

# Semiclassical Trajectory Dynamics

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## Abstract

In order to find an effective force  $F_{\text{eff}}$  that approximates  $\langle F(X) \rangle$  in the quantum regime, as well as  $F(x)$  in the classical regime, the concept of the effective potential is introduced. In the context of this thesis, the effective potential is defined as the minimum of the expectation value of the Hamiltonian operator  $H$  under the constraint that the expectation value of the position operator  $X$  is fixed. Some methods to find the effective potential for various one dimensional systems are developed. By using the Liouville equation, the classical trajectory of a collection of particles confined in a linear potential well, i.e.  $V(x) = F|x|$ , is obtained. The semiclassical trajectory of the same system is also obtained by first replacing  $V(x)$  with the corresponding  $V_{\text{eff}}(x)$ , and then solving the Liouville equation. In order to get the quantum trajectory, the Wigner-Moyal equation is considered and solved. Both the Liouville and the Wigner-Moyal equations are solved numerically by using the finite difference method. The three trajectories for various initial conditions are then compared by measuring the overlap in the density and/or the Wigner function as a function of time.

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# Chapter 1

## Introduction

In many areas of physics, one is usually interested in knowing how a system of particles evolves with time when subjected to a certain potential energy  $V$ . In classical mechanics, the time evolution of a system of point particles is governed by the Hamilton equations of motion,

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad (1.1)$$

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}, \quad (1.2)$$

where  $H$  is the classical Hamiltonian,

$$H = \sum_i \frac{p_i^2}{2m} + V. \quad (1.3)$$

More generally, if  $A$  is a quantity that depends on all  $q_i$ 's and  $p_i$ 's, the time evolution of  $A$  can be written as,

$$\begin{aligned} \dot{A} &= \sum_i \left( \frac{\partial A}{\partial q_i} \dot{q}_i + \frac{\partial A}{\partial p_i} \dot{p}_i \right) + \frac{\partial A}{\partial t} \\ &= \{A, H\} + \frac{\partial A}{\partial t}, \end{aligned} \quad (1.4)$$

where  $\{\cdot, \cdot\}$  is called the poisson bracket.

In the Schrodinger picture of quantum mechanics, there is an analogue expression for equation

(1.4),

$$\frac{d}{dt}\langle A \rangle = \frac{1}{i\hbar}\langle [A, H] \rangle + \left\langle \frac{\partial A}{\partial t} \right\rangle. \quad (1.5)$$

The above equation is called the Ehrenfest equation.  $[\cdot, \cdot]$  is the commutator between two operators, and it plays a similar role to the poisson bracket.

Let's now consider a one particle system. By setting  $A = P$ , i.e. the momentum operator, equation (1.5) becomes

$$\begin{aligned} \frac{d}{dt}\langle P \rangle &= -\left\langle \frac{\partial V}{\partial X} \right\rangle \\ &= \langle F(X) \rangle. \end{aligned} \quad (1.6)$$

Equation (1.6) is similar to equation (1.2) in some sense but not exactly the same. Even if one tries to carry equation (1.2) forward to quantum mechanics by setting  $x \rightarrow \langle X \rangle$  and  $p \rightarrow \langle P \rangle$ , the resulting equation is

$$\frac{d}{dt}\langle P \rangle = F(\langle X \rangle). \quad (1.7)$$

In general,  $F(\langle X \rangle) \neq \langle F(X) \rangle$ , and therefore equation (1.7) is not the same as equation (1.6). The purpose of this project is therefore to find an effective force  $F_{\text{eff}}$ , satisfying  $F_{\text{eff}}(\langle X \rangle) \simeq \langle F(X) \rangle$ .

## 1.1 The Effective Potential

The concept of the effective potential in the context of field theory was introduced by Coleman and Weinberg [1] in their paper in 1973. In this thesis, the idea of the effective potential is somewhat similar to that introduced in [1], with a slight modification in the sense that the expectation value of the position operator is used instead of the expectation value of some scalar field. Furthermore, since quantum field theory is beyond the scope of this thesis, a more suggestive argument will be used to introduce the concept of the effective potential rather than a formal treatment which makes use of the effective action and Feynman diagram as elucidated in [1].

In classical mechanics, the effective potential is defined to be the minimum energy of a system when its position is fixed. In order to carry this forward to quantum mechanics, a slight modification must be made. Since position and energy defined in the classical case are analogous to position and Hamiltonian operator respectively in quantum mechanics, it is instructive to define the effective potential  $V_{\text{eff}}$  as the minimum of the expectation value of the Hamiltonian operator  $H$ , under the constraint that the expectation value of the position operator  $X$  is fixed. That is, it is written  $V_{\text{eff}}(x) = \min_{|\psi\rangle} \langle H \rangle$  given  $\langle X \rangle = x$ .

## 1.2 Wigner-Weyl Transform

In classical statistical mechanics, the time evolution of a density  $\rho$  describing a collection of points in phase space is governed by the Liouville equation

$$\frac{\partial \rho}{\partial t} = \frac{\partial \rho}{\partial p} V'(x) - \frac{p}{m} \frac{\partial \rho}{\partial x}, \quad (1.8)$$

where  $x$  and  $p$  are position and momentum respectively, and  $V(x)$  is the potential energy. The equation above describes a system with only one degree of freedom, but it is easy to generalize it to the case with more than one degree of freedom.

In quantum mechanics,  $X$  and  $P$  operators, which correspond to  $x$  and  $p$  in classical mechanics, are not independent of each other, but are connected by the commutation relation  $[X, P] = i\hbar$ . As such, it makes no sense to draw a phase space diagram involving  $X$  and  $P$  directly. In order to be able to describe a trajectory in quantum mechanical system, it is therefore required to introduce new quantities which are analogues to  $X$  and  $P$  operators, but have equal footing, in the sense that these new quantities are merely numbers. It turns out that such quantities can be obtained from  $X$  and  $P$  by performing the *Wigner transform* [2],

$$X_w = \int dx' \langle x - \frac{1}{2}x' | X | x + \frac{1}{2}x' \rangle e^{\frac{ipx'}{\hbar}}, \quad (1.9)$$

$$P_w = \int dx' \langle x - \frac{1}{2}x' | P | x + \frac{1}{2}x' \rangle e^{\frac{ipx'}{\hbar}}. \quad (1.10)$$



The integral in equation (1.9) and (1.10) can be simplified to get  $X_w = x$  and  $P_w = p$ , i.e.  $X_w$  and  $P_w$  are not operators. In general, the Wigner transform can be performed on any operator via the above equations to get a non-operator version, which describes the same physical meaning as the corresponding operator version, as a function of  $X_w$  and  $P_w$  ( $x$  and  $p$ ). It is also possible to write the Wigner transform of an operator  $A$  as

$$\begin{aligned} A_w &= \text{Tr} \left\{ A \int dx' |x + \frac{1}{2}x'\rangle \langle x - \frac{1}{2}x'| e^{\frac{ipx'}{\hbar}} \right\} \\ &= \text{Tr} \{ AW(x, p) \}, \end{aligned} \quad (1.11)$$

where  $W(x, p) = \int dx' |x + \frac{1}{2}x'\rangle \langle x - \frac{1}{2}x'| \exp(\frac{ipx'}{\hbar}) = 2 \exp(-2i(X - x); (P - p))$ . The semicolon in the previous expression indicates that appearing products of  $X$  and  $P$  are written so that  $X$  stands left and  $P$  stands right.

These transformed quantities can also be converted back to their corresponding operator version by performing the *Weyl transform* [3, 4]

$$A = \frac{1}{2\pi\hbar} \int dx \int dp A_w W(x, p). \quad (1.12)$$

### 1.3 Wigner Function and Its Properties

There is an important lemma relating the Wigner transform of a product of two operators and the Wigner transform of each operator.

**Lemma 1.** *Let  $F$  and  $G$  be two operators. The Wigner transform of the product of the two operators is given by*

$$\begin{aligned} (FG)_w &= F_w \exp\left(\frac{i\hbar}{2}\Lambda\right)G_w \\ &= G_w \exp\left(-\frac{i\hbar}{2}\Lambda\right)F_w, \end{aligned}$$

where  $\Lambda = \overleftarrow{\frac{\partial}{\partial x}} \overrightarrow{\frac{\partial}{\partial p}} - \overleftarrow{\frac{\partial}{\partial p}} \overrightarrow{\frac{\partial}{\partial x}}$ . Left arrow means that the operator is acting on the left, while right arrow means that the operator is acting on the right.

The proof of the above lemma was presented in a paper by Īmre in 1967 [5]. The detail of the proof will be provided in the appendix and it will mainly follow the proof presented in [5]. The Wigner transform of the product of two operators  $F$  and  $G$  is often denoted as  $F_w \star G_w$  [6].

In order to construct an expression which is similar to the classical Liouville equation, i.e. equation (1.8), it is instructive to perform the Wigner Transform on the equation of motion for density matrix (Heisenberg equation of motion). That is,

$$\begin{aligned} \frac{\partial}{\partial t} \rho_w &= -\frac{1}{i\hbar} [\rho, H]_w \\ &= -\frac{1}{i\hbar} \rho_w \left( \exp\left(\frac{i\hbar}{2}\Lambda\right) - \exp\left(-\frac{i\hbar}{2}\Lambda\right) \right) H_w \\ &= \frac{2}{\hbar} H_w \sin\left(\frac{\hbar}{2}\Lambda\right) \rho_w. \end{aligned} \quad (1.13)$$

It can be shown that  $H_w(x, p) = \frac{p^2}{2m} + V(x)$ , and equation (1.13) can therefore be expanded to get,

$$\begin{aligned} \frac{\partial}{\partial t} \rho_w &= \frac{2\rho_w}{\hbar} \sin\left(\frac{\hbar}{2} \overleftarrow{\frac{\partial}{\partial p}} \overrightarrow{\frac{\partial}{\partial x}}\right) V(x) - \frac{p}{m} \frac{\partial \rho_w}{\partial x} \\ &= \frac{1}{i\hbar} \left[ V\left(x + \frac{i\hbar}{2} \frac{\partial}{\partial p}\right) - V\left(x - \frac{i\hbar}{2} \frac{\partial}{\partial p}\right) \right] \rho_w - \frac{p}{m} \frac{\partial \rho_w}{\partial x}. \end{aligned} \quad (1.14)$$

The above equation is called the Wigner-Moyal equation [7], and is analogous to the classical Liouville equation, i.e. equation (1.8). In fact, in the correspondence limit, equation (1.14) reduces to (1.8). This can be shown by Taylor expanding equation (1.14) up to first order in  $\hbar$ ,

$$\begin{aligned} \frac{\partial}{\partial t} \rho_w &= \frac{1}{i\hbar} \left[ V(x) + \frac{dV}{dx} \frac{i\hbar}{2} \frac{\partial}{\partial p} - V(x) + \frac{dV}{dx} \frac{i\hbar}{2} \frac{\partial}{\partial p} + \mathcal{O}[\hbar^2] \right] \rho_w - \frac{p}{m} \frac{\partial \rho_w}{\partial x} \\ \frac{\partial}{\partial t} \rho_w &= \frac{dV}{dx} \frac{\partial \rho_w}{\partial p} - \frac{p}{m} \frac{\partial \rho_w}{\partial x} + \mathcal{O}[\hbar], \end{aligned}$$

which is precisely equation (1.8) if  $\hbar \rightarrow 0$ .

The quantity  $\rho_w$  is called the Wigner function, and it can be shown to have the following properties [7]:

1. The Wigner function is real and normalized to unity, i.e.  $\int \frac{\rho_w}{2\pi\hbar} dx dp = 1$ .

2.  $\int \frac{\rho_w}{2\pi\hbar} dp = \langle x|\rho|x\rangle.$

3.  $\int \frac{\rho_w}{2\pi\hbar} dx = \langle p|\rho|p\rangle$

4. The Wigner function can take negative values. It therefore does not satisfy one of the probability axioms and cannot represent a probability density. It is usually referred to as a *quasi-probability distribution function*.

5. **Hudson Theorem:** [8] A necessary and sufficient condition for the Wigner function to be a true probability density (no negative value) is that the corresponding Schrödinger state function be the exponential of a quadratic polynomial.

## Chapter 2

# Obtaining the Effective Potential

In this chapter, some methods to obtain the effective potential for some one-dimensional systems are developed. Since obtaining an effective potential as defined in the first chapter is an optimization problem with constraint, it is instructive to introduce a Lagrange multiplier  $f$ . In terms of  $f$ , the optimization problem reduces to a single equation to solve, that is,

$$\begin{aligned}\delta\langle H \rangle - f\delta\langle X \rangle &= 0, \\ \delta\langle H_{\text{modified}} \rangle &= 0,\end{aligned}\tag{2.1}$$

where it is defined for convenience that  $H_{\text{modified}} = H - fX$ . There are two cases to be discussed in this chapter. For the first case, which is the easiest case, one dimensional systems with infinitely many bound states are considered. Furthermore, it is assumed that the potential energy of the system is symmetric and increasing to infinity faster than or at the same rate as  $k|x|$  for some constant  $k$ . Under these assumptions, the modified Hamiltonian will have a bound state. In this case, a useful lemma [9] can be introduced as follows:

**Lemma 2.** *Let  $H$  be a Hamiltonian that has at least a bound state. If  $|\psi\rangle$  is any state and  $E_g$  is the ground state of  $H$ , then  $\langle\psi|H|\psi\rangle \geq E_g$ .*

The proof of this lemma is provided in the appendix A1. According to this lemma, in order to minimize the expectation value of the modified Hamiltonian, it is sufficient to find the ground state

of the modified Hamiltonian. The effective potential can thus be obtained as

$$V_{\text{eff}}(x) = E_g(x) + f(x)x, \quad (2.2)$$

where  $x = \langle X \rangle$  is given and  $E_g(x)$  is the ground state of the modified Hamiltonian.<sup>1</sup> Some examples are illustrated in the first two sections below before moving to the second case, which is a more general case.

## 2.1 Example 1: Simple Harmonic Oscillator

As a simple example to illustrate the method previously explained, let's consider a one dimensional simple harmonic oscillator. The potential for one dimensional simple harmonic oscillator is given by  $V(x) = \frac{1}{2}m\omega^2x^2$ , where  $m$  is the mass of the particle, and  $\omega$  is the natural frequency of the oscillator.

The modified Hamiltonian in this case is

$$\begin{aligned} H_{\text{modified}} &= \frac{P^2}{2m} + \frac{1}{2}m\omega^2X^2 - fX \\ &= \frac{P^2}{2m} + \frac{1}{2}m\omega^2\left(X - \frac{f}{m\omega^2}\right)^2 - \frac{f^2}{2m\omega^2}. \end{aligned}$$

The first two terms are just the Hamiltonian of another simple harmonic oscillator with the same natural frequency centered around  $\frac{f}{m\omega^2}$ . Meanwhile, the third term is just a constant term. The ground state of the modified Hamiltonian is then  $E_g = \frac{1}{2}\hbar\omega - \frac{f^2}{2m\omega^2}$ . As a function of the expectation value  $x = \langle X \rangle$ , it can be observed from the modified Hamiltonian that  $\frac{f}{m\omega^2} = x$ , or  $f = m\omega^2x$ . Therefore,

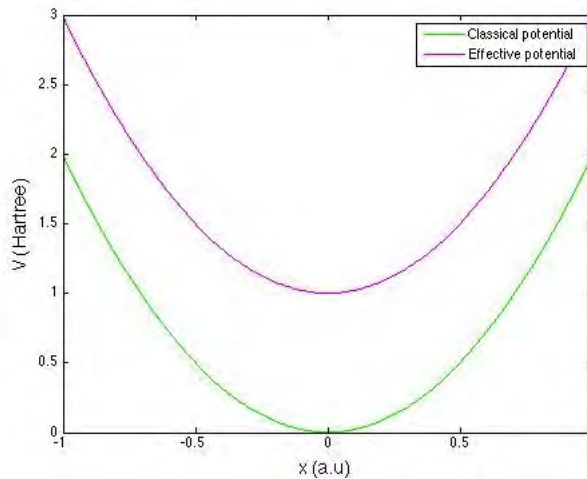
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<sup>1</sup>The ground state of the modified Hamiltonian is a function of the Lagrange multiplier  $f$ , which depends on the expectation value  $x$ . It is also noticed that the effective potential is a Legendre transform of the modified Hamiltonian ground state with respect to variable  $f$ .

$$\begin{aligned}
V_{\text{eff}}(x) &= E_g(x) + fx \\
&= \frac{1}{2}\hbar\omega + \frac{1}{2}m\omega^2x^2.
\end{aligned}
\tag{2.3}$$

This result shows that the effective potential for a simple harmonic oscillator is simply the classical potential energy, but is shifted by the amount of the zero point energy of the system. By using MATLAB, the effective potential can be plotted and compared to the classical potential in the figure below ( $\omega = 2\text{a.u.}$ ):

Figure 2.1: The effective and classical potential for simple harmonic oscillator



If  $x$  is close to 0, the value of the effective potential will tend to get closer to the zero point energy of the system. Meanwhile, for large  $|x|$ , the effective potential will approximately be the same as the classical potential, as the  $\frac{1}{2}\hbar\omega$  term will be relatively small compared to  $x^2$ . Also, in fully classical case, as  $\hbar \rightarrow 0$ , the effective potential reduces to the classical potential.

## 2.2 Example 2: Linear Potential Well

As a second example, consider a system in a linear potential well, i.e.  $V(x) = F|x|$  for some positive constant  $F$ . By limiting the values of  $f$  to  $|f| < F$ , the modified Hamiltonian will still have bound states, the previous procedure can therefore be applied.

The modified Hamiltonian for linear potential well can be written as  $H_{\text{modified}} = \frac{P^2}{2m} + F|X| - fX$ . In order to find the ground state of the modified Hamiltonian, it suffices to solve the eigenvalue equation<sup>2</sup>

$$\begin{aligned} H_{\text{modified}}\psi(x) &= E_g\psi(x), \\ -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + (F|x| - fx - E_g)\psi(x) &= 0. \end{aligned}$$

The general solution to this kind of equation can be guessed to be in the form of  $\psi(x > 0) = a_1\text{Ai}(k_1x - c_1)$  and  $\psi(x < 0) = a_2\text{Ai}(k_2x - c_2)$  where  $\text{Ai}(x)$  is the Airy function of the first kind,  $a_1$  and  $a_2$  are the normalization constants.<sup>3</sup> By differentiating  $\psi(x > 0)$  with respect to  $x$  two times,

$$\begin{aligned} \frac{d\psi(x)}{dx} &= a_1k_1\text{Ai}'(k_1x - c_1), \\ \frac{d^2\psi(x)}{dx^2} &= a_1k_1^2\text{Ai}''(k_1x - c_1) \\ &= a_1k_1^2(k_1x - c_1)\text{Ai}(k_1x - c_1). \end{aligned}$$

Substituting this to the eigenvalue equation for  $x > 0$  gives

$$\begin{aligned} -\frac{\hbar^2}{2m}a_1k_1^2(k_1x - c_1)\text{Ai}(k_1x - c_1) \\ + a_1((F - f)x - E_g)\text{Ai}(k_1x - c_1) &= 0, \\ k_1 &= \left(\frac{2m(F - f)}{\hbar^2}\right)^{\frac{1}{3}}, \end{aligned} \tag{2.4}$$

$$c_1 = \frac{2mE_g}{k_1^2\hbar^2}. \tag{2.5}$$

In a similar fashion, by evaluating the second derivative of  $\psi(x < 0)$  and substituting it into the eigenvalue equation,

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<sup>2</sup>In the following, the variable  $x$  is understood to be the coordinate variable, not the expectation value  $\langle X \rangle$ .

