

Semiclassical Fermion Densities

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2016

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A Thesis Submitted in Partial Fulfilment for the Degree of

Bachelor of Science (Honours) in Physics

ABSTRACT

We adapt the result for the semiclassical particle density of a non-interacting Fermi gas in a one-dimensional potential with two turning points in [Ribeiro *et al.*, PRL **114**, 050401 (2015)] to isotropic potentials in higher dimensions. We also propose another method for finding particle density via the quantum propagator, which is illustrated by two concrete examples in one dimension. The resultant densities in these examples are found to be the same as those given by the first method. The discussions pave the way for further refinements of semiclassical physics including Thomas-Fermi model (TF), and density functional theory (DFT).

ACKNOWLEDGEMENTS

I would like to thank *Prof.* Berthold-Georg Englert and *Dr.* Martin-Isbjörn Trappe for giving me an opportunity to work on this project and guiding me throughout the year. The discussions with them and the feedbacks I received from them have enhanced greatly my understanding of the field I am working on.

I thank my fellow honours student *Mr.* Hue Jun Hao for having collaborated with me on this project. More than once has he inspired in me ideas of how best to proceed in the project.

Finally, I want to thank an old friend *Mr.* Florent Gusdorf (literally old) for having always been a companion and a source of encouragement in both up and down moments.

CONTENTS

Abstract	2
Acknowledgements	2
I. Introduction	6
I.1. Introduction	6
I.2. Conventions and notations	8
II. Discussion of the result by Ribeiro <i>et al.</i>	9
II.1. Introduction	9
II.2. Langer wave function	9
II.3. Semiclassical particle density of a non-interacting quantum gas of fermions in one dimension	16
II.4. Leading contribution to the particle density	17
II.5. Normalization of the Langer wave function	20
III. Extension of the result by Ribeiro <i>et al.</i> to isotropic potentials in higher dimensions	22
III.1. Introduction	22
III.2. Isotropic potentials in three dimensions	23
III.2.1. Langer wave function for the radial motion and the corresponding radial particle density	23
III.2.2. TF density in three dimensions	26
III.2.3. Three-dimensional harmonic oscillator potential	26
III.2.4. Three-dimensional Coulomb potential	30
III.3. Isotropic potentials in two dimensions	34
III.3.1. Semiclassical wave function for the radial motion	34
III.3.2. Radial particle density	38
III.3.3. TF density in two dimensions	43
III.3.4. Two-dimensional harmonic oscillator potential	44
III.3.5. Two-dimensional Coulomb potential	47

IV. A new approach to finding a semiclassical particle density	51
IV.1. Introduction	51
IV.2. Particle density	51
IV.3. Quantum propagator: van Vleck-Gutzwiller formula	53
IV.4. Short-time approximation	56
IV.5. Symmetric linear potential	57
IV.5.1. Stationary states	57
IV.5.2. Exact particle density	60
IV.5.3. Particle density given by the propagator method	60
IV.5.4. Particle density given by Ribeiro <i>et al.</i> 's method	62
IV.6. One-dimensional harmonic oscillator potential	63
IV.6.1. Classically forbidden region	65
IV.6.2. Classically allowed region	67
IV.6.3. Particle density	69
Conclusions and future works	71
IV.7. Conclusions	71
IV.8. Future works	72
Appendices	74
1. F_m functions (see [1])	74
a. Expressions of F_m for some definite values of m	74
b. Recurrence formulas	74
c. Asymptotic behavior of F_m	75
2. Poisson summation formula	76
3. Airy uniform approximation to the one-dimensional time-independent Schrödinger equation	77
4. Rederivation of equations (10) and (12) in Ribeiro <i>et al.</i> 's paper	79
a. Equation (10)	79
b. Equation (12)	81
5. Energy eigenvalues of the harmonic oscillator and Coulomb potentials in three dimensions given by the JWKB quantization rule	83
a. Three-dimensional harmonic oscillator	84

b. Three-dimensional Coulomb potential	86
6. Semiclassical propagator for a symmetric linear potential in one dimension	89
7. Semiclassical propagator for a harmonic oscillator potential in one dimension	91
List of Figures	93
List of Tables	94
References	96

