a = 1$ and $b = 0$. Then using Equation (1.13) we may write

$$u(x) = cw(x) \sin(\phi(x)), \quad (2.1)$$

where $w(x)$ is the phase, $\phi(x)$ is the amplitude, c satisfies the same assumptions as in Chapter 1. The Milne method uses $k(x)$ (1.7), which is by definition always positive in the classically allowed regions. The question is how to deal with the classically forbidden regions, where $k(x)$ is always imaginary.

We will adopt approach from [1], where the authors suggest to rewrite (2.1) into

$$u(x) = c \exp(z(x)) \sin(\phi(x)), \quad (2.2)$$

where $c = \sqrt{2\mu/\pi}$ and μ represents the mass.

Our goal is to find and solve equations for $\phi(x)$ and $z(x)$, i.e. we need two equations. From the previous chapter we know that $d\phi(x)/dx = K(x) = w^{-2}(x)$. As it can be seen

$$w(x) = \exp(z(x)). \quad (2.3)$$

Then we get the first equation

$$\frac{d\phi(x)}{dx} = \exp(-2z(x)). \quad (2.4)$$

Substituting $\exp(z(x))$ into the Milne equation (1.2), we obtain

$$\frac{d}{dx} \left(\frac{dz(x)}{dx} \exp(z(x)) \right) + k^2(x) \exp(z(x)) = \exp^{-3}(z(x)),$$

$$\frac{d^2 z(x)}{dx^2} \exp(z(x)) + \exp(z(x)) \left(\frac{dz(x)}{dx} \right)^2 + k^2(x) \exp(z(x)) = \exp^{-3}(z(x)),$$

$$\frac{d^2 z(x)}{dx^2} + \left(\frac{dz(x)}{dx} \right)^2 + k^2(x) = \exp^{-4}(z(x)).$$

As $\exp^{-4}(z(x)) = \exp(-4z(x)) = (d\phi(x)/dx)^2$, we found the second equation

$$\frac{d^2 z(x)}{dx^2} + \left(\frac{dz(x)}{dx} \right)^2 - \left(\frac{d\phi(x)}{dx} \right)^2 + k^2(x) = 0. \quad (2.5)$$

The initial conditions come from the WKB theory. These hold

$$\begin{aligned} w(x_0) &= k^{-1/2}(x_0) \\ w'(x_0) &= \left. \frac{d(k^{-1/2}(x))}{dx} \right|_{x=x_0} \\ \phi(x_0) &= 0, \end{aligned} \quad (2.6)$$

where x_0 is the potential minimum. The third condition is arbitrary. We assume that $\hbar = 1$, while μ can be different from 1. Hence

$$k(x) = \sqrt{2\mu[E - V(x)]}. \quad (2.7)$$

Substituting (2.7) into (2.6), we obtain

$$w(x_0) = [2\mu(E - V(x_0))]^{-1/4} \quad (2.8)$$

and

$$w'(x_0) = \mu V'(x_0)[2\mu(E - V(x_0))]^{-5/4}. \quad (2.9)$$

Now we aim to change the first two conditions into the conditions for $z(x)$. From the reverse relation of (2.3) we gain

$$z(x_0) = \ln(w(x_0)), \quad (2.10)$$

which along with (2.8) gives

$$z(x_0) = -\frac{1}{4} \ln[2\mu(E - V(x_0))].$$

This is the first initial condition for $z(x)$. From (2.10) it is furthermore obvious that

$$z'(x)|_{x=x_0} = \left. \frac{w'(x)}{w(x)} \right|_{x=x_0}.$$

Substituting (2.8) and (2.9) into this equation yields

$$z'(x_0) = \frac{\frac{1}{2}\mu V'(x_0)[2\mu(E - V(x_0))]^{-5/4}}{[2\mu(E - V(x_0))]^{-1/4}} = \frac{V'(x_0)}{4(E - V(x_0))}.$$

This is the second initial condition for $z(x)$.

We opt for these classical conditions to simplify the calculations, i.e. the integration of Equations (2.4) and (2.5) – in this case $z(x)$ has a non-oscillatory behaviour [11].

In order to solve Equations (2.4) and (2.5), we divide the domain of $V(x)$ into classically allowed and forbidden regions. In each segment, we start the integration with different initial conditions. This means that it is needed to carry out matching of the solutions $z(x)$ and $\phi(x)$. It is conducted in the following way: we add a constant c_1 to $z(x)$ in the first region, while another constant d_1 is added to $\phi(x)$ in the second region, so that the resulting function is a C_1 function. Then, we add a constant d_2 to the just formed $\phi(x)$, so that it satisfies the third condition of (2.6).