<sup>3</sup>There is actually another term which involves the Airy function of the second kind, i.e.  $b\text{Bi}(kx - c)$  for some constant  $b$ . However, unless  $b = 0$ , this term blows up at  $x \rightarrow \pm\infty$ , which is not allowed for a normalizable solution.

$$\begin{aligned}
& -\frac{\hbar^2}{2m}a_2k_2^2(k_2x - c_2)\text{Ai}(k_2x + c_2) \\
& +a_2(-(F + f)x - E_g)\text{Ai}(k_2x + c_2) = 0, \\
& k_2 = -\left(\frac{2m(F + f)}{\hbar^2}\right)^{\frac{1}{3}}, \tag{2.6}
\end{aligned}$$

$$c_2 = \frac{2mE_g}{k_2^2\hbar^2}. \tag{2.7}$$

It now remains to determine the ground state energy  $E_g$ . Before doing so, it is required that the wave function and its derivative are continuous everywhere. In particular, the condition that they are continuous at  $x = 0$  gives

$$\begin{aligned}
ak_1\text{Ai}(-c_1) &= bk_2\text{Ai}(-c_2), \\
ak_1\text{Ai}'(-c_1) &= bk_2\text{Ai}'(-c_2), \\
\frac{k_1\text{Ai}'(-c_1)}{\text{Ai}(-c_1)} &= \frac{k_2\text{Ai}'(-c_2)}{\text{Ai}(-c_2)}, \\
\frac{\text{Ai}'(-c_1)}{\sqrt{c_1}\text{Ai}(-c_1)} + \frac{\text{Ai}'(-c_2)}{\sqrt{c_2}\text{Ai}(-c_2)} &= 0, \tag{2.8}
\end{aligned}$$

where the last line is obtained by moving the right hand side to the left hand side, and then substituting equation (2.4) - (2.7). Equation (2.8) can, in principle, be solved for  $E_g(f)$ .

This is still not the end of the story, as the effective potential is a function of the given expectation value  $x = \langle X \rangle$ , not the Lagrange multiplier. In this case, a relationship between  $f$  and  $x$  must be found. This can be done by making use of the Feynman-Hellmann theorem [9]:

**Feynman-Hellmann Theorem.** *Let  $E$  be the energy eigenvalue to the Hamiltonian  $H$  with (normalized) eigenstate  $|\psi\rangle$ . Suppose  $H$  is a function of a parameter  $\lambda$ . It follows that  $\langle\psi|\frac{\partial H}{\partial\lambda}|\psi\rangle = \langle\frac{\partial H}{\partial\lambda}\rangle = \frac{\partial E}{\partial\lambda}$ .*

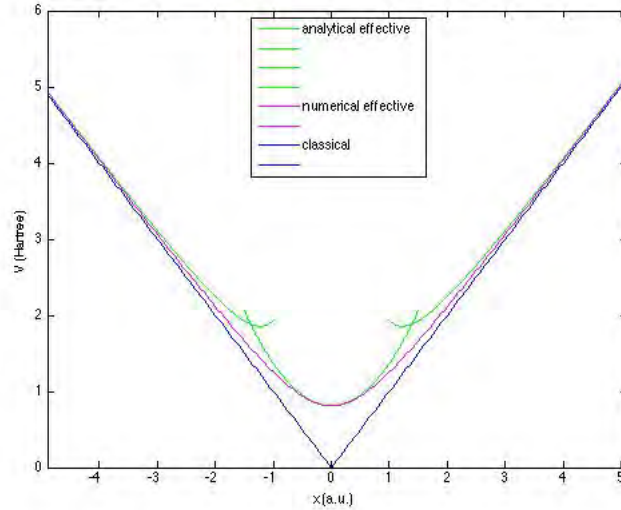
The proof of the Feynman-Hellmann theorem is provided in the appendix. By letting  $f$  as the  $\lambda$  parameter in the Feynman-Hellmann theorem,



$$\begin{aligned}
\left\langle \frac{\partial H}{\partial f} \right\rangle &= \frac{\partial E_g}{\partial f}, \\
-\langle X \rangle &= \frac{\partial E_g}{\partial f}, \\
\frac{\partial E_g}{\partial f} &= -x.
\end{aligned} \tag{2.9}$$

In principle, equation (2.9) can be inverted to give  $f(x)$ . Therefore, solving equations (2.8) and (2.9) together will give the effective potential  $V_{\text{eff}}(x)$ . It is not difficult to do this numerically. By using MATLAB, equation (2.8) can be solved for  $E_g$  some values of fixed  $f$ . After storing the values of  $E_g(f)$  evaluated previously, numerical differentiation can be performed to give the left hand side of equation (2.9). Lastly, given the expectation value  $\langle X \rangle = x$ , the value of  $E_g$  and  $f$  satisfying equation (2.9) can be determined. For further details, a MATLAB code to solve this problem is provided in the appendix A2. The effective potential associated with this system can be plotted as follows (where  $F = 1a.u.$ ):

Figure 2.2: The effective and classical potential of a linear potential well



In the above figure, the blue curve shows the classical potential, while the magenta curve shows the corresponding effective potential. The green curves show the asymptotic behaviour of the effective potential for small and large  $|x|$ , which are going to be explained in a more detail in the next two subsections.

### 2.2.1 Asymptotic Behaviour for Small $|x|$

In addition to the numerical solution, it is also interesting to consider the analytical approximation of the effective potential for small and large values of  $|x|$ . First thing to note is that  $x = 0$  when  $f = 0$ , as the modified Hamiltonian will be just the Hamiltonian, and the expectation value of  $X$  is 0 by the symmetry of the potential. Another thing to note is that as  $|f| \rightarrow F$ , the magnitude of the expectation value of  $X$  will become very large. In order to understand this, first recall that the wave function decays in the classically forbidden region, while oscillates in the classically allowed region. Without loss of generality, assume that  $f > 0$ . In this case, the potential energy part of the modified Hamiltonian for the region  $x < 0$  will have steeper slope than the region  $x > 0$ . Therefore, given the value of  $E_g$ , the wave function should decay faster in the region  $x < 0$  than in the region  $x > 0$ . Because of this, it can be deduced that the peak of the wave function, and hence the expectation value, should be somewhere in the region  $x > 0$ . If  $f \rightarrow F$ , the slope of the potential energy part of the modified Hamiltonian in the region  $x > 0$  will be very small, and thus the wave function will start decaying at very large  $x$ . Furthermore, in the region  $x < 0$ , the slope of the potential energy part of the modified Hamiltonian tends to get steeper as  $f$  is increasing. This implies the wave function to start decaying even faster in this region. By the same argument as before, it is deduced that the expectation value will be at very large  $x > 0$ .

Having understood how  $x$  and  $f$  are related qualitatively, it is now easy to find the expression for  $V_{\text{eff}}(x)$  for small and large  $|x|$ , i.e. by letting  $|f| \rightarrow 0$  and  $|f| \rightarrow F$ . In this subsection, the expression of  $V_{\text{eff}}(x)$  for small  $|x|$  is derived. The derivation for the case of large  $|x|$  is explained in the next subsection. For convenience, define  $L(c) = \frac{\text{Ai}'(-c)}{\sqrt{c\text{Ai}(-c)}}$ . In this notation, equation (2.8) becomes  $L(c_1) + L(c_2) = 0$ . If  $|f| \rightarrow 0$ , up to first order,  $c_1 \mp \epsilon_1 \approx c_2 \pm \epsilon_2 \approx y_0$  for some (small) positive numbers  $\epsilon_1$  and  $\epsilon_2$ , where  $-y_0$  is the first zero of the first derivative of the Airy function  $\text{Ai}'(x)$ .<sup>4</sup> In particular, assuming  $f > 0$ , equation (2.4) - (2.7) show that  $c_1 > c_2$  and by Taylor expanding  $L(c)$  in equation (2.8),

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<sup>4</sup>In this paper, the first zero of  $\text{Ai}(x)$  and  $\text{Ai}'(x)$  refer to the zeros that are closest to the origin.

$$\begin{aligned}
L(c_1) + L(c_2) &= L(y_0 + \epsilon_1) + L(y_0 - \epsilon_2) \\
&= L'(y_0)\epsilon_1 - L'(y_0)\epsilon_2 \\
&= 0,
\end{aligned}$$

where  $L(y_0) = 0$ , as a result of  $L(y_0) \propto \text{Ai}'(-y_0)$ , is used in the above equation. The second and the third line in the above equation implies  $\epsilon_1 = \epsilon_2 = \epsilon$ .<sup>5</sup> By dividing  $c_1$  by  $c_2$ ,

$$\begin{aligned}
\frac{c_1}{c_2} &= \frac{k_2^2}{k_1^2} \\
&= \left(\frac{F+f}{F-f}\right)^{\frac{2}{3}} \\
&= \frac{y_0 + \epsilon}{y_0 - \epsilon}, \\
\frac{f}{F} &= \frac{(y_0 + \epsilon)^{\frac{3}{2}} - (y_0 - \epsilon)^{\frac{3}{2}}}{(y_0 + \epsilon)^{\frac{3}{2}} + (y_0 - \epsilon)^{\frac{3}{2}}} \\
&\approx \frac{(y_0^{\frac{3}{2}} + \frac{3}{2}\epsilon y_0^{\frac{1}{2}}) - (y_0^{\frac{3}{2}} - \frac{3}{2}\epsilon y_0^{\frac{1}{2}})}{(y_0^{\frac{3}{2}} + \frac{3}{2}\epsilon y_0^{\frac{1}{2}}) + (y_0^{\frac{3}{2}} - \frac{3}{2}\epsilon y_0^{\frac{1}{2}})} \\
&= \frac{3}{2} \frac{\epsilon}{y_0}. \tag{2.10}
\end{aligned}$$

Equation (2.10) shows how  $f$  scales with  $\epsilon$ , the small positive parameter corresponding to the difference between  $y_0$  and  $c_1$  or  $c_2$ , valid for small values of  $|f|$ . It is also possible to find the relationship between  $E_g$  and  $\epsilon$  by looking at equation (2.4) and (2.5),

---

<sup>5</sup>This is true provided  $L'(y_0) \neq 0$ . In fact, it is easy to show that  $L'(y_0)$  is indeed non-zero by using product rule. The only non-zero term comes by differentiating  $\text{Ai}'(-c)$  in the numerator and using the fact that  $\text{Ai}''(-y_0) = -y_0 \text{Ai}(-y_0)$ . [10]

$$\begin{aligned}
c_1 &= \frac{2mE_g}{k_1^2\hbar^2} \\
&= \left(\frac{2m}{F^2\hbar^2}\right)^{\frac{1}{3}} \frac{E_g}{\left(1 - \frac{f}{F}\right)^{\frac{2}{3}}} \\
&\approx \left(\frac{2m}{F^2\hbar^2}\right)^{\frac{1}{3}} \frac{E_g}{\left(1 - \frac{3\epsilon}{2y_0}\right)^{\frac{2}{3}}}, \\
E_g &= \left(\frac{F^2\hbar^2}{2m}\right)^{\frac{1}{3}} \left(1 - \frac{3\epsilon}{2y_0}\right)^{\frac{2}{3}} c_1 \\
&= \left(\frac{F^2\hbar^2}{2m}\right)^{\frac{1}{3}} \left(1 - \frac{3\epsilon}{2y_0}\right)^{\frac{2}{3}} (y_0 + \epsilon) \\
&\approx \left(\frac{F^2\hbar^2}{2m}\right)^{\frac{1}{3}} \left(y_0 - \frac{5\epsilon^2}{4y_0}\right) \\
&= E_0 y_0 - \frac{5E_0\epsilon^2}{4y_0}. \tag{2.11}
\end{aligned}$$

In the last line above,  $E_0 = \left(\frac{F^2\hbar^2}{2m}\right)^{\frac{1}{3}}$ . Equation (2.11) and (2.10) can be combined to obtain  $E_g$  as a function of  $f$ .

$$E_g \approx E_0 y_0 - \frac{5f^2 y_0}{9F^2}. \tag{2.12}$$

Equation (2.9) can then be applied to get

$$\begin{aligned}
x &= -\frac{\partial E_g}{\partial f} \\
&\approx \frac{10f y_0 E_0}{9F^2}, \\
f &\approx \frac{9F^2 x}{10y_0 E_0}. \tag{2.13}
\end{aligned}$$

Equation (2.13) can be substituted back into equation (2.12) to find

$$E_g \approx E_0 y_0 - \frac{9F^2 x^2}{20y_0 E_0}. \tag{2.14}$$

Finally, the effective potential, valid for small  $|x|$ , is obtained by using equation (2.2),

$$\begin{aligned} V_{\text{eff}}(x) &= E_g(x) + fx \\ &\approx E_0 y_0 + \frac{9F^2 x^2}{20y_0 E_0}. \end{aligned} \tag{2.15}$$

One can identify that the first term of equation (2.15) is just the ground state energy of the linear potential well. The second term is, however, quadratic, in contrast to the classical potential  $V(x) = F|x|$  which is linear. Because of this quadratic form, the angular frequency associated with the motion near the equilibrium point can be calculated. This will be discussed further in subsection (2.2.3).

### 2.2.2 Asymptotic Behaviour for Large $|x|$

After looking at the case when  $|x|$  is small, let's now turn to the case when  $|x|$  is very large. Without loss of generality, it is assumed that  $x > 0$ , and hence  $f > 0$  from the argument in the first paragraph of this subsection. Recall also that if  $x$  is very large,  $f \rightarrow F$ . According to equation (2.4),  $k_1 \rightarrow 0$ . However, since  $c_1$  is finite, it follows that  $E_g \rightarrow 0$ . As a consequence, equation (2.7) tells that  $c_2 \rightarrow 0$ . By defining  $L(y)$  as in the previous subsection, it then follows that  $L(c_2) \rightarrow -\infty$ , where there is an overall minus sign since  $\text{Ai}(0) > 0$  while  $\text{Ai}'(0) < 0$ . On the other hand, it is required that equation (2.8) holds. This implies  $L(c_1) \rightarrow +\infty$ . This can be achieved only if  $-c_1$  is close to the zero of the Airy function  $\text{Ai}(x)$ .

From this observation, it is safe to assume that  $c_2 = \epsilon$  and  $c_1 = \alpha - \epsilon_1$ , where  $\epsilon$  and  $\epsilon_1$  are small positive numbers, and  $-\alpha$  is the first zero of Airy function  $\text{Ai}(x)$ . By expanding equation (2.8) up to first order,

$$\begin{aligned} \frac{\text{Ai}'(0)}{\sqrt{\epsilon}\text{Ai}(0)} + \frac{\text{Ai}'(-\alpha)}{\sqrt{\alpha}\text{Ai}'(-\alpha)(\epsilon_1)} &= \frac{\text{Ai}'(0)}{\sqrt{\epsilon}\text{Ai}(0)} + \frac{1}{\sqrt{\alpha}(\epsilon_1)}, \\ \epsilon_1 &= \frac{\sqrt{\epsilon}}{\sqrt{\alpha}u_0}, \end{aligned} \tag{2.16}$$

where  $u_0 = -\frac{\text{Ai}'(0)}{\text{Ai}(0)} > 0$ . As in the case for small  $|x|$  by dividing  $c_1$  by  $c_2$ ,

$$\begin{aligned}\frac{c_1}{c_2} &= \left(\frac{F+f}{F-f}\right)^{\frac{2}{3}} \\ &= \frac{\alpha - \frac{\sqrt{\epsilon}}{\sqrt{\alpha u_0}}}{\epsilon}, \\ \frac{f}{F} &\approx 1 - \frac{2\epsilon^{\frac{3}{2}}}{\alpha^{\frac{3}{2}}}.\end{aligned}\tag{2.17}$$

By considering the expression for  $c_1$ , it is possible to obtain the relationship between  $E_g$  and  $\epsilon$  as well. That is,

$$\begin{aligned}c_1 &= \frac{E_g}{E_0(1 - \frac{f}{F})^{\frac{2}{3}}} \\ &\approx \frac{E_g\alpha}{2^{\frac{2}{3}}E_0\epsilon}, \\ E_g &\approx 2^{\frac{2}{3}}\epsilon E_0.\end{aligned}\tag{2.18}$$

By combining equation (2.17) and (2.18),

$$E_g \approx \alpha\left(1 - \frac{f}{F}\right)^{\frac{2}{3}}.\tag{2.19}$$

As  $E_g(f)$  has been obtained, direct application of equation (2.9) can be performed to get

$$\begin{aligned}x &= -\frac{\partial E_g}{\partial f} \\ &\approx \frac{2\alpha E_0}{3F}\left(a - \frac{f}{F}\right)^{-\frac{1}{3}}, \\ f &\approx F - \left(\frac{2\alpha E_0}{3F^{\frac{2}{3}}x}\right)^3,\end{aligned}\tag{2.20}$$

$$E_g \approx \left(\frac{2\alpha^{\frac{3}{2}}E_0}{3Fx}\right)^2.\tag{2.21}$$

With equations (2.20) and (2.21) ready, equation (2.2) can be used to finally get the approximation of the effective potential for large  $|x|$ , which is

$$V_{\text{eff}}(x) \approx F|x| + \frac{4\alpha^3 E_0^3}{27F^2 x^2}. \quad (2.22)$$

In the correspondence limit  $\hbar \rightarrow 0$ ,  $E_0 \rightarrow 0$  and the expression above reduces to that of the classical potential.

### 2.2.3 Further Observations

In general, a Lagrange multiplier is not merely a number, rather it represents a certain physical meaning. It is therefore instructive to understand the physical meaning of the Lagrange Multiplier introduced earlier, i.e.  $f$ . To do this, let's look at the expression for the effective potential as a functional of  $f$  and  $x$ , i.e.  $V_{\text{eff}} = E_g + fx$ . By taking the functional derivative of this expression,

$$\begin{aligned} \frac{\delta V_{\text{eff}}}{\delta x} &= \frac{\delta E_g}{\delta x} + \frac{\delta fx}{\delta x} \\ &= \frac{\partial E_g}{\partial f} \frac{\delta f}{\delta x} + x \frac{\delta f}{\delta x} + f \\ &= -x \frac{\delta f}{\delta x} + x \frac{\delta f}{\delta x} + f \\ &= f. \end{aligned} \quad (2.23)$$

Equation (2.9) had been used to get the third line from the second line. According to equation (2.23),  $-f$  represents the physical force acting on the system due to the effective potential. This can also be verified by looking at some values of  $x$ . For example, if  $x = 0$ ,  $f = 0$  and therefore no force is acting on the system. If  $x > 0$ ,  $f > 0$  and therefore the force is directing to the left, i.e. toward  $x = 0$ . Finally, if  $x$  is positively large,  $f \rightarrow F$  and the magnitude of the force is approximating that due to the classical potential. These descriptions agree with figure (2.2).