I. INTRODUCTION

I.1. Introduction

Dirac once commented [2], “The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation.” The comment reflects a seemingly common situation in all sorts of physical theories. From the observation of a handful of physical phenomena, scientists try to describe nature in terms of some simple (or elegant) principles that can be applied to explain other phenomena (we are talking about the power of prediction of a physical theory). However, no matter how hard we try, there is still some gap between ideal and reality. Exact solutions to most physical systems are just unachievable. The classical chaos, the Navier-Stokes equations, the Einstein equations, and the Schrödinger equation are some examples. One simply has to resort to approximations, perturbation methods, and the like.

In quantum mechanics, the widely used approximations are the JWKB method, and the TF model [1, 3–5]. The former is along the line of solving the Schrödinger equation approximately in the semiclassical regime (where \hbar is smaller than the classical action). The latter can be derived from the statistical method and is seemingly independent of the Schrödinger equation. Soon after its birth, the TF model was applied extensively to complex atomic systems and predicted the binding energy of neutral atoms, with a precision of about 10 percent [1]. Being largely classical, the model needs to be further refined in order to give rise to better approximations. It eventually led to DFT, which was put on a firm theoretical footing by the Hohenberg-Kohn theorem [6]. DFT now is a powerful tool for predicting the electronic properties of atomic structures in condensed matter physics and chemical physics (see the review papers [7–9]).

Among the observables that are of interest in any consideration of complex systems, one of the most important is the particle density. It is also the main variable in DFT, which states that the total energy of a system is a functional of the particle density, and the ground

state particle density is the one that minimizes this density functional. In the present work, we look at the ground state particle density in a limited context of non-interacting fermions, which are subject to the same external potential. Interacting fermions, however, can be considered to move in a common effective potential, and the problem can be reduced to the non-interacting case. Of the attempts at modifying the TF particle density, which does not reflect quantum effects, a notable result for one-dimensional potentials with two turning points is reported by Ribeiro *et al.* [10]. The authors use the Langer wave function [11, 12] as an approximation to the single-particle wave function and derive from it the semiclassical ground state particle density. This semiclassical particle density is found to have a closed form expression and gives an accurate approximation to the exact density. One motivation of this project is to generalize this result to higher dimensions, starting with the isotropic case.

Another line of attack is through the Feynman path integral formalism of quantum mechanics. We propose a method for obtaining particle density via the quantum propagator. There has been a great deal of research in this field such as on the semiclassical quantum propagator, and the trace formula [5, 13]. However, they do not consider the particle density and its leading contribution specifically. Potentially, the new method can be generalized to higher dimensions, in which the propagator is well defined.

The outline of the present report is as follows. Section II is devoted to the discussion of the result by Ribeiro *et al.*, including the Langer wave function and the expression for the semiclassical ground state particle density. Section III is an extension of this semiclassical particle density to isotropic potentials in higher dimensions, where we first consider the Langer wave function (or semiclassical wave function) for the radial motion and the corresponding radial particle density. We then use the examples of the harmonic oscillator and Coulomb potentials in two and three dimensions to demonstrate the obtaining of the particle density for fully filled shells. Finally, in section IV, we derive a formula for particle density in terms of the quantum propagator. We also discuss the van Vleck-Gutzwiller semiclassical propagator formula as well as the short-time approximation in choosing classical trajectories. We illustrate the new method with two concrete examples in one dimension. Various physical insights have been deduced from these examples to prepare for the treatment of the general case.

Some theoretical works in this paper were done in collaboration with Hue Jun Hao.

Collaboration shows in the discussions on the Langer wave function in one dimension, the leading contribution to the semiclassical density by Ribeiro *et al.*, and the short-time approximation.