If we substitute these functions $z(x)$ and $\phi(x)$ into Equation (2.2), we receive a wavefunction for a certain energy E . Moving to the next subsection, our goal will be to find resonance energies E_R , for which the knowledge of $\phi(x)$ is essential.

2.1.2 Resonance Positions and Widths

In order to find E_R , one plots $\phi = \phi(E)$ for a chosen x_{out} located in the forbidden region. The resonances are characterised by jumps of ϕ by π . We will demonstrate this behaviour on the example from [1] – see the following section.

Calculating the derivative $\partial\phi(x_{\text{out}}, E)/\partial E$ and plotting it against energy E , we can read out resonance energies and then find the resonance widths Γ from the Breit-Wigner formula [1]

$$\frac{\partial\phi(x_{\text{out}}, E)}{\partial E} = \frac{\Gamma/2}{(E - E_R)^2 + (\Gamma/2)^2} + C, \quad (2.11)$$

where a constant C is the derivative of the background phase. The process of locating Γ will be described more in the next section.

2.2 Numerical Illustration

The program input consists of a grid $[x_{\text{min}}, \dots, x_{\text{max}}]$, a potential function $V(x)$, a reduced mass μ , an energy range $[E_{\text{min}}, \dots, E_{\text{max}}]$, in which we aim to find resonances, and E_{wave} , which is the energy, where the corresponding wavefunction is desired.

The first of the following subsections describes the way one solves Equations (2.4) and (2.5). The second one explains how to find resonances. In the last subsection we list an example of a resonance search.

2.2.1 Solving the Modified Milne Equations

Depending on a specific potential function, one may firstly interpolate it using the cubic spline algorithm listed in [12]. Then for each value of E from

$[E_{\min}, \dots, E_{\max}]$ we divide the grid into a classically allowed and forbidden region and calculate the initial values of $z(x)$ and $\phi(x)$, i.e. $z(x_0)$ and $\phi(x_0)$. For both regions x_0 is the potential minimum. The values $z(x_0)$ and $\phi(x_0)$ are calculated via (2.6).

Once we know the initial values of $z(x)$ and $\phi(x)$, we can start the integration of (2.4) and (2.5). We use the 4-th order fixed step size Runge-Kutta algorithm. In the case of $z(x)$, we concretely take the algorithm for the second-order ordinary differential equations, while to calculate $\phi(x)$, it is sufficient to use the algorithm for the first-order ordinary differential equations.

Once we have the solutions $z(x)$ and $\phi(x)$ in both regions, we match them as described in the previous subsection and move $\phi(x)$ by the magnitude of d_2 , so that the last condition of (2.6) is valid. Now we can proceed to locating resonances.

2.2.2 Three Criteria for a Resonance

As it was foreshadowed in the section Resonance Positions and Widths, we examine $\phi(x_{\text{out}}, E)$. We simply choose $x_{\text{out}} = x_{\text{max}}$ and look for jumps by π , which can be found due to the fact that $\phi(x_{\text{max}}, E)$ is a monotonic function. In order to locate all jumps by π , the difference between adjacent values of $\phi(x_{\text{max}}, E)$ is set to be less than $\pi/40$ radians.

We calculate $\partial\phi(x_{\text{max}}, E)/\partial E$. We classify its local maxima as resonance peaks. With these data using (2.11) we find resonance widths Γ . In some cases it may happen that not all of the peaks are true resonances. We demand for the resonance peaks to satisfy three criteria:

- The phase $\phi(x_{\text{max}}, E)$ has a jump of π .
- The peak has the form of (2.11).
- The wavefunction $u(x)$ is strongly peaked in the well region of $V(x)$ at E_R .

For example, some of the “fake” resonances have the Breit-Wigner form, but the jump in the $\phi(x_{\text{max}}, E)$ -dependence does not equal π .

2.2.3 Examples

As an illustrative example we choose ${}^3\text{He}^4\text{He}^{2+}$ from [1]. They use the potential curve from [13] and take $\mu = 3134.3$ a.u. We present the potential curve with the interpolated values from [13] in Figure 2.1. Our program could not have been debugged due to time constraints.

In the first figure of the article there are shown the calculated functions for certain energies near the second resonance energy $E_{\nu=1} = -3.658682803223646$ a.u. The local minimum of the curve lies at $r = 1.328$ a.u. and its local maximum is located at $r \sim 2.172$ a.u. It can be seen that $\gamma_{\text{above}}(r)$, which is $z_{\text{above}}(x)$ in the language of our previous notation, reaches high values near $r = 0$ a.u., i.e.