In subsection (2.2.1), the effective potential expression for small values of  $|x|$  was derived. Equation (2.15) shows that the effective potential is approximately quadratic for small  $|x|$ . As a result, a particle weakly disturbed from the equilibrium position will undergo a simple harmonic motion. By noting that equation (2.15) takes the form  $V_{\text{eff}}(x) = a + \frac{1}{2}m\omega^2 x^2$ , it is easy to see that  $\omega = \sqrt{\frac{9F^2}{10m\gamma_0 E_0}}$ .

In this expression,  $\omega$  represents the angular frequency of the system under the influence of the effective potential. This angular frequency can be compared with the angular frequency corresponding to the energy transition from the first excited state to the ground state for linear potential well. The angular frequency that corresponds to this energy transition is given by  $\omega_{\text{trans}} = \frac{E_1 - E_g}{\hbar}$ .<sup>6</sup> By modifying equation (2.8) to the case  $f = 0$ , it is easy to see that  $E_1 = E_0\alpha$  and  $E_g = E_0y_0$ , where  $E_0$ ,  $\alpha$ , and  $y_0$  are as defined previously. Therefore,  $\omega_{\text{trans}} = \frac{E_0(\alpha - y_0)}{\hbar}$ . Upon comparing  $\omega$  with  $\omega_{\text{trans}}$ , all the system dependent parameters such as  $m$  and  $F$  nicely cancel, leaving only a fixed number  $\frac{\omega_{\text{trans}}}{\omega} \approx 0.9926$  that is independent of any parameters.

This result is useful. In general, any given state can be expressed as a linear combination of all the eigenstates. For small values of  $\langle H \rangle$ , which classically corresponds to small energy values, this linear combination is dominated by the ground state and the first excited. Furthermore, the time evolution of the probability density corresponding to a state that consists of the ground state and the first excited state will be periodic with angular frequency  $\omega_{\text{trans}}$ . The above results therefore shows that for small energy values, the effective potential gives a nice description of the quantum behaviour. This will also be verified more clearly in chapter 3, when the semiclassical and the quantum trajectory are compared.

## 2.3 More General Methods

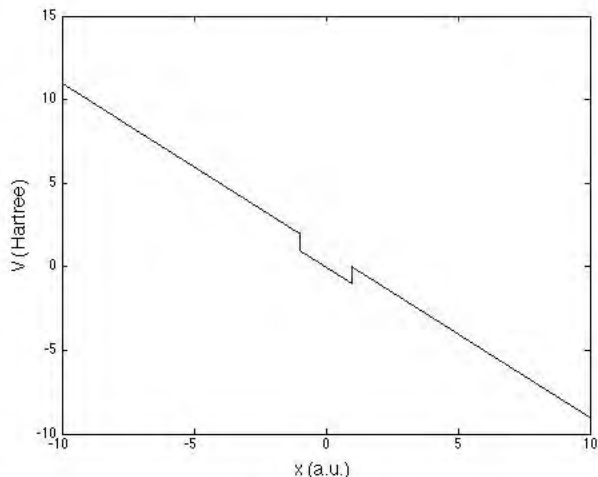
The method developed previously will not work in general. As an illustration, consider a finite square potential  $V(x) = V_0$  when  $|x| < a$  and 0 otherwise. The modified Hamiltonian that corresponds to this potential is  $H_{\text{modified}} = \frac{P^2}{2m} - fX + V_0(\eta(X + a) - \eta(X - a))$ , where  $\eta(x)$  is the step function. The potential part of this modified Hamiltonian can be plotted in the following figure:

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<sup>6</sup>In this subsection,  $E_g$  refers to the ground state of the linear potential well Hamiltonian, not that of the modified Hamiltonian as used in the previous subsections, e.g. in the first line of equation (2.3).



Figure 2.3: Plot of  $V_{\text{modified}}(x)$  with  $f = 1\text{a.u.}$  and  $V_0 = 1\text{Hartree}$



According to the figure above, the modified Hamiltonian is quantum mechanically unbounded. In other words, it does not have a bound state. Equation (2.2) cannot be applied here because there is no  $E_g$ . In order to solve equation (2.1), all possible forms of wave functions must therefore be considered. This is clearly not an easy work and not very effective either. In this section, more general methods to solve this minimization problem will be elucidated.

### 2.3.1 Method 1

If introducing one Lagrange Multiplier causes a trouble, it is natural to think that introducing another Lagrange Multiplier might solve the problem. This is actually the main idea of the more general methods.

In order to be able to introduce the second Lagrange Multiplier, a second constraint must be added to the system. Suppose that in addition to fixing  $\langle X \rangle = x$ , the expectation value of  $X^2$  is also fixed to a value  $\langle X^2 \rangle = \chi > x^2$ . It is now possible to introduce two Lagrange Multipliers  $f_1$  and  $f_2$  and write the modified Hamiltonian as  $H_{\text{modified}} = H - f_1 X + f_2 X^2$ , where  $f_2 > 0$ .<sup>7</sup> By considering a certain range of values for  $f_2$ , the modified Hamiltonian will have a bound state, and the procedure used in the previous sections can be applied, with a slight modification that equation

<sup>7</sup>The sign in front of  $f_1$  and  $f_2$  are arbitrary. However, the unboundedness problem when only one Lagrange Multiplier is used leads to the conclusion that the term multiplying  $X^2$  must be a positive real number. It is of course also possible to write  $H_{\text{modified}} = H - f_1 X - f_2 X^2$ , where  $f_2 < 0$ .

(2.2) now takes the form

$$\langle H \rangle_{\min}(x, \chi) = E_g(x, \chi) + f_1(x, \chi)x - f_2(x, \chi)\chi. \quad (2.24)$$

In the expression above,  $E_g$  is the ground state energy of the modified Hamiltonian. Equation (2.24) is not the end of the story yet, as the original problem only involves one constraint, i.e.  $\langle X \rangle = x$ , and the second constraint is completely artificial. In order to find the correct effective potential, the minimum of equation (2.24) over all values of  $\chi$  must first be found, and the final expression for the effective potential will then take the form

$$V_{\text{eff}}(x) = \min_{\chi} \langle H \rangle_{\min}(x, \chi). \quad (2.25)$$

To understand how this method works, consider the following reasoning. Suppose that there are two particles in a one dimensional line. One of the particle is fixed in a certain position, and the other particle is allowed to move freely along that line. If one is asked to find the minimum interaction energy between the two particles (Suppose that the interaction energy depends only on the relative distance between the two particles), one obvious way is to measure the interaction energy between the two particles at some particular position of particle 2, and then compare it with that obtained when particle 2 is at another fixed position. In the end, all these values are compared, and the minimum over all is taken.

An example to illustrate the use of this method will be presented in the next section. In the remainder of this subsection, a drawback to this method will be elucidated. In most systems, an analytic expression for equation (2.24) is very difficult to obtain. As such, numerical method must be used to compute  $\langle H \rangle_{\min}(x, \chi)$  as an array of numbers representing the values of  $\langle H \rangle_{\min}$  given  $x$  and  $\chi$ . In that case, applying (2.25) will be very difficult, since it is impossible to construct an infinite array of numbers containing the values of  $\langle H \rangle_{\min}$  for all possible values of  $\chi$ . Nevertheless, this method has simplified the original minimization problem, as now the problem reduces to finding a number, rather than a function, that minimizes the Hamiltonian. There are of course some approximation methods to solve this kind of problems numerically, for example the simulated annealing method [11].

### 2.3.2 Method 2

The second method has the same basic idea as the first method, i.e. by introducing additional constraints. By writing  $\langle X \rangle = x$  in coordinate representation,

$$\int_{-\infty}^{\infty} dx' |\psi(x')|^2 x' = x,$$

$$\int_{-\infty}^0 dx' |\psi(x')|^2 x' + \int_0^{\infty} dx' |\psi(x')|^2 x' = x,$$

where  $\psi(x) = \langle x | \psi \rangle$  is the wavefunction in coordinate representation. By fixing  $\int_{-\infty}^0 dx' |\psi(x')|^2 x' = \langle X \eta(-X) \rangle = x_1$  and  $\int_0^{\infty} dx' |\psi(x')|^2 x' = \langle X \eta(X) \rangle = x_2$ , where  $\eta(x)$  is the Heaviside step function, the equation above reads

$$x_1 + x_2 = x. \quad (2.26)$$

By treating  $x_1$  and  $x_2$  as fixed values, two additional constraints are introduced into the system, which are related to the original constraint by equation (2.26). As before, two Lagrange Multipliers can then be introduced, and the modified Hamiltonian becomes

$$H_{\text{modified}} = H - f_1 X \eta(-X) + f_2 X \eta(X). \quad (2.27)$$

By choosing appropriate values for  $f_1$  and  $f_2$ , bound state for  $H_{\text{modified}}$  exists, and again the procedure used in the previous section follows. In this case, equation (2.2) also needs a slight modification to become

$$\langle H \rangle_{\min}(x_1, x_2) = E_g(x_1, x_2) + f_1(x_1, x_2)x_1 - f_2(x_1, x_2)x_2. \quad (2.28)$$

In order to get the correct effective potential, all possible values of  $x_1$  and  $x_2 = x - x_1$  must be considered, and the minimum over all is taken as the value of  $V_{\text{eff}}(x)$ .

As in the first method, the difficulty of applying this method is in minimizing equation (2.28)

over all  $x_1$  and  $x_2$ . For symmetric potential, however, we have developed a method to obtain the correct effective potential without having to consider all possible values of  $x_1$  and  $x_2$ . To understand this method, let's first refer to the figure below:

Figure 2.4: The potential part of the modified Hamiltonian for free particle motion

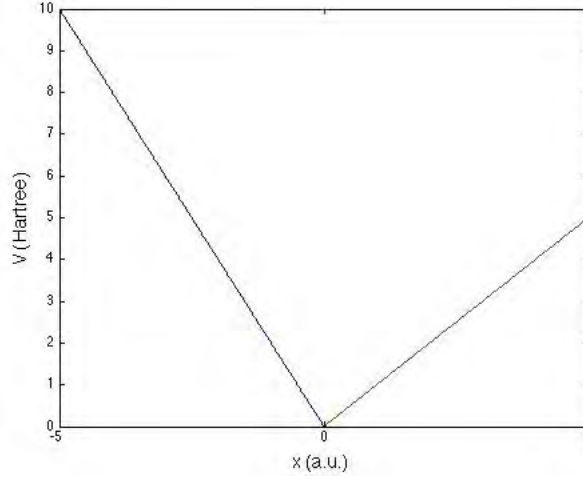


Figure (2.4) shows the plot of the potential part of equation (2.27) for the case of free particle motion. In that figure,  $f_1$  and  $f_2$  correspond to the left and right slopes respectively. Since the modified Hamiltonian is required to have a bound state, both  $f_1$  and  $f_2$  must be non-negative. By looking at the figure above, there are some useful facts, which are listed as follows:

1. As  $f_1$  get larger or  $f_2$  get smaller, the expectation value of the position operator  $X$  will be shifted to the right.
2. As  $f_2$  get larger or  $f_1$  get smaller, the expectation value of the position operator  $X$  will be shifted to the left.
3. If  $\langle X \rangle = x$  is fixed, and  $\langle H \rangle_{\min}(x_1, x_2)$  is minimized,  $E_g$  will have to be minimized<sup>8</sup>, and therefore the two slopes must be as small as possible.

While figure (2.4) only illustrates the case of free particle motion, the three facts above still hold for any symmetric potential. For various systems with symmetric potentials, there are two cases in which one can predetermine the relationship between  $f_1$  and  $f_2$  by using the three facts above.

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<sup>8</sup>One property of the Legendre transform is the reverse ordering property. Since equation (2.28) is in the form of the negative Legendre transform of  $\langle H \rangle_{\min}$ , it preserves the order, i.e.  $E_g(f_1, f_2) > 0$  implies  $\langle H \rangle_{\min}(x_1, x_2) > 0$  and vice versa. Therefore, the minimum of  $E_g(f_1, f_2)$  will also give the minimum of  $\langle H \rangle_{\min}(x_1, x_2)$ .

In the first case, the potential part of the Hamiltonian goes to  $\infty$  as  $x \rightarrow \infty$  faster than or at the same rate as  $k|x|$  for some positive constant  $k$ . This is the case where the method in the previous section works. The method introduced in this subsection can of course be used instead to solve such problems. In this case,  $f_1$  and  $f_2$  are allowed to take negative values as long as  $|f_1| > k$  and  $|f_2| > k$ . Suppose now that, without loss of generality,  $x > 0$  is fixed. According to fact 1 and 2 above,  $f_1 > f_2$ . Meanwhile, according to fact 3,  $f_1$  and  $f_2$  must be as small as possible. As such, as  $f_1$  and  $f_2$  keep decreasing, they will eventually reach the values in which  $f_1 = -f_2$ . Equation (2.27) then becomes  $H_{\text{modified}} = H - f_1 X$ , which leads to equation (2.2), i.e. reduces to the method used in the previous section.

Now, let's consider the case where the method used in the previous section fails, i.e. when the potential part of the Hamiltonian does not go to  $\infty$  as  $x \rightarrow \infty$  or it goes to infinity very slowly. In this case, both  $f_1$  and  $f_2$  must be non-negative in order for  $H_{\text{modified}}$  to have bound states. Following the previous reasoning, if  $x > 0$  is fixed,  $f_1$  and  $f_2$  will have to be as small as possible, while preserving  $f_1 > f_2$ . However, since  $f_2$  cannot be negative, the smallest possible value for  $f_2$  is 0. As such, equation (2.27) becomes  $H_{\text{modified}} = H - f_1 X \eta(-X)$ , where  $f_1 > 0$ . Since  $H_{\text{modified}}$  now only depends on unknown parameter  $f_1$ , it is easier to solve to get  $f_1(x_1, x_2)$ . Furthermore, since  $x_1$  and  $x_2$  have one-to-one correspondence to  $f_1$  and  $f_2$ , these  $x_1$  and  $x_2$  are values that correspond to the minimum of equation (2.28). Therefore, the next step is to find  $x_1(x)$  and  $x_2(x) = x - x_1(x)$ . After it is done, the effective potential  $V_{\text{eff}}(x)$  will be obtained. Some examples to illustrate this method are given in section (2.5) and (2.6).

## 2.4 Example 3: Free Motion System

Without the presence of any potential energy,  $V = 0$  and  $H = \frac{P^2}{2m}$ . With only one Lagrange Multiplier introduced, the modified Hamiltonian clearly does not have a bound state. By following the first method introduced in the previous section, let  $\langle X^2 \rangle = \chi$  be fixed. The modified Hamiltonian for this case is  $H_{\text{modified}} = \frac{P^2}{2m} - f_1 X + f_2 X^2$ , which is similar in form to the modified Hamiltonian for simple harmonic oscillator, cf. section (2.1). By following the procedure presented in section

(2.1),

$$\begin{aligned} H_{\text{modified}} &= \frac{P^2}{2m} + f_2 \left( X - \frac{f_1}{2f_2} \right)^2 - \frac{f_1^2}{4f_2}, \\ x &= \frac{f_1}{2f_2}, \\ E_g &= \hbar \sqrt{\frac{f_2}{2m}} - \frac{f_1^2}{4f_2}. \end{aligned}$$

$\chi$  as a function of  $f_1$  and  $f_2$  can be found by applying the Feynman-Hellmann theorem,

$$\begin{aligned} \chi(f_1, f_2) &= \frac{\partial E_g}{\partial f_2} \\ &= \frac{1}{2} \hbar \sqrt{\frac{1}{2mf_2}} + \frac{f_1^2}{4f_2^2}. \end{aligned}$$

By substituting  $f_1$  into the above equation,

$$\begin{aligned} \chi &= \frac{1}{2} \hbar \sqrt{\frac{1}{2mf_2}} + x^2, \\ f_2 &= \frac{\hbar^2}{8m(\chi - x^2)^2}, \\ f_1 &= 2x \frac{\hbar^2}{8m(\chi - x^2)^2}. \end{aligned}$$

By substituting these  $f_1(x, \chi)$ ,  $f_2(x, \chi)$ , and  $E_g(x, \chi)$  into equation (2.24),

$$\langle H \rangle_{\min}(x, \chi) = \frac{\hbar^2}{8m(\chi - x^2)}. \quad (2.29)$$

The remaining task is now to minimize equation (2.29) over all  $\chi$  while  $x$  is fixed. By looking at equation (2.29),  $\chi$  appears at the denominator, and therefore the whole expression will become smaller as  $\chi$  is set larger. In particular, by setting  $\chi \rightarrow \infty$ ,  $\langle H \rangle_{\min}(x, \chi) \rightarrow 0$ .<sup>9</sup> Therefore,  $V_{\text{eff}}(x) =$

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<sup>9</sup>In this particular case, the minimum of  $\langle H \rangle_{\min}(x, \chi)$  does not exist in the mathematical sense. Instead, it has an infimum. Therefore, it is reasonable to take the effective potential  $V_{\text{eff}}(x)$  as the infimum of  $\langle H \rangle_{\min}(x, \chi)$  over all  $\chi$ , which is 0 for all values of  $x$ .

0.

## 2.5 Example 4: Dirac Delta Potential

Consider a Dirac delta potential energy, where  $V(x) = -\alpha\delta(x)$ , where  $\alpha$  is a positive constant and  $\delta(x)$  is the Dirac delta function. Modified Hamiltonian with only one Lagrange Multiplier clearly does not have a bound state. The procedure introduced in the beginning of this chapter will not be applicable for this particular problem. In fact, this potential energy is symmetric by definition, and the second method introduced in section (2.3) can be applied.

Let  $\langle X\eta(-X) \rangle = x_1$  and  $\langle X\eta(X) \rangle = x_2$  be fixed, where  $x_1 + x_2 = x = \langle X \rangle$ . Equation (2.27) becomes

$$H_{\text{modified}} = \frac{P^2}{2m} - \alpha\delta(X) - f_1X\eta(-X) + f_2X\eta(X). \quad (2.30)$$

The case where  $x = 0$  is easy, since the effective potential is merely given by the ground state energy of the Dirac delta potential. The task is therefore to find the effective potential at  $x \neq 0$ . Without loss of generality, assume  $x < 0$ . The argument presented in section (2.3.2) shows that  $f_1 = 0$ , while  $f_2 > 0$ . The next step is then to find the ground state energy for  $H_{\text{modified}}$ , which can be done by solving the eigenvalue equation

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(y)}{dy^2} - \alpha\delta(y)\psi(y) + f_2y\eta(y)\psi(y) = E_g\psi(y),$$

where  $E_g < 0$ . In order to solve this equation, divide the region into two,  $y > 0$  and  $y < 0$ . For  $y < 0$ , the last term in the left hand side vanishes, and the normalizable solution to the differential equation is well-known, which is  $\psi(y < 0) = a \exp(ky)$ , where  $k = \frac{\sqrt{-2mE_g}}{\hbar}$  and  $a$  is a constant. For  $y > 0$ ,  $\eta(y) = 1$  in the last term, and the normalizable solution to this kind of differential equation has been obtained in section (2.2). By making some slight changes, the solution to the differential equation is  $\psi(y > 0) = b\text{Ai}(k_1y + c_1)$ , where  $k_1 = (\frac{2mf_2}{\hbar^2})^{\frac{1}{3}}$  and  $c_1 = -\frac{2mE_g}{k_1^2\hbar^2}$ .