I.2. Conventions and notations

In this report, we use extensively the family of functions $F_m(z)$ employed, for example by Englert in [1]. This class of functions, related to the Airy function and its derivative, is defined as

$$F_0(z) = [\text{Ai}(z)]^2 \quad (1)$$

and

$$F_m(z) = \left(-\frac{d}{dz}\right)^{-m} F_0(z), \text{ for integer } m, \quad (2)$$

where $(d/dz)^{-1}$ signifies

$$\left(\frac{d}{dz}\right)^{-1} f(z) = -\int_z^\infty dz' f(z') \quad (3)$$

Appendix 1 summarizes some recurrence and asymptotic properties of the functions F_m as well as the expressions of the functions for some values of m that are useful in this work.

Throughout the report, the derivatives w.r.t time of certain quantities may be found denoted by overdots, and those w.r.t position by primes.

We also assume that all fermions are spin-polarized. In other words, they have the same spin and we neglect the spin multiplicity of 2 for each orbital.

There are several technical calculations in the appendices that the reader can skip in the first reading.

It is also worth clarifying the units used in various numerical calculations in the present report. Throughout, we work in the units where the mass of the particle m , the reduced Planck constant \hbar , and the charge of the particle e are equal to one. For the example of the Morse potential, $V(x) = D(e^{-2\beta x} - 2e^{-\beta x})$, in section II, we choose $D = 15$ and $\beta = \frac{1}{4}$. For the harmonic oscillator in all dimensions in sections III and IV, we choose $\omega = 1$. Finally, for the symmetrical linear potential in section IV, we choose $f = 1$.

II. DISCUSSION OF THE RESULT BY RIBEIRO *ET AL.*

II.1. Introduction

In this section, the semiclassical particle density for non-interacting fermions in a one-dimensional potential with two turning points by Ribeiro *et al.* [10] will be presented. An analysis of the authors' arguments starts with a discussion on the Langer wave function (19), continuous in the entire domain, as an approximation to the single-particle wave function. The authors derive from this semiclassical wave function a closed form formula for the particle density (25), which is a correction to the TF density. We discuss some features of this formula including its dominant term (27) and illustrate it by a one-dimensional Morse potential, as done in [10].

II.2. Langer wave function

The one-dimensional time-independent *Schrödinger equation* for one particle with mass m can be written as

$$\frac{d^2}{dx^2}\psi(x) + \frac{p^2(x)}{\hbar^2}\psi(x) = 0, \quad (4)$$

where $\psi(x)$ is the wave function and the classical momentum $p(x)$ is given by

$$p^2(x) = 2m(E - V(x)),$$

where E is the energy eigenvalue, and $V(x)$ is the one-dimensional potential energy.

There are only a limited number of problems that have exact solutions. There have been, therefore, various schemes for finding approximate solutions to the Schrödinger equation, notably in the semiclassical regime, where the *reduced Planck constant* \hbar is small compared to the classical action.

One such scheme is well known under the name *JWKB method*, after Jeffreys [14], Wentzel [15], Kramers [16], and Brillouin [17]. Concise rederivation can be consulted in many texts (see for example [5, 18]). In this method, the wave function is expressed as the product of an amplitude and a phase factor, which can be expanded in orders of \hbar . The method yields an approximation to the wave function to first order, valid on both sides of a *turning point* (one of the zeros of the classical momentum). A connection between these two solutions is obtained by comparing them with the asymptotic solution by the local analysis of the

Schrödinger equation at the turning point. One remarkable result is the quantization rule for the bound state energy eigenvalues of a potential well, obtained by requiring the wave function to be single-valued.