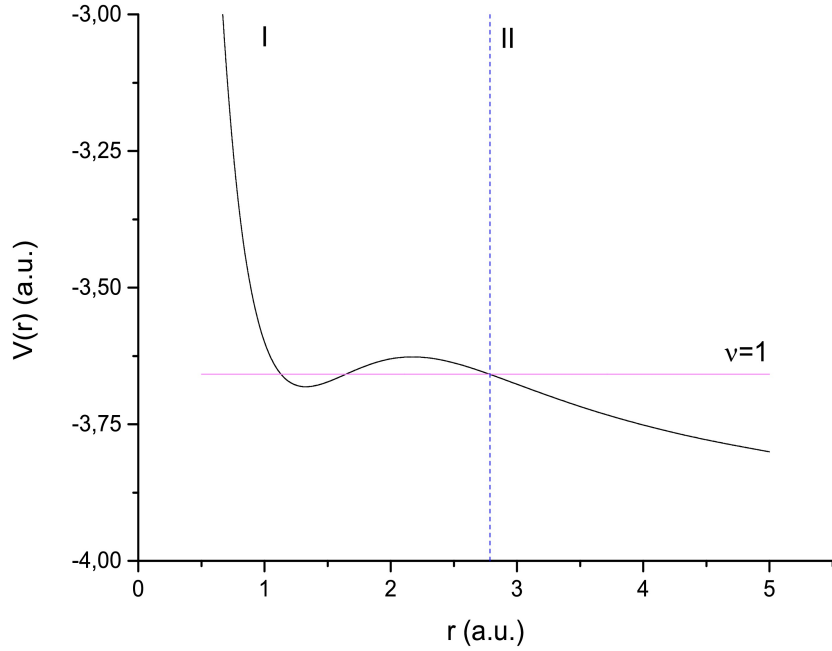


Figure 2.1: Interpolated potential energy curve of ${}^3\text{He}^4\text{He}^{2+}$ from [13]. Resonance energy $E_{\nu=1}$ and regions I and II are marked.

$x = 0$ a.u., and $r = 2.7$ a.u., i.e. $x = 2.7$ a.u. This illustrates the standard Milne approach, which the phase-amplitude modifies.

Also, one can observe the discontinuity of γ_{above} and ϕ_{above} between two regions (classically forbidden and allowed region) separated by the dashed line. As it was mentioned before, this is caused by the different initial conditions in regions I and II for the two functions. In region I the integration started at $r = 1.328$ a.u., while in region II the integration began at $r = 5$ a.u.

Let us focus strictly on resonance energies E_R . In the next figure of [1] we observe four true resonances E_R of ${}^3\text{He}^4\text{He}^{2+}$. There is another jump in $\phi(r)$ but its magnitude is different from π . Therefore, it is not a vibrational state. It is the case of above mentioned “fake” resonance. The figure also shows (see graph below) the shape of the peak of $\partial\phi(r_{\text{out}}, E)/\partial E$. The resonance width Γ is marked.

In an analogical way we can find resonances of a variety of 1D potentials. As for the accuracy of the method, we are only limited by the numerical accuracy of the calculations. Therefore, it is highly convenient to use a quadruple precision. With a double precision, not all resonance widths can be calculated. In the case of the examples listed in [1], Γ ranges from $\sim 10^{-4}$ to $\sim 10^{-22}$ a.u.

Conclusion

In the beginning of this thesis, in the theoretical part of the first chapter, we have derived the relation between the Schrödinger and the Milne equations. We have explained how to solve the Milne equation via the predictor-corrector method. We have chosen the classical initial conditions. We have defined the quantum number function and found out that it grows with energy. We have illustrated this behaviour on examples. Another important quantity is the quantum action, which has served us as a standing point for the definition of the derivative of the quantum number function and the density of states.

In the practical part of the first chapter, we have listed numerical tools used in our program and described the calculation of bound states. As the first example we have taken the linear harmonic oscillator. We have calculated the first eleven bound states. Considering the input parameters, we have found out that the ideal number of iterations counts three and that we can choose from a wider range of trial energies. Similarly, we have tested the method on the octic oscillator and discussed the case of double-wells.

We have calculated the first eight bound states of the Morse potential. In that case the ideal number of iterations is five. Trial energies can be, again, chosen from a wider range.