For a Dirac delta potential, while the wave function is continuous everywhere, the derivative of the wave function has a discontinuity at  $y = 0$  by  $\Delta\psi'(0) = -\frac{2m\alpha}{\hbar^2}\psi(0)$  [9]. By imposing the wave

function to be continuous at  $y = 0$ ,

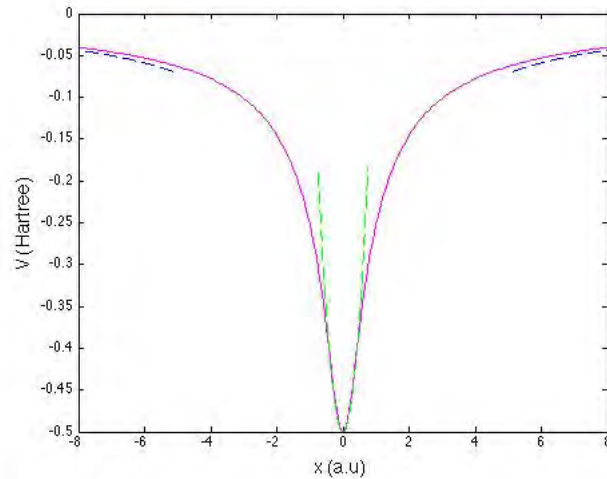
$$\begin{aligned}\lim_{y \rightarrow 0^+} \psi(y) &= \lim_{y \rightarrow 0^-} \psi(y), \\ b\text{Ai}(c_1) &= a, \\ \frac{a}{b} &= \text{Ai}(c_1).\end{aligned}\tag{2.31}$$

Furthermore, the discontinuity of the first derivative of the wave function at  $y = 0$  gives

$$\begin{aligned}\lim_{y \rightarrow 0^+} \psi'(y) - \lim_{y \rightarrow 0^-} \psi'(y) &= -\frac{2m\alpha}{\hbar^2} \psi(0), \\ bk_1\text{Ai}'(c_1) - ka &= -\frac{2m\alpha}{\hbar^2} a, \\ \frac{2m\alpha}{\hbar^2} - k &= -k_1\text{Ai}'(c_1) \frac{b}{a}, \\ \frac{2m\alpha}{\hbar^2} - k &= -k_1 \frac{\text{Ai}'(c_1)}{\text{Ai}(c_1)}.\end{aligned}\tag{2.32}$$

For a given  $f_2$ , equation (2.32) can be solved numerically for  $E_g$ . In order to get  $E_g(x)$ , a relationship between  $f_2$  and  $x$  must be found. In particular, this can be done by using the constraint equation  $\int_{-\infty}^{\infty} y|\psi(y)|^2 dy = x$ . A MATLAB code that solves this problem will be provided in the appendix A2. The effective potential corresponding to this system is shown in the following figure:

Figure 2.5: The effective potential of an attractive Dirac delta system



In the above, the purple line shows the numerical solution, whereas green and blue lines show



the asymptotic approximation for small and large  $|x|$  respectively. The small and large  $|x|$  approximation will be explained in the following subsections.

### 2.5.1 Small $|x|$ Approximation

As before, assume without loss of generality that  $x < 0$  so that  $f_1 = 0$ . If  $x \rightarrow 0$ ,  $f_2 \rightarrow 0$  and  $c_1$  in equation (2.32) will be very large. As such,  $\text{Ai}'(c_1)$  and  $\text{Ai}(c_1)$  can be approximated by [10]

$$\text{Ai}'(c_1) \approx -\frac{1}{2}\pi^{-\frac{1}{2}}c_1^{\frac{1}{4}}\exp\left(-\frac{2}{3}c_1^{\frac{3}{2}}\right)\left(1 - b_1\left(\frac{2}{3}c_1^{\frac{3}{2}}\right)^{-1} + b_2\left(\frac{2}{3}c_1^{\frac{3}{2}}\right)^{-2}\right), \quad (2.33)$$

$$\text{Ai}(c_1) \approx \frac{1}{2}\pi^{-\frac{1}{2}}c_1^{-\frac{1}{4}}\exp\left(-\frac{2}{3}c_1^{\frac{3}{2}}\right)\left(1 - a_1\left(\frac{2}{3}c_1^{\frac{3}{2}}\right)^{-1} + a_2\left(\frac{2}{3}c_1^{\frac{3}{2}}\right)^{-2}\right), \quad (2.34)$$

where  $a_k = \frac{\Gamma(3k+\frac{1}{2})}{54^k k! \Gamma(k+\frac{1}{2})}$  and  $b_k = -\frac{6k+1}{6k-1}a_k$ . By using this approximation, equation (2.32) can be simplified to:

$$\alpha = \frac{\hbar^2 k_1}{m} + \frac{3}{4k_1^2}f_2 - \frac{5m}{16\hbar^2 k_1^5}f_2^2. \quad (2.35)$$

Before proceeding any further, let's find a normalized wave function in the small  $|x|$  approximation. Before entering this subsection, the form of the wave function in the region  $y < 0$  and  $y > 0$  has been deduced, which is

$$\psi(y) = \begin{cases} a \exp(ky) & \text{for } y < 0 \\ b \text{Ai}(k_1 y + c_1) & \text{for } y > 0 \end{cases}. \quad (2.36)$$

The normalization constant  $a$  and  $b$  are connected by equation (2.31). Furthermore, normalized wave function requires that

$$\int_{-\infty}^{\infty} |\psi(y)|^2 dy = 1. \quad (2.37)$$

The left hand side of equation (2.37) consists of two terms, the first term is

$$\int_{-\infty}^0 a^2 \exp(2ky) dy = \frac{a^2}{2k}. \quad (2.38)$$

The second term involves the integration of  $\psi(y)$  from 0 to  $\infty$ ,

$$\begin{aligned}
\int_0^\infty b^2 \text{Ai}(k_1 y + c_1)^2 dy &= \frac{a^2}{\text{Ai}(c_1)^2} \int_0^\infty \text{Ai}(k_1 y + c_1)^2 dy \\
&= \frac{a^2}{\text{Ai}(c_1)^2} \left[ y \text{Ai}(k_1 y + c_1)^2 \Big|_0^\infty - 2 \int_0^\infty (k_1 y + c_1) \text{Ai}(k_1 y + c_1) \text{Ai}'(k_1 y + c_1) dy \right. \\
&\quad \left. + 2c_1 \int_0^\infty \text{Ai}(k_1 y + c_1) \text{Ai}'(k_1 y + c_1) dy \right] \\
&= \frac{a^2}{\text{Ai}(c_1)^2} \left[ y \text{Ai}(k_1 y + c_1)^2 \Big|_0^\infty - 2 \int_0^\infty \text{Ai}''(k_1 y + c_1) \text{Ai}'(k_1 y + c_1) dy \right. \\
&\quad \left. + 2c_1 \int_0^\infty \text{Ai}(k_1 y + c_1) \text{Ai}'(k_1 y + c_1) dy \right] \\
&= \frac{a^2}{\text{Ai}(c_1)^2} \left[ y \text{Ai}(k_1 y + c_1)^2 - \frac{1}{k_1} \text{Ai}'(k_1 y + c_1)^2 + \frac{c_1}{k_1} \text{Ai}(k_1 y + c_1)^2 \right]_0^\infty \\
&= a^2 \left[ \frac{1}{k_1} \left( \frac{\text{Ai}'(c_1)}{\text{Ai}(c_1)} \right)^2 - \frac{c_1}{k_1} \right] \\
&\approx a^2 \left[ \frac{c_1}{k_1} \left( 1 + \frac{1}{2} c_1^{-\frac{3}{2}} - \frac{1}{4} c_1^{-3} + \frac{25}{64} c_1^{-\frac{9}{2}} \right) - \frac{c_1}{k_1} \right] \\
&= \frac{a^2}{2k} - \frac{ma^2}{2\hbar^2 k^4} f_2 + \frac{25 m^2 a^2}{64 \hbar^4 k^6} f_2^2. \tag{2.39}
\end{aligned}$$

In the third line above,  $\text{Ai}''(y) = y \text{Ai}(y)$  is used. In the second last line above, small  $|x|$  approximation is used to approximate  $\left( \frac{\text{Ai}'(c_1)}{\text{Ai}(c_1)} \right)^2$ . By substituting these results into equation (2.37),

$$a^2 = \frac{k}{\left( 1 - \frac{mf_2}{2\hbar^2 k^3} + \frac{25m^2 f_2^2}{16\hbar^4 k^6} \right)}. \tag{2.40}$$

The relationship between  $f_2$  and  $x$  can now be determined by calculating the expectation value  $\langle X \rangle = x$  explicitly. Since  $x = x_1 + x_2$ , let's calculate  $x_1$  and  $x_2$  separately.  $x_1$  is easy to calculate,

$$\begin{aligned}
x_1 &= \int_{-\infty}^0 a^2 y \exp(2ky) dy \\
&= -\frac{a^2}{4k^2}. \tag{2.41}
\end{aligned}$$

In order to calculate  $x_2$ , which involves Airy function, integration by parts will be used repeatedly, along with the property of the Airy function  $\text{Ai}''(y) = y\text{Ai}(y)$ .

$$\begin{aligned}
x_2 &= b^2 \int_0^\infty x \text{Ai}(k_1 y + c_1)^2 dy \\
&= \frac{b^2}{k_1} \left[ \int_0^\infty (k_1 y + c_1) \text{Ai}(k_1 y + c_1)^2 dy - \int_0^\infty c_1 \text{Ai}(k_1 y + c_1)^2 dy \right] \\
&= \frac{b^2}{k_1} \left[ \int_0^\infty \text{Ai}(k_1 y + c_1) \text{Ai}''(k_1 y + c_1) dy - \int_0^\infty c_1 \text{Ai}(k_1 y + c_1)^2 dy \right].
\end{aligned}$$

The integral in the second term has been calculated previously, which leads to equation (2.39). The result is

$$-\int_0^\infty c_1 \text{Ai}(k_1 y + c_1)^2 dy = \frac{c_1^2}{k_1} \text{Ai}(c_1)^2 - \frac{c_1}{k_1} \text{Ai}'(c_1)^2. \quad (2.42)$$

The remaining task is therefore to solve the integral in the first term. Let's focus on calculating

$$\begin{aligned}
\int_0^\infty \text{Ai}''(k_1 y + c_1) \text{Ai}(k_1 y + c_1) dy &= -\frac{1}{k_1} \text{Ai}'(c_1) \text{Ai}(c_1) - \int_0^\infty \text{Ai}'(k_1 y + c_1)^2 dy \\
&= -\frac{1}{k_1} \text{Ai}'(c_1) \text{Ai}(c_1) - 0 + \int_0^\infty 2k_1 y \text{Ai}'(k_1 y + c_1) \text{Ai}''(k_1 y + c_1) dy \\
&= -\frac{1}{k_1} \text{Ai}'(c_1) \text{Ai}(c_1) + 2 \int_0^\infty (k_1 y + c_1) \text{Ai}'(k_1 y + c_1) \text{Ai}''(k_1 y + c_1) dy \\
&\quad - 2c \int_0^\infty \text{Ai}'(k_1 y + c_1) \text{Ai}''(k_1 y + c_1) dy \\
&= -\frac{1}{k_1} \text{Ai}'(c_1) \text{Ai}(c_1) - 2c \int_0^\infty \text{Ai}'(k_1 y + c_1) \text{Ai}''(k_1 y + c_1) dy \\
&\quad + 2 \int_0^\infty (\text{Ai}'''(k_1 y + c_1) - \text{Ai}(k_1 x + c_1)) \text{Ai}''(k_1 y + c_1) dy \\
&= -\frac{1}{k_1} \text{Ai}'(c_1) \text{Ai}(c_1) + \frac{c_1}{k_1} \text{Ai}'(c_1)^2 \\
&\quad - \frac{1}{k_1} \text{Ai}''(c_1)^2 + \frac{2}{k_1} \text{Ai}'(c_1) \text{Ai}(c_1) + 2 \int_0^\infty \text{Ai}'(k_1 y + c_1)^2 dy.
\end{aligned}$$

The last term in the last line has the same form as the last term in the first line. Since the first and the last line are equal,

$$\begin{aligned}
-\frac{1}{k_1} \text{Ai}'(c_1) \text{Ai}(c_1) - \int_0^\infty \text{Ai}'(k_1 y + c_1)^2 dy &= -\frac{1}{k_1} \text{Ai}'(c_1) \text{Ai}(c_1) + \frac{c_1}{k_1} \text{Ai}'(c_1)^2 \\
&\quad - \frac{1}{k_1} \text{Ai}''(c_1)^2 + \frac{2}{k_1} \text{Ai}'(c_1) \text{Ai}(c_1) + 2 \int_0^\infty \text{Ai}'(k_1 y + c_1)^2 dy, \\
\int_0^\infty \text{Ai}'(k_1 y + c_1)^2 dy &= -\frac{c_1}{3k_1} \text{Ai}'(c_1)^2 + \frac{c_1^2}{3k_1^2} \text{Ai}(c_1)^2 - \frac{2}{3k} \text{Ai}'(c_1) \text{Ai}(c_1). \quad (2.43)
\end{aligned}$$

By substituting this result back into the computation of  $\int_0^\infty \text{Ai}''(k_1 y + c_1) \text{Ai}(k_1 y + c_1) dy$ ,

$$\int_0^\infty \text{Ai}''(k_1 y + c_1) \text{Ai}(k_1 y + c_1) dy = -\frac{1}{3k_1} \text{Ai}'(c_1) \text{Ai}(c_1) + \frac{c_1}{3k_1} \text{Ai}'(c_1)^2 - \frac{c_1^2}{3k_1} \text{Ai}(c_1)^2. \quad (2.44)$$

Equation (2.44) can be combined with equation (2.42) to get the expression for  $x_2$ , along with the small  $|x|$  approximation for Airy function and the relationship  $b = \frac{a}{\text{Ai}(c_1)}$ ,

$$\begin{aligned}
x_2 &= \frac{a^2}{k_1^2} \left[ \frac{2}{3} c_1^2 - \frac{2c_1}{3} \left( \frac{\text{Ai}'(c_1)}{\text{Ai}(c_1)} \right)^2 - \frac{1}{3} \frac{\text{Ai}'(c_1)}{\text{Ai}(c_1)} \right] \\
&\approx \frac{a^2}{k_1^2} \left[ \frac{2}{3} c_1^2 - \frac{2}{3} c_1^2 \left( 1 + \frac{1}{2} c_1^{-\frac{3}{2}} - \frac{1}{4} c_1^{-3} + \frac{25}{64} c_1^{-\frac{9}{2}} \right) + \frac{c_1^{\frac{1}{2}}}{3} \left( 1 + \frac{1}{4} c_1^{-\frac{3}{2}} - \frac{5}{32} c_1^{-3} \right) \right] \\
&= \frac{a^2}{k^2} \left[ \frac{1}{4} - \frac{5}{16} c_1^{-\frac{3}{2}} + \frac{45}{64} c_1^{-3} \right] \\
&= \frac{a^2}{k^2} \left[ \frac{1}{4} - \frac{5}{8} \frac{m}{\hbar^2 k^3} f_2 + \frac{45m^2}{16\hbar^4 k^6} f_2^2 \right]. \quad (2.45)
\end{aligned}$$

Denote  $\frac{m}{\hbar^2 k^4} = q$ . By requiring that  $x_1 + x_2 = x$ , substituting equation (2.40) and expanding the result up to second order,

$$\begin{aligned}
-\frac{5q}{8} f_2 + \frac{45}{16} q^2 k f_2^2 &= x \left( 1 - \frac{q}{2} k f_2 + \frac{25}{16} q^2 k^2 f_2^2 \right), \\
\frac{45}{16} q^2 k \left( 1 - \frac{5}{9} kx \right) f_2^2 + \frac{5}{8} q \left( \frac{4}{5} kx - 1 \right) f_2 - x &= 0. \quad (2.46)
\end{aligned}$$

Equation (2.46) is a quadratic equation, and therefore  $f_2$  can be expressed in terms of  $x$  as

$$\begin{aligned} f_2 &= \frac{\frac{5}{8}q \left(1 - \frac{4}{5}kx\right) - \sqrt{\frac{1}{64}q^2 (25 + 680kx - 384k^2x^2)}}{\frac{45}{8}q^2k \left(1 - \frac{5}{9}kx\right)} \\ &\approx -\frac{8x}{5q} + \frac{256}{25} \frac{kx^2}{q}. \end{aligned} \quad (2.47)$$

In the above, only the negative solution in the quadratic equation is considered. The reason for this is because the positive solution contains a term that goes  $\propto \frac{1}{x}$ , which is not physical as  $x \rightarrow 0$ .

This result can be substituted back into equation (2.35), while keeping  $x$  up to second order,

$$\frac{\hbar^2 k}{m} - \frac{2\hbar^2 k^2 x}{5m} + \frac{44\hbar^2 k^3 x^2}{25m} - \alpha = 0. \quad (2.48)$$

This is a cubic equation in  $k$ . It is possible to obtain an approximate solution for  $k$  up to second order in  $x$  by writing  $k \approx k_0 + \epsilon$ , where  $\epsilon \propto x^2$  is a small quantity and  $k_0$  is a solution to equation (2.48) with  $k^3$  term is neglected. That is,

$$\begin{aligned} k_0 &= \frac{5}{4x} - \frac{1}{x} \sqrt{\left(\frac{5}{4}\right)^2 - \frac{5x\alpha m}{2\hbar^2}} \\ &\approx \frac{m\alpha}{\hbar^2} + \frac{m^2\alpha^2 x}{5\hbar^4} + \frac{8m^3\alpha^3 x^2}{25\hbar^6}. \end{aligned} \quad (2.49)$$

In terms of  $k_0$  and  $\epsilon$ , and by still maintaining  $x$  up to second order, equation (2.48) becomes

$$\begin{aligned} \frac{\hbar^2}{m}\epsilon + \frac{44}{25} \frac{\hbar^2 k_0^3 x^2}{m} &= 0, \\ \epsilon &= -\frac{44}{25} \left(\frac{m\alpha}{\hbar^2}\right)^3 x^2. \end{aligned} \quad (2.50)$$

This gives  $k = \frac{m\alpha}{\hbar^2} + \frac{2}{5} \left(\frac{m\alpha}{\hbar^2}\right)^2 - \frac{36}{25} \left(\frac{m\alpha}{\hbar^2}\right)^3 x^2 + \mathcal{O}[x^3]$ . As a result,

$$f_2 \approx -\frac{8}{5} \frac{m^3 \alpha^4}{\hbar^6} x + \frac{192}{25} \frac{m^4 \alpha^5}{\hbar^8} x^2, \quad (2.51)$$

$$x_2 \approx \frac{\hbar^2}{4m\alpha} + \frac{7x}{10} + \frac{21m\alpha x^2}{25\hbar^2}, \quad (2.52)$$

$$\begin{aligned} E_g &= -\frac{\hbar^2 k^2}{2m} \\ &\approx -\frac{m\alpha^2}{2\hbar^2} - \frac{2m^2\alpha^3}{5\hbar^4} x + \frac{34}{25} \frac{m^3\alpha^4}{\hbar^6} x^2. \end{aligned} \quad (2.53)$$

Now, all the ingredients are complete, and the effective potential can be approximated up to second order in  $x$  as

$$\begin{aligned} V_{\text{eff}}(x) &= E_g(x) - f_2(x)x_2(x) \\ &\approx -\frac{m\alpha^2}{2\hbar^2} + \frac{14}{25} \frac{m^3\alpha^4 x^2}{\hbar^6}. \end{aligned} \quad (2.54)$$

The first term of equation (2.54), which corresponds to  $x \rightarrow 0$ , is just the bound state energy of the Dirac delta potential. Furthermore, there is also no linear term, because the lowest order correction is quadratic. These facts show that the effective potential is a smooth continuous function in the approximation of small  $x$ , in contrast to the classical potential which is discontinuous at the origin.