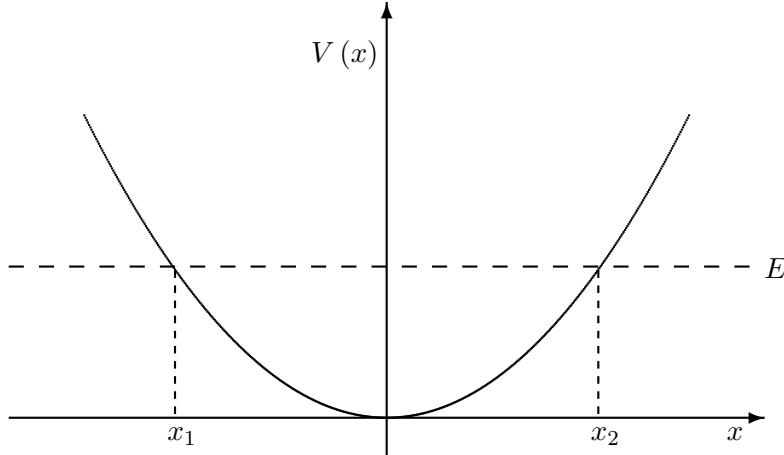


Figure 1. A typical potential in one dimension with two turning points x_1 and x_2 .

For a typical potential well with two turning points x_1 and x_2 as shown in figure 1, the energy eigenvalues are given approximately by

$$\int_{x_1}^{x_2} p(x) dx = \int_{x_1}^{x_2} \sqrt{2m(E - V(x))} dx = \left(n + \frac{1}{2}\right) \pi \hbar, \quad (5)$$

where the integral is taken from one turning point to another and n is a non-negative integer, which is also the number of nodes of the wave function [5].

The condition for the approximation to work to the first order is that the variation of the potential should be small enough (see [5]), so that

$$\sqrt{\frac{\hbar^2}{2m}} \frac{|V'(x)|}{(E - V(x))^{3/2}} \ll 1. \quad (6)$$

This is essentially a condition on the *de Broglie wave length* $\lambda = \frac{\hbar}{p(x)}$

$$\left| \frac{\partial \lambda}{\partial x} \right| \ll 1. \quad (7)$$

This method, however, has the disadvantage that the wave function diverges as $\frac{1}{\sqrt{|p(x)|}}$ in the neighborhood of a turning point.

Langer [19] generalized the JWKB method to get a semiclassical wave function that is continuous in the whole domain including the turning point(s). The general method is known as *Airy uniform approximation* to the one-dimensional Schrödinger equation (cf. [20]). A

review is given in Appendix 3. Near the *left turning point* x_1 , the semiclassical wave function is found by this method to be

$$\psi(x) = \left[\frac{z(x)}{p^2(x)} \right]^{1/4} \text{Ai}(-z(x)), \quad (8)$$

where

$$z(x) = \begin{cases} \left[\frac{3}{2\hbar} \int_{x_1}^x p(x') dx' \right]^{2/3}, & \text{for } x > x_1, \\ - \left[\frac{3}{2\hbar} \int_x^{x_1} |p(x')| dx' \right]^{2/3}, & \text{for } x < x_1. \end{cases} \quad (9)$$

$z(x)$ can be written in terms of a quantity called the *abbreviated action* or the *reduced action* (see [21]) with respect to the left turning point x_1 , given by

$$S_1(x) = \int_{x_1}^x p(x') dx' = \int_{x_1}^x \sqrt{2m(E - V(x'))} dx'. \quad (10)$$

The abbreviated action $S_1(x)$ (in short, “action”, if there is no ambiguity) can be continued analytically into the classically forbidden region if the phase of the classical momentum $p(x)$ is suitably chosen in that region. When $x < x_1$, we put

$$p(x) = e^{i\pi/2} |p(x)|.$$

This gives rise to

$$\begin{aligned} S_1(x) &= \int_x^{x_1} (-e^{i\pi/2}) |p(x')| dx' \\ &= e^{i3\pi/2} \int_x^{x_1} |p(x')| dx', \end{aligned} \quad (11)$$

and $z(x)$ can then be defined as

$$z(x) = \left[\frac{3}{2\hbar} S_1(x) \right]^{2/3}. \quad (12)$$

The phase factor $e^{i3\pi/2}$ gives $z(x)$ the negative sign and ensures that the wave function in equation (8), following the property of Airy function (see [20]), tends to zero rapidly in the forbidden region. The Airy uniform approximation method applies equally well near the *right turning point* x_2 . In this case, we simply replace the action with respect to the left turning point by that with respect to the right turning point

$$S_2(x) = \int_x^{x_2} p(x') dx' = \int_x^{x_2} \sqrt{2m(E - V(x'))} dx'. \quad (13)$$