We have plotted function $K(x)$ for our systems and have shown that for symmetrical potentials it is symmetrical. We have illustrated the shape of wavefunctions and have shown their even and odd character for symmetrical potentials. We have plotted energy levels of the Morse oscillator and demonstrated the decreasing level spacing between energies.

We have conducted a brief discussion on the end points of the calculated functions and set boundary conditions equal to 10^{-15} . From the results in our tables it can be seen that the accuracy of calculated bound states depends on the number of integration points and the step; with the Milne method we can reach the accuracy up to 10^{-11} - 10^{-12} .

In the second chapter, we have introduced an altered form of the wavefunction. We have derived the modified Milne equation for the phase and the amplitude function. We have derived the corresponding initial conditions. In the next sections we have explained the resonance search. We have described the method on the example of ${}^3\text{He}^4\text{He}^{2+}$. We have examined its phase and amplitude functions. ${}^3\text{He}^4\text{He}^{2+}$ has four true resonances. The accuracy of the phase-amplitude method is given by the numerical precision of the calculations.

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A. Attachments

A.1 Attachment 1 - Source Code

```
*****
* BOUND-STATE PROBLEM
*****

include 'globc_20D.f'

INTEGER NMINM, NMAXM, j, k, NMINM_FIXED, NMAXM_FIXED
DOUBLE PRECISION E1, E2, E3, hM
DOUBLE PRECISION N1, N2, N3, N4, N5, N6, N7, N8, N9
DOUBLE PRECISION det, detNN, detNN1, detNN2, detNN3
DOUBLE PRECISION alpha1, alpha2, alpha3
INTEGER N_ENERGY, NUE_MIN, NUE_MAX
PARAMETER (N_ENERGY = 100)
DOUBLE PRECISION E_T(0:N_ENERGY), E_WAVE
INTEGER N_WAVE
DOUBLE PRECISION EN_WAVE(0:N_ENERGY)

*****
* MAIN PROGRAM
*****

* choose one of the systems:
** CIAL=1...Morse oscillator
** CIAL=2...LHO
** CIAL=8...octic oscillator

CIAL=2

* hM...step
* NMINM, NMAXM...range

hM= 0.0025d0
NMINM = -4000
NMAXM = 4000

NMINM_FIXED=NMINM
NMAXM_FIXED=NMAXM

* choose trial energies:
E1 = 12.d0
E2 = 5.d0
E3 = 0.3d0
```



```

* potencial CIAL = 1, calculation of exact energies:
*       DO j=0,9
*           EN_WAVE(j) = DBLE(j)+0.5d0
*           EN_WAVE(j)=EN_WAVE(j)-0.05d0*(DBLE(j)+0.5d0)**(2.d0)
*       ENDDO
*       open(100, file='j,EN_WAVE(j).dat')
*       do j=0, 9
*           write(100,12) j,',' ,EN_WAVE(j)
*       enddo
*12     FORMAT(I4,A4,F25.8)
*       close(100)

* number of energies we look for plus one:
NUE_MIN = 0
NUE_MAX = 11

* calculation of alpha(i) for i=1,2,3:
CALL Quant(E1,hM,NMINM,NMAXM)
N1 = NQ
write(*,*)'Quant called 1'
write(*,*) NMINM, NMAXM
write(*,*) E1,N1

CALL Quant(E2,hM,NMINM,NMAXM)
N2 = NQ
write(*,*)'Quant called 2'
write(*,*) NMINM, NMAXM
write(*,*) E2,N2

CALL Quant(E3,hM,NMINM,NMAXM)
N3 = NQ
write(*,*)'Quant called 3'
write(*,*) NMINM, NMAXM
write(*,*) E3,N3

N4 = N1**2
N5 = N2**2
N6 = N3**2
N7 = N1**3
N8 = N2**3
N9 = N3**3

detNN=det(N1,N2,N3,N4,N5,N6,N7,N8,N9)
detNN1=det(E1,E2,E3,N4,N5,N6,N7,N8,N9)
detNN2=det(N1,N2,N3,E1,E2,E3,N7,N8,N9)
detNN3=det(N1,N2,N3,N4,N5,N6,E1,E2,E3)