Similar to the linear potential well case, this small  $|x|$  approximation of  $V_{\text{eff}}$  contains a quadratic term. The angular frequency associated with this quadratic term is  $\omega = \sqrt{\frac{28}{25} \frac{m\alpha^2}{\hbar^3}} \approx 1.05 \frac{m\alpha^2}{\hbar^3}$ . This is about two times the frequency corresponding to the minimum energy required to excite one particle in the ground state to the unbounded state. Since the Dirac delta potential only has one bound state, the interpretation of this result is not obvious. However, as in the linear potential well case, this may correspond to the frequency of the probability density when  $\langle H \rangle$  is small.

## 2.5.2 Large $|x|$ Approximation

Let's now consider the case when  $|x| \rightarrow \infty$ . In particular,  $f_2 \rightarrow \infty$ ,  $c_1 \rightarrow 0$ , and  $k \rightarrow 0$ .

Let  $a_1 = \text{Ai}(0) = \frac{1}{3^{\frac{2}{3}}\Gamma(\frac{2}{3})}$  and  $a_2 = -\text{Ai}'(0) = \frac{1}{3^{\frac{1}{3}}\Gamma(\frac{1}{3})}$ . Furthermore, let  $b = \frac{a_2}{a_1}$ .<sup>10</sup> Equation (2.32)

<sup>10</sup>This  $b$  is not to be confused with the normalization constant  $b$  of the wave function in equation (2.36).

can then be approximated as

$$\begin{aligned}
-k + \frac{2m\alpha}{\hbar^2} &\approx -\frac{k}{\sqrt{c_1}} \frac{\text{Ai}'(0)}{\text{Ai}(0) + \text{Ai}'(0)c_1} \\
&= \frac{kb}{\sqrt{c_1}} \frac{1}{1 - bc_1} \\
&\approx \frac{kb}{\sqrt{c_1}} (1 + bc_1).
\end{aligned} \tag{2.55}$$

The normalization constant  $a$  of the wave function in equation (2.36) can be found by again recalling equation (2.38) and (2.39), and then substituting them into equation (2.37),

$$\begin{aligned}
\frac{a^2}{k^2} \left( \frac{1}{2} + b^2 \sqrt{c_1} \right) &= 1, \\
a^2 &= \frac{k}{\frac{1}{2} + b^2 \sqrt{c_1}}.
\end{aligned} \tag{2.56}$$

In the large  $|x|$  approximation, the first line of equation (2.45) can be approximated by

$$\begin{aligned}
x_2 &\approx \frac{a^2}{3k_1^2} b \\
&= \frac{a^2}{3k^2} bc_1.
\end{aligned}$$

Furthermore, the requirement  $x_1 + x_2 = x$  gives

$$\begin{aligned}
\frac{a^2}{3k^2} bc_1 - \frac{a^2}{4k^2} &= x, \\
\frac{1}{3} bc_1 - kxb^2 \sqrt{c_1} - \left( \frac{1}{4} + \frac{1}{2} kx \right) &= 0,
\end{aligned} \tag{2.57}$$

where the value of  $a$  has been substituted and expanded up to second order in  $\sqrt{c_1}$ .

Let  $\sqrt{c_1} \approx c_0 + \epsilon$  where  $\epsilon$  is a small correction, and  $c_0 = -\frac{1}{2b^2} - \frac{1}{4kxb^2}$  is a solution to equation (2.57) with its first term is neglected. Since  $c_1 \rightarrow 0$ ,  $c_0 \rightarrow 0$  as well. In order for this to be true,  $k \approx -\frac{1}{2x} + \epsilon_2$  where  $\epsilon_2$  is another small quantity. In terms of  $\epsilon_2$ ,  $c_0 = \frac{x\epsilon_2}{b^2}$ . This can be plugged back into equation (2.57) to get  $\epsilon = -\frac{2x^2\epsilon_2^2}{3b^5}$ . Since  $\epsilon_2$  is a second order in  $\frac{1}{x}$ ,  $\epsilon$  is very small and can be ignored, leaving  $\sqrt{c_1} \approx c_0 = \frac{x\epsilon_2}{b^2}$ .

This result can be substituted back into equation (2.55), which yields

$$\frac{2m\alpha}{\hbar^2}\epsilon_2 - \frac{b^3}{2x^2} = 0. \quad (2.58)$$

Equation (2.58) can be easily solved to get  $\epsilon_2 \approx -\frac{b^3\hbar^2}{4m\alpha x^2}$ . This is sufficient to get all  $x_2$ ,  $f_2$ , and  $E_g$  via

$$\begin{aligned} k &\approx -\frac{1}{2x} - \frac{b^3\hbar^2}{4m\alpha x^2}, \\ \sqrt{c_1} &= \left(\frac{\hbar^2 k^3}{2mf_2}\right)^{\frac{1}{3}} \\ &\approx -\frac{b\hbar^2}{4m\alpha x}, \\ f_2 &\approx \frac{4m\alpha^3}{b^3\hbar^4}, \end{aligned} \quad (2.59)$$

$$x_2 \approx -\frac{b^3\hbar^4}{12m^2\alpha^2 x}, \quad (2.60)$$

$$\begin{aligned} E_g &= -\frac{\hbar^2 k^2}{2m} \\ &\approx -\frac{\hbar^2}{8m^2 x^2} \end{aligned} \quad (2.61)$$

The effective potential in large  $|x|$  approximation is therefore

$$V_{\text{eff}}(x) \approx -\frac{\alpha}{3|x|} - \frac{\hbar^2}{8m^2 x^2} \quad (2.62)$$

This effective potential will go to 0 as  $x$  go larger and larger, as it should.

## 2.6 Example 5: Finite Square Well Revisited

In the beginning of section 2.3, a finite square well potential is used to illustrate how the method introduced in the beginning of this chapter may fail.

Since a finite square well potential can be oriented to be an even function, the method used to find the effective potential of an attractive Dirac delta potential can also be applied for this case. Let's now consider the finite square well potential as described in the beginning of section (2.3). As



before, let  $x_1 = \langle X\eta(-X) \rangle$ ,  $x_2 = \langle X\eta(X) \rangle$ , and  $x_1 + x_2 = x = \langle X \rangle$  be fixed. The next step is to write equation (2.27) as

$$H_{\text{modified}} = \frac{P^2}{2m} + V_0 (\eta(X+a) - \eta(X-a)) - f_1 X\eta(-X) + f_2 X\eta(X). \quad (2.63)$$

For  $x = 0$ , the effective potential is just the ground state energy of the finite square well. Without loss of generality, suppose  $x < 0$ . As in the previous section,  $f_1$  can then be set to 0.

The next step is to solve the Schrödinger equation corresponding to this  $H_{\text{modified}}$ . In coordinate representation,

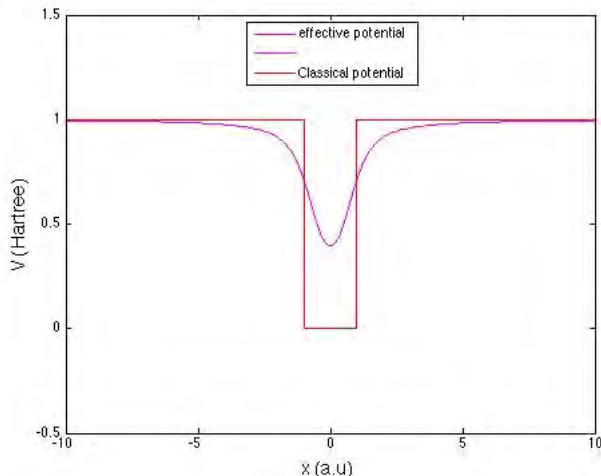
$$\left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial y^2} + V_0 (\eta(y+a) - \eta(y-a)) + f_2 y\eta(y) \right) \psi(y) = E_g \psi(y). \quad (2.64)$$

Equation (2.64) can be solved by first dividing the region into 4,  $y < -a$ ,  $-a < y < 0$ ,  $0 < y < a$ , and  $y > a$ . For each region, equation (2.64) is solved to get  $\psi(y)$ .  $\psi(y)$  and its derivative are then required to be continuous everywhere, which leads to 6 continuity conditions. These continuity conditions can be summarized in a  $6 \times 6$  matrix,

$$\det \begin{pmatrix} \text{Ai}(k_1 a_0 + c_1) & \text{Bi}(k_1 a_0 + c_1) & -\text{Ai}(k_1 a_0 + c_2) & 0 & 0 & 0 \\ k_1 \text{Ai}'(k_1 a_0 + c_1) & k_1 \text{Bi}'(k_1 a_0 + c_1) & -k_1 \text{Ai}'(k_1 a_0 + c_2) & 0 & 0 & 0 \\ \text{Ai}(c_1) & \text{Bi}(c_1) & 0 & -1 & 0 & 0 \\ k_1 \text{Ai}'(c_1) & k_1 \text{Bi}'(c_1) & 0 & 0 & -c & 0 \\ 0 & 0 & 0 & \cos(ca_0) & -\sin(ca_0) & \exp(-ka_0) \\ 0 & 0 & 0 & c \sin(ca_0) & c \cos(ca_0) & -k \exp(-ka_0) \end{pmatrix} = 0,$$

where  $k_1 = \left(\frac{2mf_2}{\hbar}\right)^{\frac{1}{3}}$ ,  $c_1 = -\frac{2mE_g}{k_1^2 \hbar^2}$ ,  $c_2 = \frac{2m(V_0 - E_g)}{k_1^2 \hbar^2}$ ,  $k = \frac{\sqrt{2m(V_0 - E_g)}}{\hbar}$ , and  $c = \frac{\sqrt{2mE_g}}{\hbar}$ . The first to the last rows correspond to the continuity of  $\psi(y)$  and its derivative at  $y = a$ ,  $y = 0$ , and  $y = -a$  respectively. If a value of  $f_2$  is given, the equation above can be solved for  $E_g$ , the ground state energy of the modified Hamiltonian  $H_{\text{modified}}$ . A numerical procedure of solving the effective potential for this case is similar to that for an attractive Dirac delta potential case. The effective potential obtained numerically is shown in the following figure

Figure 2.6: The effective potential of an attractive finite square well



In the figure above, the red curve shows the finite square well potential considered, while the magenta curve shows the corresponding effective potential. Since obtaining this effective potential involves solving the determinant of a  $6 \times 6$  matrix, it is difficult to obtain an analytical expression for the effective potential, even in the small and large  $|x|$  approximations. Figure 2.6 therefore does not show curves for small and large  $|x|$  approximations.

## 2.7 Remarks

Two more methods have been introduced to obtain the effective potential of a more general system where the method in the first section does not apply. In general, the two methods introduced can be used to find the effective potential of any one-dimensional system in an attractive potential. There are of course some remaining questions, for example

1. How to obtain the effective potential of a one-dimensional system in a repulsive potential?
2. How to obtain the effective potential of a system with more than one degree of freedom, i.e. more than one dimensional?

Quantum mechanically, under a repulsive potential energy, the energy spectrum is continuous. The Hamiltonian is however still bounded from below by the minimum of the potential. If an arbitrary wave function is given, it is possible to spread the wave function by making it wider while keeping the

expectation value  $\langle X \rangle$  fixed. This corresponds to lowering the expectation value of the Hamiltonian while keeping the expectation value of the position fixed. As a result, the expectation value of the Hamiltonian will reach the minimum of the potential, and this will be taken as the effective potential. Therefore, the effective potential will just be a constant everywhere and is given by the minimum of the potential.

For a system with more than one degree of freedom, there will be more than one position operator. By carrying forward the definition of the effective potential of a one-dimensional system, the effective potential of a three-dimensional system shall be defined as the minimum of  $\langle H \rangle$  when  $\langle \mathbf{r} \rangle$  is fixed. The effective potential of a system with more than one degree of freedom has not however been explored in a more detail in this project due to the time constraint and therefore will be left for future work.

# Chapter 3

## Trajectory Dynamics

In chapter 2, the effective potential for various systems has been obtained, either analytically or numerically. The remaining task to do is therefore to verify how good this semiclassical approximation, when compared to the quantum and classical case.

The cases of the simple harmonic oscillator and free particle motion are trivial. Meanwhile, there is no classical trajectory for a system in a Dirac delta potential. The best example to consider is therefore a linear potential well potential. In this chapter, the trajectories for the classical, semiclassical, and quantum case of linear potential well will be obtained and compared. The trajectories for the case of simple harmonic oscillator will also be used to verify the numerical implementation.

### 3.1 Classical and Semiclassical Trajectory

#### 3.1.1 Solving the Hamiltonian Equations of Motion

One way of obtaining the trajectory of a collection of particles for the classical and semiclassical cases is by solving the Hamilton equations of motion for a collection of point particles. Suppose there are  $N$  particles initially located at points  $\{(x_0(0), p_0(0)), (x_1(0), p_1(0)), \dots (x_{N-1}(0), p_{N-1}(0))\}$ . Under the influence of a certain potential energy  $V(\mathbf{x})$ , the Hamilton equations of motion for each particle can be written as (ignore any interaction force between the particles)

$$\dot{\eta} = \mathbf{J} \frac{\partial H}{\partial \eta}, \quad (3.1)$$

where  $H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x})$  and

$$\begin{aligned}\boldsymbol{\eta} &= \begin{pmatrix} \mathbf{q} \\ \mathbf{p} \end{pmatrix}, \\ \mathbf{J} &= \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \\ \frac{\partial H}{\partial \boldsymbol{\eta}} &= \begin{pmatrix} \frac{\partial H}{\partial \mathbf{q}} \\ \frac{\partial H}{\partial \mathbf{p}} \end{pmatrix}.\end{aligned}$$

equation (3.1) is exactly the same as equation (1.1) and (1.2), and is called the Hamilton equations of motion in symplectic notation [12]. The advantage of using the symplectic notation is its compact form if one intends to solve the Hamilton equations of motion for a system of  $N$  particles. Rather than solving  $N$  equations of type (1.1) and another  $N$  equations of type (1.2), it is sufficient to just solve one matrix equation (3.1).

Let's now set  $V(x) = |x|$ . In this case, the Hamiltonian  $H$  is separable, and equation (3.1) becomes a non-coupled ordinary differential equation. Numerically, an ordinary differential equation can be solved by using the fourth-order Runge-Kutta method [13]. Suppose an initial condition  $\boldsymbol{\eta}(0)$  is given,  $\boldsymbol{\eta}(t)$  can be obtained by first defining a very small time step  $\Delta t$ , and then finding  $\boldsymbol{\eta}(n\Delta t)$  recursively via

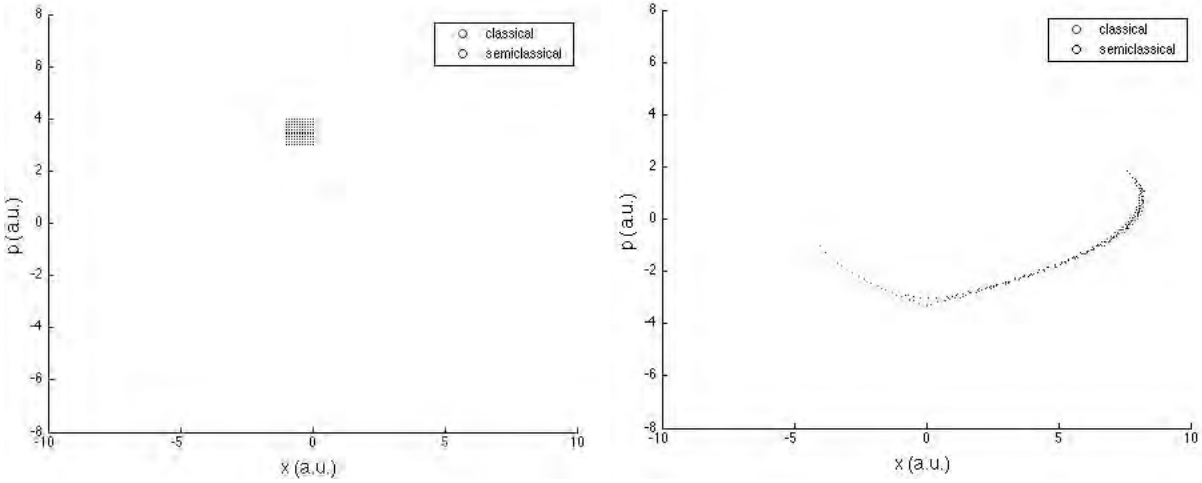
$$\boldsymbol{\eta}(n\Delta t) = \boldsymbol{\eta}((n-1)\Delta t) + \frac{\Delta t}{6} (\mathbf{f}_0 + 2\mathbf{f}_1 + 2\mathbf{f}_2 + \mathbf{f}_3), \quad (3.2)$$

where

$$\begin{aligned}\mathbf{f}_0 &= \dot{\boldsymbol{\eta}}((n-1)\Delta t, \boldsymbol{\eta}((n-1)\Delta t)), \\ \mathbf{f}_1 &= \dot{\boldsymbol{\eta}}\left(\left(n - \frac{1}{2}\right)\Delta t, \boldsymbol{\eta}((n-1)\Delta t) + \frac{\Delta t}{2}\mathbf{f}_0\right), \\ \mathbf{f}_2 &= \dot{\boldsymbol{\eta}}\left(\left(n - \frac{1}{2}\right)\Delta t, \boldsymbol{\eta}((n-1)\Delta t) + \frac{\Delta t}{2}\mathbf{f}_1\right), \\ \mathbf{f}_3 &= \dot{\boldsymbol{\eta}}(n\Delta t, \boldsymbol{\eta}((n-1)\Delta t) + \Delta t\mathbf{f}_2).\end{aligned}$$

By considering a number of points in phase space which are initially equally spaced and contained in a square  $-1 < x < 0$  and  $3 < p < 4$  (see figure 3.1 (left)), the distribution of these particles at a later time can be obtained (see figure 3.1 (right)),

Figure 3.1: The initial distribution of a collection of particles in a phase space



In the figure above, it is shown that initially the two distributions are in the shape of a square. Since the period of motion depends on the initial location in phase space, after about one and half cycle, the two distributions have deformed from their original shape. The classical and semiclassical distributions are quite similar in general. For the classical distribution, there is a cusp at  $x = 0$ , which corresponds to the discontinuity in the first derivative of  $p$  with respect to time.