```

```

alpha1=detNN1/detNN
alpha2=detNN2/detNN
alpha3=detNN3/detNN

* Newton iteration:
DO j=NUE_MIN,NUE_MAX-1
write(*,*) 'Energy',j
E_T(j+1) = alpha1*DBLE(j+1)+alpha2*DBLE(j+1)**2
E_T(j+1) = E_T(j+1)+alpha3*DBLE(j+1)**3
DO k=1,3
CALL DensG(E_T(j+1),hM,NMINM_FIXED,NMAXM_FIXED,0)
write(*,*) E_T(j+1)
write(*,*) NMINM_FIXED,NMAXM_FIXED
open(219,position='append',file='NMINM_FIXED,NMAXM_FIXED.dat')
write(219,90) NMINM_FIXED,' ',NMAXM_FIXED
90      FORMAT(I15,A4,I15)
close(219)
NMINM_FIXED=NMINM_FIXED+DIFF_MIN
NMAXM_FIXED=NMAXM_FIXED+DIFF_MAX
write(*,*) NMINM_FIXED,NMAXM_FIXED
open(219,position='append',file='NMINM_FIXED,NMAXM_FIXED.dat')
write(219,90) NMINM_FIXED,' ',NMAXM_FIXED
close(219)
E_T(j+1) = E_T(j+1)+(DBLE(j+1)-NQ)/DD
write(*,*) 'energie'
write(*,*) E_T(j+1)
IF (k .eq.10)THEN
open(219,position='append',file='NMINM_FIXED,NMAXM_FIXED.dat')
write(219,*) ' '
close(219)
ENDIF
ENDDO
ENDDO

open(111, file='energie.dat')
do j=NUE_MIN,NUE_MAX-1
write(111,38) E_T(j+1)
enddo
38      FORMAT(F25.14)
close(111)

write(*,*)'energies were calculated'
stop

* calculation of the wavefunction:
* odd / even bound state:
*      wave_const = 1
* choose energy for which the wavefunction is desired:

```



```

V(N) = 0.5d0*(X(N))**2.d0
ENDDO
ELSEIF(CIAL .EQ. 8) THEN
DO N = NMIN, NMAX
V(N) = 0.5d0*(X(N))**8.d0
ENDDO
ELSEIF(CIAL .EQ. 1) THEN
DO N = NMIN, NMAX
V(N) = 5.d0*(EXP((-1/(SQRT(10.d0))))*X(N))-1.d0)**(2.d0)
ENDDO
ENDIF

* PREDICTOR-CORRECTOR METHOD (Milne (1933)) for solving
* the Milne equation

DO N = NMIN, NMAX
K2(N) = 2.d0*(E-V(N))
ENDDO
P2(0)= K2(0)

* cutting of the integration interval:
PRC = 1.d-15
NMIN_FIXED=NMIN
NMAX_FIXED=NMAX

* integration 'to the right':
*****

* initial points depend on the derivatives of V(N) at N=0:
IF(CIAL .EQ. 2) THEN
DO N = -1, 2
WR(N) =(1.d0+((X(N)-X(0))**4.d0)/12.d0)/((K2(0))**(1.d0/4.d0))
ENDDO
ELSEIF(CIAL .EQ. 8) THEN
DO N = -1, 2
WR(N) =1.d0/((K2(0))**(1.d0/4.d0))
ENDDO
ELSEIF(CIAL .EQ. 1) THEN
DO N = -1, 2
WR1(N)= 1.d0+((X(N)-X(0))**4)/12.d0
WR2(N)= -2.d0*SQRT(2.d0)/SQRT(5.d0)
WR2(N)= (WR2(N)+(1.d0/(SQRT(10.d0))))*((X(N)-X(0))**5)/60.d0
WR(N) = (WR1(N)+WR2(N))/((K2(0))**(1.d0/4.d0))
IF (N.EQ.0) THEN
write(*,*) 'WR(0)'
write(*,*) WR(N)
ENDIF
ENDDO

```

```

ENDIF

DO N = 0, 2
WR3(N)= WR(N)**(-3.d0)
FR(N) = RHS(WR3(N),WR(N),K2(N))
ENDDO

DO N = 2, 3
WRA(N+1)= WR(N)+WR(N-2)-WR(N-3)
WRB(N+1)=(h**2)*(5.d0*FR(N)+2.d0*FR(N-1)+5.d0*FR(N-2))/4.d0
WR(N+1) = WRA(N+1)+WRB(N+1)
WR3(N+1)= WR(N+1)**(-3.d0)
FR(N+1) = RHS(WR3(N+1),WR(N+1),K2(N+1))

WR(N+1) = 2.d0*WR(N)-WR(N-1)
WR(N+1) = WR(N+1)+(h**2)*(FR(N+1)+10.d0*FR(N)+FR(N-1))/12.d0
WR3(N+1)= WR(N+1)**(-3.d0)
FR(N+1) = RHS(WR3(N+1),WR(N+1),K2(N+1))
ENDDO

DO N = 4, NMAX-1
WR(N+1) = WR(N)+WR(N-4)-WR(N-5)
WA(N+1)= 67.d0*FR(N)-8.d0*FR(N-1)+122.d0*FR(N-2)-8.d0*FR(N-3)
WA(N+1)= (h**2)*(WA(N+1)+67.d0*FR(N-4))/48.d0
WR(N+1) = WR(N+1)+ WA(N+1)
WR3(N+1)= WR(N+1)**(-3.d0)

IF(WR3(N+1) .LT. PRC) THEN
NMAX = N
EXIT
ELSE
FR(N+1) = RHS(WR3(N+1),WR(N+1),K2(N+1))
WR(N+1) = WR(N)+WR(N-2)-WR(N-3)
WB(N+1)= 17.d0*FR(N+1)+232.d0*FR(N)+222.d0*FR(N-1)
WB(N+1)= WB(N+1)+232.d0*FR(N-2)
WB(N+1)= (h**2)*(WB(N+1)+17.d0*FR(N-3))/240.d0
WR(N+1) = WR(N+1)+ WB(N+1)
WR3(N+1)= WR(N+1)**(-3.d0)
FR(N+1) = RHS(WR3(N+1),WR(N+1),K2(N+1))
ENDIF
ENDDO

* integration 'to the left'
*****
IF(CIAL .EQ. 1)THEN
DO N = 1, -2, -1
WL1(N)= 1.d0+((X(N)-X(0))**4)/12.d0
WL2(N)= -2.d0*SQRT(2.d0)/SQRT(5.d0)

```

```

WL2(N)= (WL2(N)+(1.q0/(SQRT(10.d0))))*((X(N)-X(0))**5)/60.d0
WL(N) = (WL1(N)+WL2(N))/((K2(0))**(1.q0/4.d0))
ENDDO

```

```

DO N = 0, -2, -1
WL3(N)= WL(N)**(-3.d0)
FL(N) = RHS(WL3(N),WL(N),K2(N))
ENDDO

```

```

DO N = -2, -3, -1
WLA(N-1) = WL(N)+WL(N+2)-WL(N+3)
WLB(N-1)=(h**2)*(5.d0*FL(N)+2.d0*FL(N+1)+5.d0*FL(N+2))/4.d0
WL(N-1)= WLA(N-1)+WLB(N-1)
WL3(N-1)= WL(N-1)**(-3.d0)
FL(N-1) = RHS(WL3(N-1),WL(N-1),K2(N-1))

```

```

WL(N-1) = 2.d0*WL(N)-WL(N+1)
WL(N-1) = WL(N-1)+(h**2)*(FL(N-1)+10.d0*FL(N)+FL(N+1))/12.d0
WL3(N-1)= WL(N-1)**(-3.d0)
FL(N-1) = RHS(WL3(N-1),WL(N-1),K2(N-1))
ENDDO

```

```

DO N = -4, NMIN+1, -1
WL(N-1) = WL(N)+WL(N+4)-WL(N+5)
WA(N-1)= 67.d0*FL(N)-8.d0*FL(N+1)+122.d0*FL(N+2)-8.d0*FL(N+3)
WA(N-1)= (h**2)*(WA(N-1)+67.d0*FL(N+4))/48.d0
WL(N-1) = WL(N-1)+ WA(N-1)
WL3(N-1)= WL(N-1)**(-3.d0)

```

```

IF(WL3(N-1) .LT. PRC) THEN
NMIN = N
EXIT
ELSE
FL(N-1) = RHS(WL3(N-1),WL(N-1),K2(N-1))
WL(N-1) = WL(N)+WL(N+2)-WL(N+3)
WB(N-1)= 17.d0*FL(N-1)+232.d0*FL(N)+222.d0*FL(N+1)
WB(N-1)= WB(N-1)+232.d0*FL(N+2)
WB(N-1)= (h**2)*(WB(N-1)+17.d0*FL(N+3))/240.d0
WL(N-1) = WL(N-1)+ WB(N-1)
WL3(N-1)= WL(N-1)**(-3.d0)
FL(N-1) = RHS(WL3(N-1),WL(N-1),K2(N-1))
ENDIF
ENDDO

```

```

ELSE
DO N = 0, NMIN
WL(N) = WR(-N)