### 3.1.2 Solving the Liouville Equation

Another way of obtaining a classical and semiclassical description of the time evolution of a continuous system of particles is by solving the Liouville equation, i.e. equation (1.8).

Unlike the Hamilton equations of motion, Liouville equation is a partial differential equation. One way to solve such equation numerically is by using the finite difference method [13]. The idea of this method is to discretize phase space and time into grids. Suppose that each point in position space, momentum space, and time are separated by a distance  $\Delta x$ ,  $\Delta p$ , and  $\Delta t$  respectively. Also suppose that position space, momentum space, and time cover  $(x_0, x_0 + n_i \Delta x)$ ,  $(p_0, p_0 + n_j \Delta p)$ , and

$(t_0, t_0 + n_k \Delta t)$  respectively. In this discretized space, The Liouville equation can be written as

$$\begin{aligned} \frac{\rho_{ijk+1} - \rho_{ijk-1}}{2\Delta t} &= V'(x_0 + i\Delta t) \frac{\rho_{ij+1k} - \rho_{ij-1k}}{2\Delta p} - \frac{p_0 + j\Delta p}{m} \frac{\rho_{i+1jk} - \rho_{i-1jk}}{2\Delta x}, \\ \rho_{ijk+1} &= \rho_{ijk-1} + 2\Delta t \left( V'(x_0 + i\Delta t) \frac{\rho_{ij+1k} - \rho_{ij-1k}}{2\Delta p} - \frac{p_0 + j\Delta p}{m} \frac{\rho_{i+1jk} - \rho_{i-1jk}}{2\Delta x} \right). \end{aligned} \quad (3.3)$$

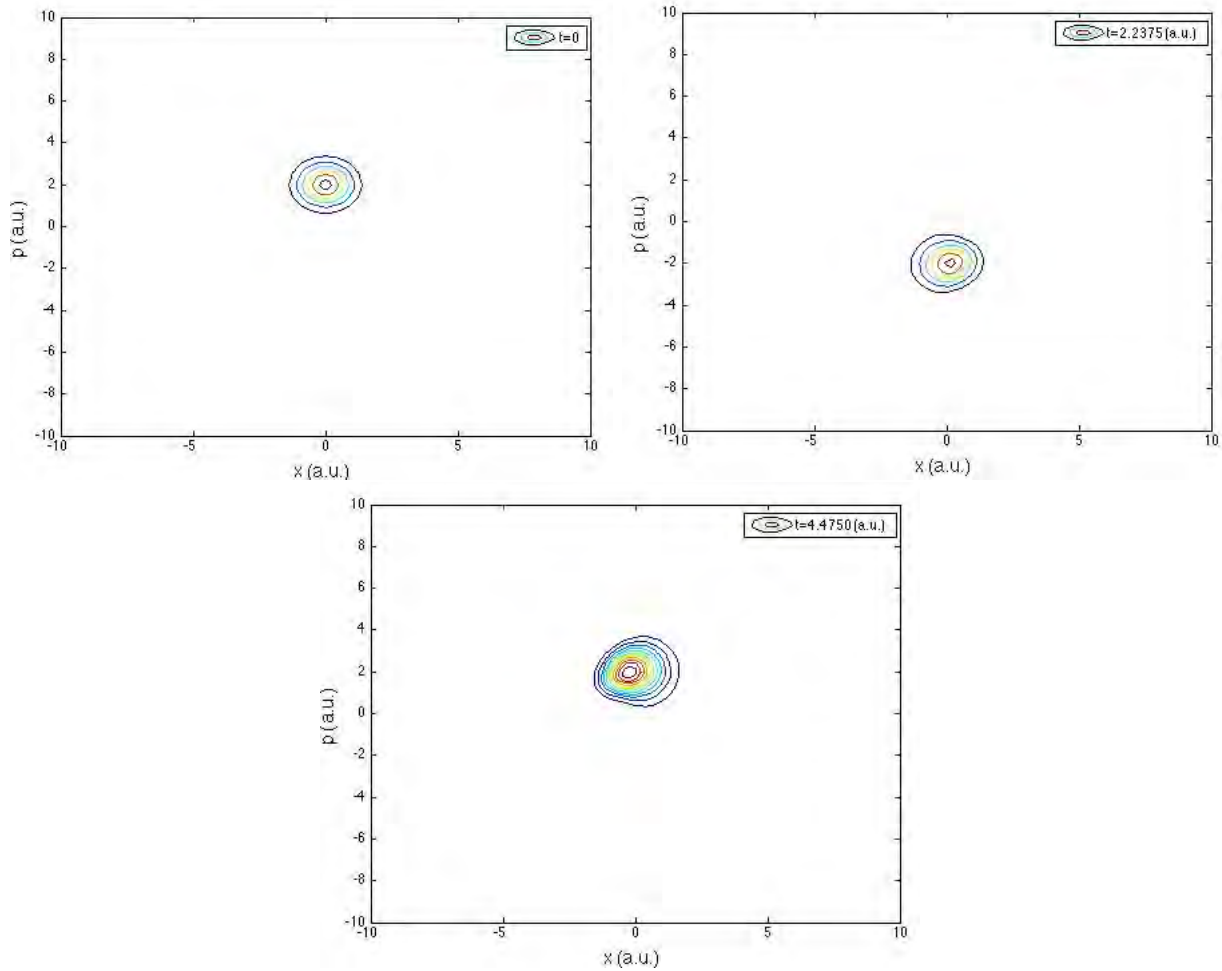
By using this method, the values of the density at time  $t + \Delta t$  can be determined from the density at time  $t$  and  $t - \Delta t$ . The density as a function of time in  $(t_0, t_0 + n_k \Delta t)$  can therefore be obtained and plotted.<sup>1</sup> The classical and semiclassical trajectories of a system in linear potential well for various initial conditions will be shown and discussed in section 3.3.

Before moving to the next section, it is instructive to verify that the numerical implementation of the method introduced above works as expected by applying it to the simple harmonic oscillator potential. The following figure shows the time evolution of the density of a system under a simple harmonic potential,

---

<sup>1</sup>Since there is no information about the values of the density at time  $t = t_0 - \Delta t$ , in order to find the density at time  $t = t_0 + \delta t$ , the time derivative in the Liouville equation is approximated by  $\frac{\rho_{ijk+1} - \rho_{ijk}}{\Delta t}$  instead when  $k = 0$ .

Figure 3.2: The time evolution of the density of a system in simple harmonic oscillator, calculated numerically using finite difference method.



In the case of simple harmonic oscillator, each point in phase space will be moving periodically with equal angular frequency  $\omega$ . Therefore, it is expected that the distribution should maintain its shape during the motion. It is verified in the above figure.

## 3.2 Quantum Trajectory

A quantum analogue to the classical Liouville equation is the Wigner-Moyal equation, i.e. equation (1.14). The Wigner-Moyal equation is also a partial differential equation, and therefore the procedure in the previous section can be used to solve it. There is actually one problem with the Wigner-Moyal equation, which makes it not so easy to solve. The first term in the right hand side of equation (1.14) contains high order partial differentiations. As such, turning each partial



differentiation into its discretized version will require a lot of effort. One way to overcome this problem is by writing the first term in the right hand side of equation (1.14) in terms of its Fourier transform. In that case, equation (1.14) becomes

$$\frac{\partial}{\partial t} \rho_w = \int_{-\infty}^{\infty} \frac{dy}{\sqrt{2\pi\hbar}} \frac{\tilde{\rho}_w(t, x, y) e^{\frac{ipy}{\hbar}}}{i\hbar} \left[ V\left(x - \frac{y}{2}\right) - V\left(x + \frac{y}{2}\right) \right] - \frac{\partial \rho_w}{\partial x} \frac{p}{m}, \quad (3.4)$$

where  $\tilde{\rho}_w(t, x, y) = \int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi\hbar}} \rho_w e^{-\frac{ipy}{\hbar}}$ , is the Fourier transform of  $\rho_w$ . In order to be able to apply the finite difference method on equation (3.4), the Fourier integral in equation (3.4) is approximated by using a discrete Fourier sum [13]. Instead of infinity, let the integration ranges from  $-v$  to  $v$ , where  $v$  is a certain large positive number. Before continuing the discussion, consider the following theorem,

**Theorem.** *Let  $n$  and  $m$  be integers.*

$$\sum_{l=0}^{N-1} e^{-\frac{2i\pi nl}{N}} e^{\frac{2i\pi ml}{N}} = \begin{cases} N & \text{for } n = m \\ 0 & \text{for } n \neq m \end{cases}$$

The proof of the theorem is straightforward and will be given in the appendix. Therefore, in order to realize a discrete Fourier transform from  $\rho_w(x, p, t)$  to  $\tilde{\rho}_w(x, y, t)$  which resembles a continuous Fourier transform, the momentum and  $y$  space will be discretized into  $N$  equally separated points, where the distance between two adjacent points in momentum space and  $y$  space are  $\Delta p$  and  $\Delta y = \frac{2\pi}{N}$  respectively. In this case, the relationship between  $\rho_w(x, p, t)$  and  $\tilde{\rho}_w(x, y, t)$  can be written as

$$\tilde{\rho}_w(x, -v + k\Delta y, t) = \sum_{l=0}^{N-1} \rho_w(x, -p_0 + l\Delta p, t) e^{-i(-v + \frac{2\pi k}{N})(-p_0 + l\Delta p)}, \quad (3.5)$$

$$\rho_w(x, -p_0 + l\Delta p, t) = \frac{1}{N} \sum_{k=0}^{N-1} \tilde{\rho}_w(x, -v + k\Delta y, t) e^{i(-v + \frac{2\pi k}{N})(-p_0 + l\Delta p)}. \quad (3.6)$$

It is easy to check that the two equations above are consistent by substituting equation (3.5) into

equation (3.6) and using the theorem above,

$$\begin{aligned}
\rho_w(x, -p_0 + l\Delta p, t) &= \frac{1}{N} \sum_{k=0}^{N-1} \sum_{l'=0}^{N-1} \rho_w(x, -p_0 + l'\Delta p, t) e^{i\frac{2\pi k(l-l')}{N}} e^{iv(l'-l)} \\
&= \frac{1}{N} \sum_{l'=0}^{N-1} \rho_w(x, -p_0 + l'\Delta p, t) e^{iv(l'-l)} N \delta_{ll'} \\
&= \rho_w(x, -p_0 + l\Delta p, t).
\end{aligned}$$

Having introduced a discrete Fourier transform, there is still another minor problem. If  $N$  is chosen to be very large, performing a discrete Fourier transform and its inverse may require a lot of computation, and therefore even a computer will take a long time to compute. Fortunately, there is a method which can be used to compute a discrete Fourier transform faster. This method is called the *fast Fourier transform* method [13]. To get the idea of the fast Fourier transform, consider the following discrete Fourier transform, where  $N$  is assumed to be even,

$$\begin{aligned}
g(j\Delta\omega) &= \sum_{i=0}^{N-1} f(i\Delta t) e^{-\frac{2i\pi ij}{N}} \\
&= \sum_{i=0}^{\frac{N}{2}-1} f(2i\Delta t) e^{-\frac{2i\pi(2i)j}{N}} + \sum_{i=0}^{\frac{N}{2}-1} f((2i+1)\Delta t) e^{-\frac{2i\pi(2i+1)j}{N}} \\
&= g_{\text{even}}(j\Delta\omega) + e^{-\frac{2i\pi j}{N}} g_{\text{odd}}(j\Delta\omega).
\end{aligned}$$

In the above equation  $g_{\text{even}}$  and  $g_{\text{odd}}$  are just discrete Fourier transforms which use even and odd points respectively. By using fast Fourier transform, the discrete Fourier transform is computed by using the result of the discrete Fourier transforms with  $\frac{N}{2}$  number of points via the above equation. In particular, if  $N$  is a multiple of 2, the discrete Fourier transform can be computed by performing successive fast Fourier transform methods. The original discrete Fourier transform method with  $N$  number of points requires  $N^2$  number of operation. By performing a fast Fourier transform, the number of operations is reduced to  $2 \times (\frac{N}{2})^2$ . If,  $N$  is a multiple of 2, performing successive fast Fourier transforms reduces the number of operation to the order of  $N \log_2 N$ .

Let's now apply the finite difference method on equation (3.4). As in the previous section, the first step is to discretize position space, momentum space,  $y$  space, and time into grids. Suppose

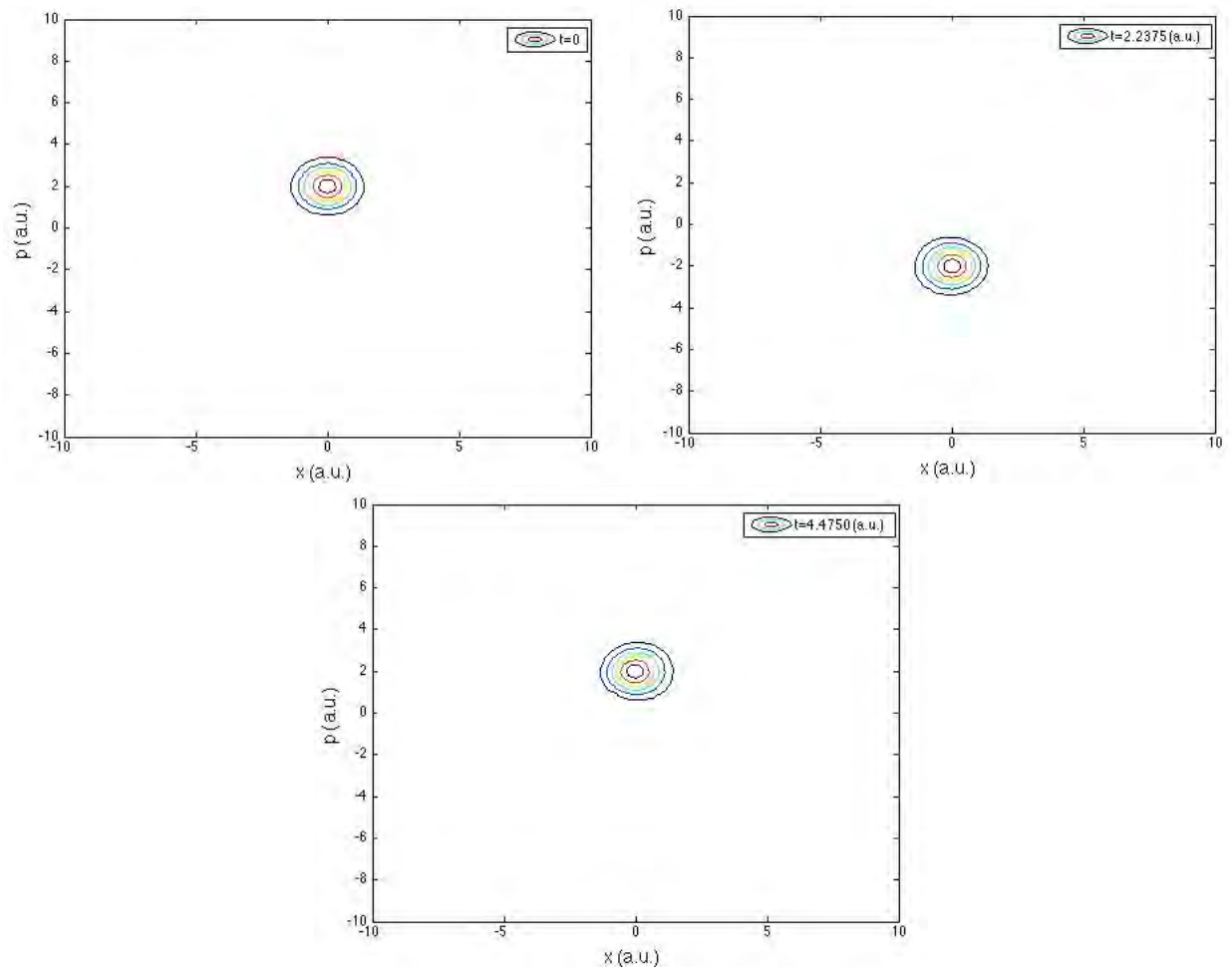
the position space, momentum space,  $y$  space, and time cover  $(-x_0, x_0)$ ,  $(-p_0, p_0)$ ,  $(-v, v)$ , and  $(0, t)$  respectively. In addition, suppose these regions are divided into  $N_x$ ,  $N_p$ ,  $N_y$ , and  $N_t$  equally spaced points respectively. Since momentum space and  $y$  space are related by a discrete Fourier transform, it is necessary to set  $N_p = N_y = N$ , and therefore  $v = \frac{\pi(N-1)^2}{2Np_0}$ . Furthermore, in order to be able to use successive fast Fourier transform method,  $N = 2^r$ , where  $r$  is a positive integer. In this discretized space, equation (3.4) becomes

$$\begin{aligned}
\frac{\rho_{w,ijk+1} - \rho_{w,ijk-1}}{2\Delta t} &= \frac{1}{N} \sum_{l=0}^{N-1} \frac{\tilde{\rho}_{w,ilk}}{i\hbar} e^{i(-v + \frac{2\pi l}{N})(-p_0 + k\Delta p)} \left[ V(-x_0 + i\Delta x - \frac{\hbar}{2}(-v + l\Delta y)) \right. \\
&\quad \left. - V(-x_0 + i\Delta x + \frac{\hbar}{2}(-v + l\Delta y)) \right] - \frac{p_0 + j\Delta p}{m} \frac{\rho_{w,i+1jk} - \rho_{w,i-1jk}}{2\Delta x}, \\
\rho_{w,ijk+1} &= \rho_{w,ijk-1} \\
&\quad + 2\Delta t \left\{ \frac{1}{N} \sum_{l=0}^{N-1} \frac{\tilde{\rho}_{w,ilk}}{i\hbar} e^{i(-v + \frac{2\pi l}{N})(-p_0 + k\Delta p)} \left[ V(-x_0 + i\Delta x - \frac{\hbar}{2}(-v + l\Delta y)) \right. \right. \\
&\quad \left. \left. - V(-x_0 + i\Delta x + \frac{\hbar}{2}(-v + l\Delta y)) \right] - \frac{p_0 + j\Delta p}{m} \frac{\rho_{w,i+1jk} - \rho_{w,i-1jk}}{2\Delta x} \right\}, \tag{3.7}
\end{aligned}$$

where  $\Delta t = \frac{t}{N_t-1}$ ,  $\Delta x = \frac{2x_0}{N_x}$ ,  $\Delta p = \frac{2p_0}{N}$ , and  $\Delta y = \frac{2v}{N}$ . As in the previous method, the Wigner function at time  $t + \Delta t$  can be determined from the Wigner function at time  $t$  and  $t - \Delta t$ .