```

```

ENDDO
ENDIF

* correction of NMIN, NMAX for the Simpson's rule:
DO WHILE(MOD(NMAX,4).NE.0)
NMAX=NMAX-1
ENDDO

IF (CIAL .EQ. 1) THEN
DO WHILE(MOD(NMIN,4).NE.0)
NMIN=NMIN+1
ENDDO
ELSE
NMIN=-NMAX
ENDIF

DIFF_MIN=NMIN_FIXED-NMIN
DIFF_MAX=NMAX_FIXED-NMAX

DO N=0,NMAX
W(N)=WR(N)
ENDDO
DO N=0,NMIN,-1
W(N)=WL(N)
ENDDO

* quantum momentum K(x)...KK:
DO N = 0,NMAX
KK(N)=(WR(N))**(-2.d0)
ENDDO
IF(CIAL .NE. 1)THEN
DO N=0,NMIN,-1
KK(N)=KK(-N)
ENDDO
ELSE
DO N = 0,NMIN,-1
KK(N)=(WL(N))**(-2.d0)
ENDDO
ENDIF

* right-hand NQR and left-hand NQL integrals:
* (Simpson's rule)
QR = SIMPS(0,NMAX,h,KK)
NQR = QR/PI

IF(CIAL .NE. 1)THEN
NQL = -NQR
ELSE

```



```

KK_int(N-DNMIN+1)=KK(N)
enddo
do N=DNMIN,DNMAX
X_int(N-DNMIN+1)=X(N)
enddo

CALL spline(X_int, KK_int, NMIN_f, NMAX_f, KYD1, KYDN)
do N=NMIN_f, NMAX_f
KYDD(N)=y2(N)
enddo

h_int = hh/2.d0
NMAX_f = (2*NMAX_f)-1

KX_INT(NMIN_f)=X_int(NMIN_f)

DO M=NMIN_f, NMAX_f-1
KX_INT(M+1)=KX_INT(NMIN_f)+DBLE(M)*h_int
ENDDO

kklo = NMIN_f
kkhi = NMAX_f

DO M=NMIN_f, NMAX_f
CALL splint(X_int, KK_int, KYDD, NMAX_f, KX_INT(M))
KY_INT(M)=y
ENDDO
* end of the interpolation

DNMIN = DNMIN*2
DNMAX = DNMAX*2

do N=NMIN_f, NMAX_f
KK(N+DNMIN-1)=KY_INT(N)
enddo

do N=NMIN_f, NMAX_f
X(N+DNMIN-1)=KX_INT(N)
enddo

DO k = 0, DNMAX, 2
RBL(k) = SIMPS(DNMAX, k, h_int, KK)
R(k) = ((SIN(RBL(k)))**2.d0)/KK(k)
ENDDO

TR = TRAPEZ(0, DNMAX, hh, R)
FR = (SIN(2.d0*PI*NQR))/(2.d0*PI*P2(0))
DR = 2.d0*TR/PI + FR

```

```

IF (CIAL .EQ. 1) THEN
DO k = 0, DNMIN, -2
RBL(k) = SIMPS(DNMIN,k,h_int,KK)
R(k) = ((SIN(RBL(k)))**2.d0)/KK(k)
ENDDO
TL = TRAPEZ(0, DNMIN, hh, R)
FL = (SIN(2.d0*PI*NQL))/(2.d0*PI*P2(0))
DL = 2.d0*TL/PI + FL
ELSE
DO k = 0, DNMIN, -2
RBL(k) = RBL(-k)
R(k) = R(-k)
ENDDO
TL = -TR
FL = -FR
DL = -DR
ENDIF

DD = DR-DL

* calculation of the wavefunction:
IF (WF .EQ. 1) THEN
* normalisation constant of the wavefunction:
c = 2.d0/(DD*PI)
c = SQRT(c)

IF (CIAL .EQ. 1) THEN
DO k = DNMIN, DNMAX, 2
RBL(k) = SIMPS(DNMIN,k,h_int,KK)
u(k) = c*SIN(RBL(k))/SQRT(KK(k))
ENDDO
ELSEIF (MOD(wave_const,2).EQ.0) THEN
write(*,*) 'sign is being changed'
DO k = DNMIN, 0, 2
RBL(k) = SIMPS(DNMIN,k,h_int,KK)
u(k) = c*SIN(RBL(k))/SQRT(KK(k))
ENDDO
DO k = 0, DNMAX, 2
RBL(k) = -RBL(-k)
u(k) = -u(-k)
ENDDO
ELSE
write(*,*) 'sign stays the same'
DO k = DNMIN, 0, 2
RBL(k) = SIMPS(DNMIN,k,h_int,KK)
u(k) = c*SIN(RBL(k))/SQRT(KK(k))
ENDDO