The trajectory of the Wigner function for a system in a linear potential well is shown in the next section. In the rest of this section, the procedure above is applied to the simple harmonic oscillator case to verify that the numerical implementation of the procedure above is correct. As in the previous section, it is expected that the shape of the distribution is preserved during the motion. This is verified in the following figure,

Figure 3.3: The time evolution of the density of a system in simple harmonic oscillator, calculated numerically using finite difference method.



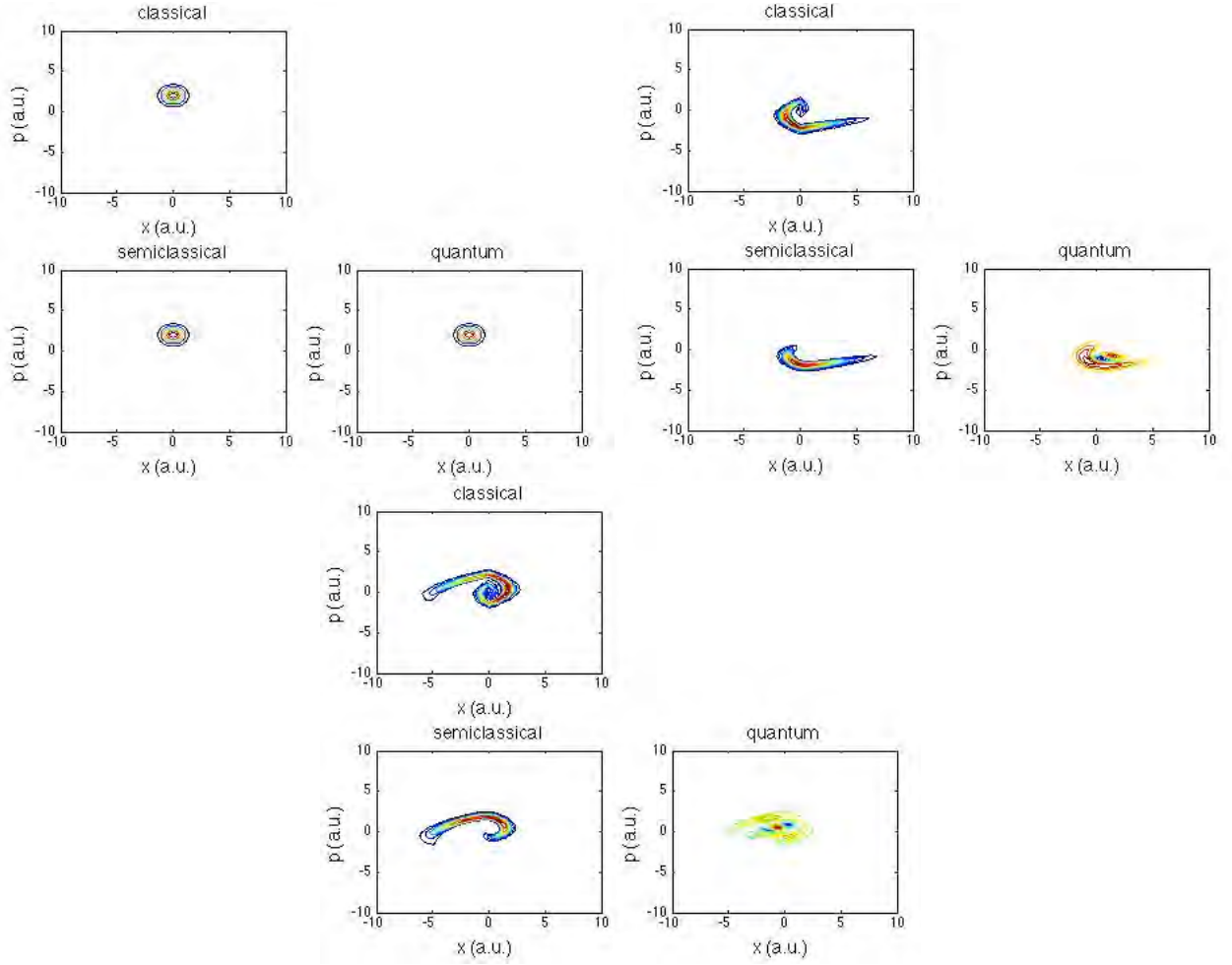
### 3.3 Comparison of Trajectories

Having obtained the density and Wigner function as a function of time, the classical, semiclassical, and quantum trajectory can be plotted. As an example, suppose the initial density is given by

$$\rho(x, p, 0) = \frac{1}{\pi} e^{-x^2 - (p-2)^2}. \quad (3.8)$$

By using the method introduced in the previous two sections, the classical and semiclassical density, as well as the Wigner function for a system in a linear potential well with  $V = |x|$  are plotted in the following figure,

Figure 3.4: The initial classical and semiclassical density, as well as the initial Wigner function (top left). The density and Wigner function after about half period ( $t = 5.0a.u.$ ) (top right) and after a period ( $t = 10a.u.$ ) (bottom)



In figure 3.4, while the classical and semiclassical density are always non-negative, the Wigner function shows a negative region at time  $t > 0$ , as indicated by the blue island. In order to check the similarity between the two densities and the Wigner function, the overlap between them will be measured. This can be done by first defining an inner-product in phase space,

$$\langle \rho_1(x, p, t), \rho_2(x, p, t) \rangle = \int dx dp \rho_1(x, p, t) \rho_2(x, p, t), \quad (3.9)$$

where the integration covers the whole phase space. Therefore, the similarity between the quantum and classical trajectory, classical and semiclassical trajectory, and quantum and semiclassical

trajectory respectively can be measured by

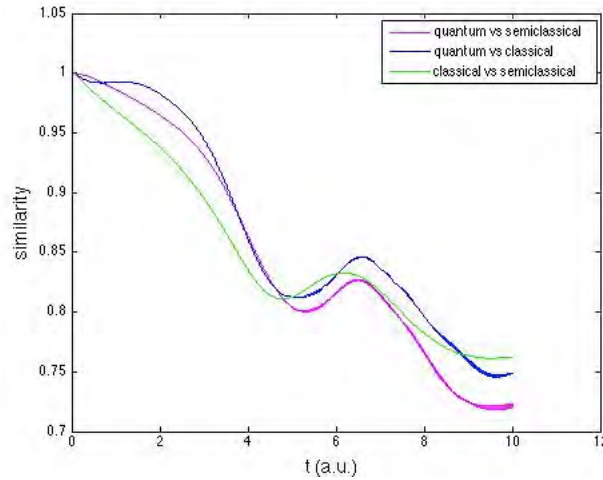
$$S_{q,c} = \frac{\langle \rho_w, \rho_c \rangle}{\sqrt{\langle \rho_w, \rho_w \rangle} \sqrt{\langle \rho_c, \rho_c \rangle}}, \quad (3.10)$$

$$S_{sc,c} = \frac{\langle \rho_{sc}, \rho_c \rangle}{\sqrt{\langle \rho_{sc}, \rho_{sc} \rangle} \sqrt{\langle \rho_c, \rho_c \rangle}}, \quad (3.11)$$

$$S_{q,sc} = \frac{\langle \rho_w, \rho_{sc} \rangle}{\sqrt{\langle \rho_w, \rho_w \rangle} \sqrt{\langle \rho_{sc}, \rho_{sc} \rangle}}. \quad (3.12)$$

As a function of time, these similarities are shown in the following figure,

Figure 3.5: The similarity between the quantum, classical, and semiclassical trajectory as a function of time



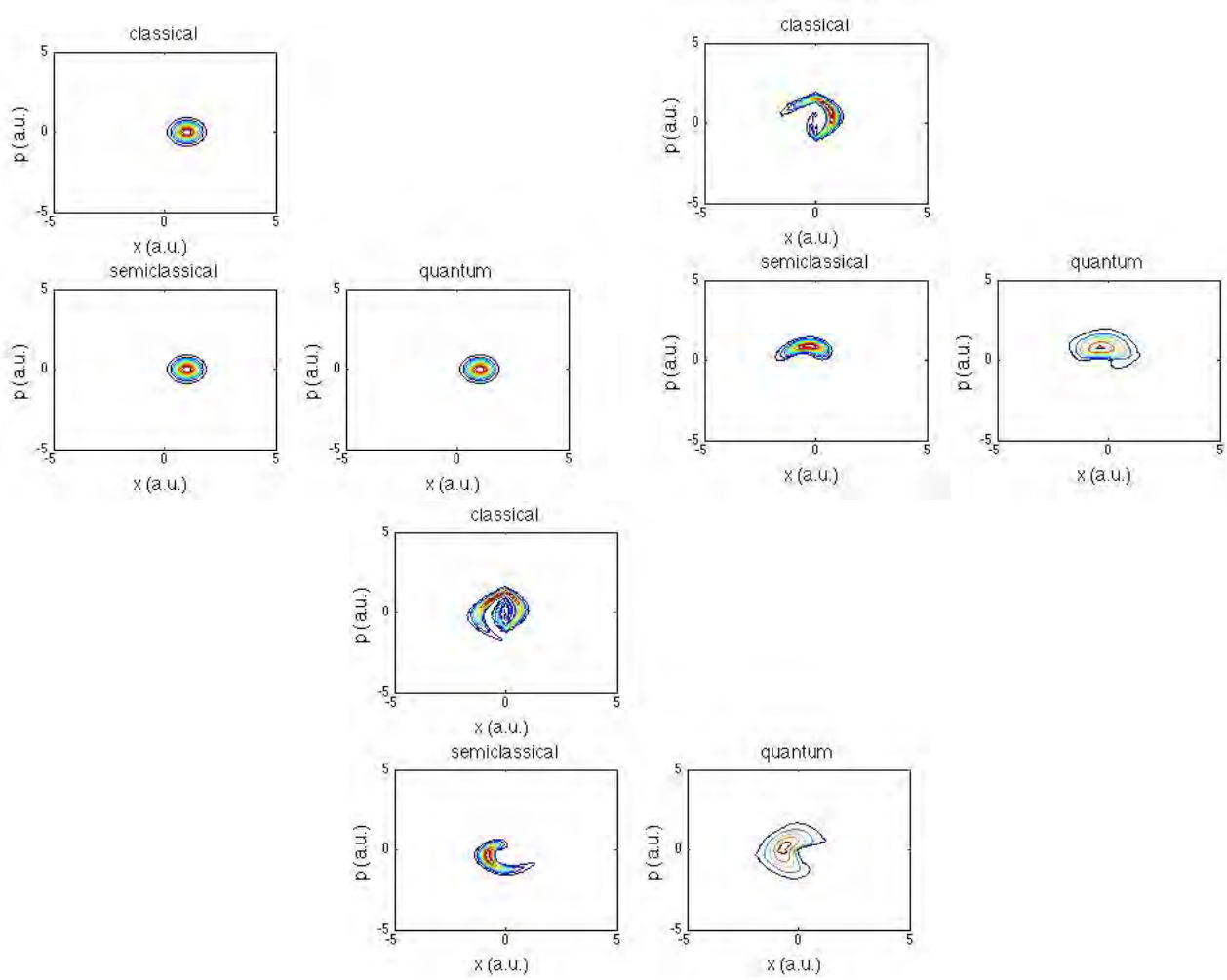
In the above figure, the semiclassical trajectory does not seem to be a very good approximation to both classical and quantum trajectory. One possible reason for this is that the distribution contains a range of energies from very low energies (comparable to the ground state energy) to very large energies (far larger than the ground state energy). In order to get a better understanding on how good this semiclassical approximation is, two cases are considered. In the first case, the distribution is chosen such that it covers a range of very low energies. In the second case, the distribution is chosen to cover a range of large energies.

For the first case, suppose the initial distribution is given by

$$\rho(x, p, 0) = \frac{1}{\pi} e^{-3((x-1)^2 + p^2)}. \quad (3.13)$$

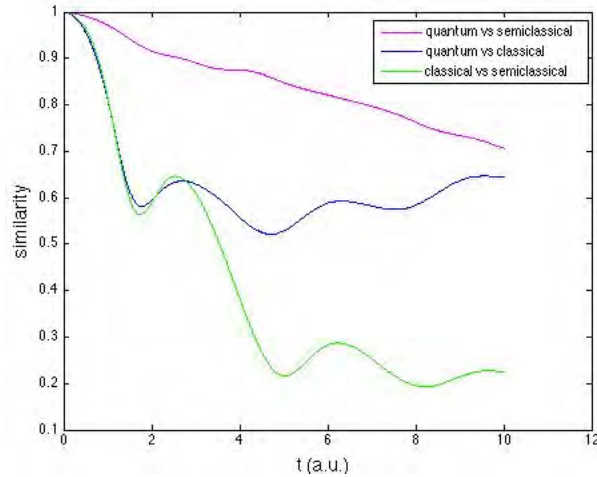
The time evolution of the density and the Wigner function for this case is shown in the following figure,

Figure 3.6: The initial classical and semiclassical density, as well as the initial Wigner function (left). The density and Wigner function after about  $\frac{3}{4}$  period ( $t = 5.0a.u.$ ) (right) and after one and a half period ( $t = 10a.u.$ ) (bottom)



As before, the similarity between the trajectories as a function of time can be computed and is shown in the figure below,

Figure 3.7: The similarity between the quantum, classical, and semiclassical trajectory as a function of time



In this second example, the semiclassical trajectory nicely resembles the quantum trajectory. The reason for this is that for low energies, the ground state and the first few excited states of the linear potential well will be dominant. In addition, for low energies, the effective potential will become very close to the ground state energy of the linear potential well. Therefore, it is not surprising that the two trajectories are very similar. On the other hand, since the ground state energy is different from the classical lowest allowed energy, it is also expected that the semiclassical and classical trajectory are not very similar.

For the second case, consider the initial distribution

$$\rho(x, p, 0) = \frac{1}{\pi} e^{-(x-5)^2 + p^2}. \quad (3.14)$$

The time evolution of the density and the Wigner function, as well as the similarity between them are shown in the two following figures,



Figure 3.8: The initial classical and semiclassical density, as well as the initial Wigner function (left). The density and Wigner function after about half period ( $t = 5.0a.u.$ ) (right) and after about  $\frac{3}{4}$  period ( $t = 10a.u.$ ) (bottom)

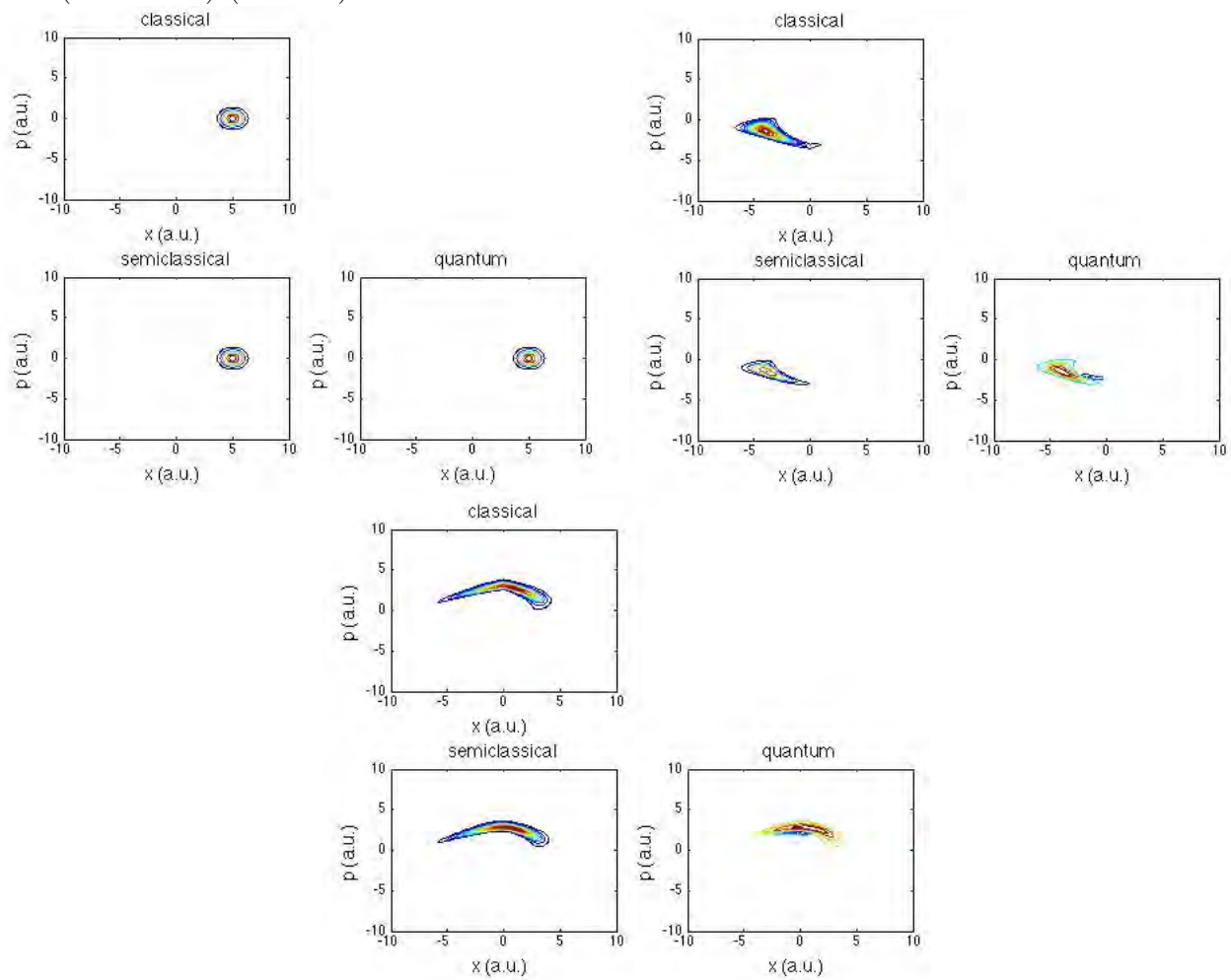
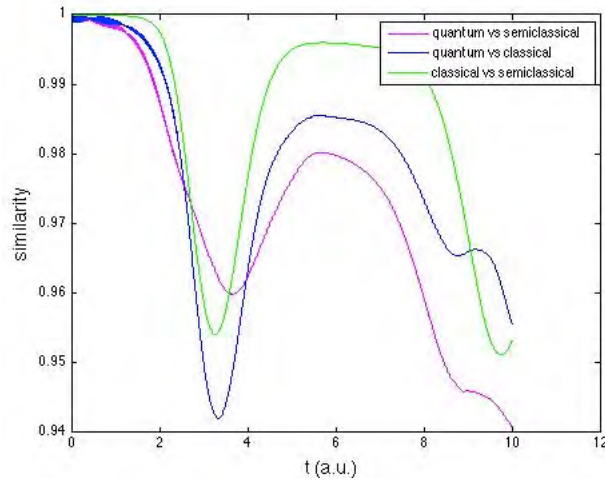


Figure 3.9: The similarity between the quantum, classical, and semiclassical trajectory as a function of time



In figure 3.9, all the densities are very similar, i.e. the similarities are all above 0.9. Furthermore, it is shown that the similarity between the classical and the semiclassical density are the highest. The similarity is at its best when  $x$  is very far from 0. The reason for this is that for  $x \gg 0$ , the effective potential  $V_{\text{eff}}$  is almost the same as the classical potential  $V(x)$ .

### 3.4 Summary and conclusion

The main purpose of this project is to find an effective force that approximates equation (1.6) and (1.7). In order to do this, the concept of the effective potential is introduced, which is defined as the minimum of the expectation value of the Hamiltonian  $\langle H \rangle$  when the expectation value of the position operator  $\langle X \rangle$  is fixed. In chapter 2, some methods have been developed to obtain the effective potential for various one-dimensional systems. The method is based on the use of Lagrange multipliers to include the constraints in the modified Hamiltonian. By limiting the values of the Lagrange Multipliers, the bound state of the modified Hamiltonian exists, and lemma 2 explains that the minimum of  $\langle H_{\text{modified}} \rangle$  is just its ground state energy.

In this chapter, the classical and semiclassical trajectory for a system in a linear potential well have been obtained by numerically solving the Liouville equation, where  $V(x) = |x|$  for the classical trajectory and  $V(x) = V_{\text{eff}}(x)$  for the semiclassical trajectory. By numerically solving the Wigner-Moyal equation, the quantum trajectory has been obtained as well. For various initial

distributions, the three trajectories are compared by calculating the overlap between the classical and semiclassical density, as well as the Wigner function. If the initial distribution covers a range of low energies, the semiclassical trajectory and the quantum trajectory are very similar. If the initial distribution covers a range of large energies, the semiclassical trajectory nicely approximates the classical trajectory.

# Appendix

## A1. Proof of Lemmas and Theorems

**Lemma 1.** *Let  $F$  and  $G$  be two operators. The Wigner transform of the product of the two operators is given by*

$$\begin{aligned}(FG)_w &= F_w \exp\left(\frac{i\hbar}{2}\Lambda\right)G_w \\ &= G_w \exp\left(-\frac{i\hbar}{2}\Lambda\right)F_w,\end{aligned}$$

where  $\Lambda = \overleftarrow{\frac{\partial}{\partial x}}\overrightarrow{\frac{\partial}{\partial p}} - \overleftarrow{\frac{\partial}{\partial p}}\overrightarrow{\frac{\partial}{\partial x}}$ . Left arrow means that the operator is acting on the left, while right arrow means that the operator is acting on the right.

*Proof.* Denote  $\tilde{F}_w = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dx dp F_w(x, p) \exp(-\frac{i}{\hbar}(xy + pq))$  and  $\tilde{G}_w = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dx dp G_w(x, p) \exp(-\frac{i}{\hbar}(xy + pq))$  as the Fourier transform of  $F_w$  and  $G_w$ . To start the proof, let's find the relationship between  $\langle x|A|x'\rangle$  and  $\tilde{A}_w$ . By using the Weyl transformation expression of  $A$ , i.e equation(1.5),

$$\begin{aligned}\langle x|A|x'\rangle &= \int \frac{dx'' dp}{2\pi\hbar} A_w(x'', p) \langle x|W(x'', p)|x'\rangle \\ &= \int \frac{dx'' dp dp'}{2\pi\hbar} A_w(x'', p) \langle x|p'\rangle \langle p'|W(x'', p)|x'\rangle \\ &= 2 \int \frac{dx'' dp dp'}{2\pi\hbar} A_w(x'', p) \exp\left(-\frac{2i(x-x'')(p'-p)}{\hbar}\right) \langle x|p'\rangle \langle p'|x'\rangle \\ &= 2 \int \frac{dx'' dp dp'}{(2\pi\hbar)^2} A_w(x'', p) \exp\left(-\frac{2i(x-x'')(p'-p)}{\hbar}\right) \exp\left(\frac{ip'(x-x')}{\hbar}\right) \\ &= 2 \int \frac{dx'' dp dp'}{(2\pi\hbar)^2} A_w(x'', p) \exp\left(-\frac{2i(\frac{1}{2}(x+x')-x'')p'}{\hbar}\right) \exp\left(\frac{2ip(x-x'')}{\hbar}\right)\end{aligned}$$

$$\begin{aligned}
&= \int \frac{dx'' dp}{\pi \hbar} A_w(x'', p) \delta(x'' - \frac{1}{2}(x + x')) \exp(\frac{2ip(x - x'')}{\hbar}) \\
&= \int \frac{dp}{2\pi \hbar} A_w(\frac{1}{2}(x + x'), p) \exp(\frac{ip(x - x')}{\hbar}) \\
&= \int \frac{dy}{2\pi \hbar} \tilde{A}_w(y, x' - x) \exp(\frac{iy(x + x')}{2\hbar}).
\end{aligned}$$

By using this result, let's now calculate  $(FG)_w$ :

$$\begin{aligned}
(FG)_w &= \int dx' \langle x - \frac{1}{2}x' | FG | x + \frac{1}{2}x' \rangle \exp(\frac{ipx'}{\hbar}) \\
&= \int dx' dx'' \langle x - \frac{1}{2}x' | F | x' \rangle \langle x' | G | x + \frac{1}{2}x' \rangle \exp(\frac{ipx'}{\hbar}) \\
&= \int \frac{dx' dx'' dy dy'}{(2\pi \hbar)^2} \tilde{F}_w(y, x'' - x + \frac{1}{2}x') \tilde{G}_w(y', x + \frac{1}{2}x' - x'') \exp(\frac{ipx'}{\hbar}) \exp(\frac{iy(x'' + x - \frac{1}{2}x')}{2\hbar}) \\
&\quad \exp(\frac{iy(x'' + x + \frac{1}{2}x')}{2\hbar}).
\end{aligned}$$

In the above, let  $\alpha = x'' - x + \frac{1}{2}x'$  and  $\beta = x - x'' + \frac{1}{2}x'$ . In particular,  $x' = \alpha + \beta$  and  $x'' = x + \frac{\alpha - \beta}{2}$ .

The above equation then becomes:

$$\begin{aligned}
(FG)_w &= \int \frac{d\alpha d\beta dy dy'}{(2\pi \hbar)^2} \tilde{F}_w(y, \alpha) \tilde{G}_w(y', \beta) \exp(\frac{ip(\alpha + \beta)}{\hbar}) \exp(\frac{i\beta y}{2\hbar}) \exp(\frac{ixy}{\hbar}) \\
&\quad \exp(\frac{i\alpha y'}{2\hbar}) \exp(\frac{ixy'}{\hbar}) \\
&= \int \frac{d\alpha d\beta dy dy'}{(2\pi \hbar)^2} (\exp(\frac{i(xy + \alpha p)}{\hbar}) \tilde{F}_w(y, \alpha)) \exp(-\frac{i(\beta y - \alpha y')}{2\hbar}) (\exp(\frac{i(xy' + p\beta)}{\hbar}) \tilde{G}_w(y', \beta)) \\
&= \int \frac{d\alpha d\beta dy dy'}{(2\pi \hbar)^2} (\exp(\frac{i(xy + \alpha p)}{\hbar}) \tilde{F}_w(y, \alpha)) \exp(\frac{i\hbar}{2} (\overleftarrow{\frac{\partial}{\partial x}} \overrightarrow{\frac{\partial}{\partial p}} - \overleftarrow{\frac{\partial}{\partial p}} \overrightarrow{\frac{\partial}{\partial x}})) \\
&\quad (\exp(\frac{i(xy' + p\beta)}{\hbar}) \tilde{G}_w(y', \beta)) \\
&= (\int \frac{dy d\alpha}{2\pi \hbar} \exp(\frac{i(xy + \alpha p)}{\hbar}) \tilde{F}_w(y, \alpha)) \exp(\frac{i\hbar}{2} \Lambda) (\int \frac{dy' d\beta}{2\pi \hbar} \exp(\frac{i(xy' + p\beta)}{\hbar}) \tilde{G}_w(y', \beta)) \\
&= F_w(x, p) \exp(\frac{i\hbar}{2} \Lambda) G_w(x, p),
\end{aligned}$$

which completes the proof. □

**Lemma 2.** *Let  $H$  be a Hamiltonian that has at least a bound state. If  $|\psi\rangle$  is any state and  $E_g$  is*

the ground state of  $H$ , then  $\langle \psi | H | \psi \rangle \geq E_g$ .

*Proof.* Let's consider the case where all the eigenvalues are discrete. The case when some are continuous is similar. Let  $\{|\psi_m\rangle\}$  be the set of all eigenstates of  $H$ . The Hamiltonian operator can be expanded in terms of its eigenstates as  $H = \sum_m E_m |\psi_m\rangle\langle\psi_m| \geq E_g \sum_m |\psi_m\rangle\langle\psi_m| = E_g$ . Where the inequality comes from the fact that  $E_m > E_g$  for  $E_m \neq E_g$   $\square$

**Feynman-Hellmann Theorem.** Let  $E$  be the energy eigenvalue to the Hamiltonian  $H$  with (normalized) eigenstate  $|\psi\rangle$ . Suppose  $H$  is a function of a parameter  $\lambda$ . It follows that  $\langle \psi | \frac{\partial H}{\partial \lambda} | \psi \rangle = \frac{\partial E}{\partial \lambda}$

*Proof.* The eigenvalue equation for  $H$  is given by  $H|\psi\rangle = E|\psi\rangle$ , where  $|\psi\rangle$  is the corresponding eigenvector. In particular:

$$\begin{aligned} E &= \langle H \rangle, \\ \frac{\partial E}{\partial \lambda} &= \frac{\partial}{\partial \lambda} \langle H \rangle \\ &= \left\langle \frac{\partial H}{\partial \lambda} \right\rangle + \frac{\partial \langle \psi |}{\partial \lambda} H | \psi \rangle + \langle \psi | H \frac{\partial | \psi \rangle}{\partial \lambda} \\ &= \left\langle \frac{\partial H}{\partial \lambda} \right\rangle + E \frac{\partial \langle \psi | \psi \rangle}{\partial \lambda} \\ &= \left\langle \frac{\partial H}{\partial \lambda} \right\rangle. \end{aligned}$$

The third line is obtained from the second line by using the fact that  $H|\psi\rangle = E|\psi\rangle$ , as well as  $\langle \psi | H = \langle \psi | E$ . Using the fact that  $\langle \psi | \psi \rangle = 1$ , the last line follows.  $\square$

**Theorem.** Let  $n$  and  $m$  be integers.

$$\sum_{l=0}^{N-1} e^{-\frac{2i\pi nl}{N}} e^{\frac{2i\pi ml}{N}} = \begin{cases} N & \text{for } n = m \\ 0 & \text{for } n \neq m \end{cases}$$

*Proof.* Recall the geometric series,

$$\sum_{l=0}^{N-1} x^l = \frac{1 - x^{l+1}}{1 - x}.$$

By setting  $x = e^{\frac{2i\pi k}{N}}$ , where  $k$  is an integer, it follows that the right hand side of the equation above is 0 unless  $k = 0$ . The case  $k = 0$  corresponds to  $x = 1$ , in which the sum is just  $N$ . The theorem then follows as a corollary of this result.  $\square$

## A2. MATLAB Codes

### Code 1. The effective potential for a linear potential well

```
function Lineareff()
% To plot the effective versus classical linear potential well in one graph.
% The plot ranges from -2 to 2

F=1; % Assign the slope to be one
f=-F+0.001:0.001:F-0.001;
e=0; % initialize the ground state energy e
for i=1:length(f)
    e(i)=- (F-f(i))^(2/3)*suppl(F,f(i))/2^(1/3);
end
de=diff(e)./diff(f); %numerical differentiation
Veff=0; % initialize the effective potential
x=-2:0.05:2;
for i=1:length(x)
    Veff(i)=task1(de,f,e,x(i));
end
V=F*abs(x);
plot(x,Veff,'m',x,V,'b')

function c=suppl( F,f )
% Find c that satisfies continuity conditions (method used: Bisection method).
c=0;
dc=-10^-2;
Tol=10^-8;
w=0;
```

```

while w==0
%define wavefunction at x=0 from the left and the right resp.
h1=airy(0,c*((F-f)/(F+f))^(2/3));
h2=airy(0,c);
%define derivative to wavefunction at x=0 from the left and the right resp.
g1=(f+F)^(1/3)*airy(1,c*((F-f)/(F+f))^(2/3));
g2=-(F-f)^(1/3)*airy(1,c);
    r=h1*g2-h2*g1; % define the continuity condition
if abs(r)<Tol
    w=1;
else
    e=0;
while e==0;
    c=c+dc;
    h11=airy(0,c*((F-f)/(F+f))^(2/3));
h21=airy(0,c);
g11=(f+F)^(1/3)*airy(1,c*((F-f)/(F+f))^(2/3));
g21=-(F-f)^(1/3)*airy(1,c);
    r1=h11*g21-h21*g11;
if real(r1)*real(r)<0
    c=c-dc;
    dc=dc/2;
else
    e=1;
end
end
end
end

function Veff=task1( de,f,e,x )
% To find the effective potential
Tol=10^-3;
q=0;
while q==0

```



```

for i=1:length(f)-1
    w=de(i)+x;
    if abs(w)<Tol
        r=i;
        q=1;
        break
    end
end
if q==0 && Tol<10^-1
    Tol=Tol*5;
elseif q==0 && Tol>=10^-1
    break
end
end
e1=e(r);
f1=f(r);
Veff=e1+f1*x;

```

**Code 2. The effective potential for an attractive dirac delta potential**

```

function deltaeff()
% To plot the effective potential for delta potential well. Plot ranges
% from -8 to 8.

x=-8:0.1:0;
for i=1:length(x)
    Veff(i)=task2(x(i));
end

plot(x,Veff,'b',-x,Veff,'b')

function Veff=task2(x)
% Find the effective potential for delta well with alpha=1 given <x>
Tol=10^-5;

```

```

q=0;
f1=0:0.1:10;
y1=f1-f1; % initiate the expectation value of x
y2=f1-f1; % initiate the energy eigenvalue
y11=f1-f1; % initiate the value of <x eta(x)>
for i=1:length(f1)
    [y1(i),y11(i)]=xpec(f1(i));
end
for i=1:length(f1)
    y2(i)=supp3(f1(i));
end
f=0:0.001:10;
y=pchip(f1,y1,f);
e=pchip(f1,y2,f);
x1=pchip(f1,y11,f);
r=0;
while q==0
    for i=1:length(y)
        w=x-y(i);
        if abs(w)<Tol
            r=i;
            q=1;
        end
    end
end
if r==0
    Tol=Tol*5;
end
if Tol>10^-1
    disp('error')
    return
end
end
Veff=e(r)-f(r)*x1(r);

```

```

function [ y,y1 ] = xpec( f1 )
% Calculate <x> (y) and <x eta(x)> (y1)

% set parameters
m=1;
hb=1;

[e, rat]=supp3(f1);
if f1~=0
k1=(2*m*f1/hb^2)^(1/3);
c1=-2*m*e/k1^2/hb^2;
k2=sqrt(-2*m*e)/hb;
p1=@(x) (airy(0,k1*x+c1)).^2;
p2=@(x) (1/rat*exp(k2*x)).^2;
y1=integral(p1,0,inf);
y2=integral(p2,-inf,0);
norm=1/sqrt(y1+y2);
p1=@(x) x.*(norm*airy(0,k1*x+c1)).^2;
p2=@(x) x.*(norm*1/rat*exp(k2*x)).^2;
y1=integral(p1,0,inf);
y2=integral(p2,-inf,0);
y=y1+y2;
else
k=sqrt(-2*m*e)/hb^2;
p1=@(x) (exp(-k*x)).^2;
p2=@(x) (1/rat*exp(k*x)).^2;
y1=integral(p1,0,inf);
y2=integral(p2,-inf,0);
norm=1/sqrt(y1+y2);
p1=@(x) x.*(norm*exp(-k*x)).^2;
p2=@(x) x.*(norm*1/rat*exp(k*x)).^2;
y1=integral(p1,0,inf);
y2=integral(p2,-inf,0);
y=y1+y2;

```

```

end

function [ e, rat ] = supp3(f1)
% Dirac delta potential V=- d(x), rat=coef[psi(r)/psi(l)]

%set parameters
hb=1;
m=1;
alpha=-1;

e=-1; %initial guess for the energy;
de=0.01; % initial increment
Tol=10^-5;
q=0; % For conditional purpose
if f1~=0
while q==0
    k1=(2*m*f1/hb^2)^(1/3);
    c1=-2*m*e/k1^2/hb^2;
    k2=sqrt(-2*m*e)/hb;
    w=(2*m*alpha/hb^2+k2)*airy(0,c1)-k1*airy(1,c1);
    if abs(w)<Tol
        q=1;
    else
        r=0;
        while r==0
            e=e+de;
            k1=(2*m*f1/hb^2)^(1/3);
            c1=-2*m*e/k1^2/hb^2;
            k2=sqrt(-2*m*e)/hb;
            w1=(2*m*alpha/hb^2+k2)*airy(0,c1)-k1*airy(1,c1);
            if w1*w<0
                e=e-de;
                de=de/2;
            else

```

```
        r=1;
    end
    end
end
rat=1/airy(0,c1);
end
else
e=-m*alpha^2/2/hb^2;
rat=1;
end
```

# Bibliography

- [1] Coleman, S. and Weinberg, E. *Radiative Corrections as the Origin of Spontaneous Symmetry Breaking*. Phys. Rev. D. **7**, 1888-1910, (1973)
- [2] Wigner, E. *On the Quantum Correction For Thermodynamic Equilibrium*. Phys. Rev. **40**, 749-459, (1932)
- [3] Weyl, H. *Quantenmechanik und Gruppentheorie*. Z. Phys. **46**, 1-46, (1927)
- [4] Groenewold, H.J. *On the Principles of Elementary Quantum Mechanics*. Physica. **12**, 405-460, (1946)
- [5] Īmre, K. et al. *Wigner Method in Quantum Statistical Mechanics*. J. Math. Phys. **8**, 1097-1108, (1967)
- [6] Curtright, T. L., and Zachos, C. K. *Quantum Mechanics in Phase Space*, arXiv:1104.5269v2 [physics.hist-ph]
- [7] Wyatt, R. E., and Corey J. T. *Quantum Dynamics with Trajectories: Introduction to Quantum Hydrodynamics*. New York: Springer, (2005)
- [8] Hudson, R.L. *When is the Wigner Quasi-probability Density Non-negative?*. Rep. Math. Phys. **6**, 249-252, (1974)
- [9] Griffiths, D. J. *Introduction to Quantum Mechanics*. Upper Saddle River, NJ: Pearson Prentice Hall, (2005)
- [10] Abramowitz, M., and Stegun, I. A. *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*. Washington: U.S. Govt. Print. Off, (1964)

- [11] Press, W. H., Teukolsky, S. A., Vetterling, W. T., and Flannery, B. P. *Numerical Recipes: The Art of Scientific Computing*. Cambridge: Cambridge UP, (2007)
- [12] Goldstein, H., Poole, C.P., Safko, J. L. *Classical Mechanics*. Addison-Wesley, (2002)
- [13] DeVries, P.L. *A first course in computational physics*. New York: Wiley, (1994)