```

```

DO k = 0, DNMAX, 2
RBL(k) = RBL(-k)
u(k) = u(-k)
ENDDO
ENDIF
ENDIF

RETURN
END

* end of the subroutine DensG
*****
SUBROUTINE spline(fx,fy,minn,maxx,yp1,ypn)

include 'globc_20D.f'

INTEGER maxx, minn
DOUBLE PRECISION yp1,ypn,fx(MAX_PT),fy(MAX_PT)
INTEGER i,k
DOUBLE PRECISION p,qn,sig,un
DOUBLE PRECISION u(MAX_PT)

if (yp1.gt..99d30) then
y2(minn)=0.d0
u(minn)=0.d0
else
y2(minn)=-0.5d0
u(minn)=3.d0/(fx(minn+1)-fx(minn))
u(minn)=u(minn)*((fy(minn+1)-fy(minn))/(fx(minn+1)-fx(minn))-yp1)
endif

do 11 i=minn+1,maxx-1
sig=(fx(i)-fx(i-1))/(fx(i+1)-fx(i-1))
p=sig*y2(i-1)+2.d0
y2(i)=(sig-1.d0)/p
u(i)=(fy(i+1)-fy(i))/(fx(i+1)-fx(i))
u(i)= u(i)-(fy(i)-fy(i-1))/(fx(i)-fx(i-1))
u(i)=(6.d0*u(i)/(fx(i+1)-fx(i-1))-sig*u(i-1))/p
11 continue

if (ypn.gt..99d30) then
qn=0.d0
un=0.d0
else
qn=0.5d0
un=3.d0/(fx(maxx)-fx(maxx-1))
un=un*(ypn-(fy(maxx)-fy(maxx-1))/(fx(maxx)-fx(maxx-1)))
endif

```

```

y2(maxx)=(un-qn*u(maxx-1))/(qn*y2(maxx-1)+1.d0)
do 12 k=maxx-1,1,-1
y2(k)=y2(k)*y2(k+1)
y2(k)=y2(k)+u(k)
12  continue
return
END SUBROUTINE

* end of the subroutine spline
*****
SUBROUTINE splint(xa,ya,y2a,maxx,xx)

include 'globc_20D.f'

INTEGER maxx
DOUBLE PRECISION xx,xa(maxx),y2a(maxx),ya(maxx),z
INTEGER k,khi,klo
DOUBLE PRECISION a,b,hh

klo=kklo
khi=kkhi

IF(xx.GT.xa(khi))THEN
kkhi=kkhi+1
kklo=kklo+1
klo=kklo
khi=kkhi
ENDIF

IF (((khi-klo).GT.1).AND.(MOD(khi-klo,2)).NE.0)THEN
1  if (khi-klo.gt.1) then
k=(khi+klo)/2
if(xa(k).gt.xx)then
khi=k
else
klo=k
endif
goto 1
endif
ENDIF

IF (((khi-klo).GT.1).AND.(MOD(khi-klo,2)).EQ.0)THEN
2  if (khi-klo.gt.1) then
k=(khi+1+klo)/2
if(xa(k).gt.xx)then
khi=k
else
klo=k
endif
endif

```



```

* Global constants (in all program units must be identical):
*
* MAX_PT - Maximum number of points for the integration.
*
*****
*
INTEGER MAX_PT
PARAMETER (MAX_PT = 2000001)
DOUBLE PRECISION PI
PARAMETER (PI=3.1415926535897932384626433832795028d0)
*
*****
* Global variables
*
*****
* General variables
*

INTEGER divisor, DIFF_MIN, DIFF_MAX, CIAL
INTEGER kklo, kkhi, wave_const
DOUBLE PRECISION NQ, DD, D, NQQ
DOUBLE PRECISION NQR, NQL
DOUBLE PRECISION P2(0:0)
DOUBLE PRECISION y
COMMON /GenVarsI/ divisor, DIFF_MIN, DIFF_MAX, CIAL, kklo, kkhi
COMMON /GenVarsII/ P2, wave_const
COMMON /GenVarsD1/ NQL, NQR, NQ, D, DD, NQQ, y

DOUBLE PRECISION X(-MAX_PT:MAX_PT),R(-MAX_PT:MAX_PT)
DOUBLE PRECISION KK(-MAX_PT:MAX_PT)
DOUBLE PRECISION V(-MAX_PT:MAX_PT)
DOUBLE PRECISION y2(-MAX_PT:MAX_PT)
COMMON /ContVarsD/ V, KK, X, R, y2

*****

```