For the approximate eigenfunction to be continuous everywhere, Miller [12] suggests a connection formula, whereby the action from the left and from the right turning points are matched at a mid-phase point x_m defined by

$$\int_{x_1}^{x_m} p(x) dx = \int_{x_m}^{x_2} p(x) dx = \frac{1}{2} \int_{x_1}^{x_2} p(x) dx. \quad (14)$$

With the JWKB quantization rule (5), the mid-phase point x_m is found to satisfy

$$\int_{x_1}^{x_m} p(x) dx = \frac{1}{2} \left(n + \frac{1}{2} \right) \pi \hbar. \quad (15)$$

Altogether, the function $z_n(x)$ corresponding to each bound state energy eigenvalue E_n for a potential well with two turning points x_1 and x_2 is given by

In the classically allowed region:

$$\begin{aligned} z_n(x) &= \left[\frac{3}{2\hbar} \int_{x_1}^x dx' \sqrt{2m(E_n - V(x'))} \right]^{2/3}, \text{ for } x < x_m, \\ z_n(x) &= \left[\frac{3}{2\hbar} \int_x^{x_2} dx' \sqrt{2m(E_n - V(x'))} \right]^{2/3}, \text{ for } x > x_m. \end{aligned} \quad (16)$$

In the classically forbidden region:

$$\begin{aligned} z_n(x) &= - \left[\frac{3}{2\hbar} \int_x^{x_1} dx' \sqrt{2m(V(x') - E_n)} \right]^{2/3}, \text{ for } x < x_1, \\ z_n(x) &= - \left[\frac{3}{2\hbar} \int_{x_2}^x dx' \sqrt{2m(V(x') - E_n)} \right]^{2/3}, \text{ for } x > x_2. \end{aligned} \quad (17)$$

In passing, we deduce from these relations that

$$\frac{\partial z_n(x)}{\partial x} = \begin{cases} \frac{p_n(x)}{\hbar \sqrt{z_n(x)}}, & \text{for } x < x_m, \\ -\frac{p_n(x)}{\hbar \sqrt{z_n(x)}}, & \text{for } x > x_m. \end{cases} \quad (18)$$

The normalized semiclassical eigenfunctions (called the *Langer wave functions*) are given by [10–12]

$$\psi_n(x) = \sqrt{\frac{2m\omega_n}{p_n(x)}} z_n^{1/4}(x) \text{Ai}(-z_n(x)), \quad (19)$$

where ω_n is the angular frequency of the classical orbit corresponding to the energy level E_n , given by the JWKB quantization rule (5). By taking derivative w.r.t n of

$$S_1(x_2) = \int_{x_1}^{x_2} dx' \sqrt{2m(E_n - V(x'))} = \pi \hbar \left(n + \frac{1}{2} \right), \quad (20)$$

we infer for later reference that

$$\begin{aligned}
& \frac{\partial E_n}{\partial n} \frac{\partial}{\partial E_n} \int_{x_1}^{x_2} dx' \sqrt{2m(E_n - V(x'))} = \pi \hbar \\
\iff & \frac{\partial E_n}{\partial n} \underbrace{\int_{x_1}^{x_2} dx' \frac{1}{\sqrt{\frac{2}{m}(E_n - V(x'))}}}_{\frac{T_n}{2}} = \pi \hbar \\
\iff & \omega_n = \frac{2\pi}{T_n} = \hbar^{-1} \left. \frac{\partial E_\lambda}{\partial \lambda} \right|_{\lambda=n},
\end{aligned} \tag{21}$$

where T_n is the period of the periodic classical orbit of energy E_n . The Langer wave function (19) is up to a phase factor. Observe that, as given by (19), the wave function is positive and decays to zero at $\pm\infty$. In view of the fact that n is the number of nodes, the correct wave function should change sign n times from $-\infty$ to $+\infty$. We, therefore, add in a factor $e^{in\pi}$ when $x < x_m$. The wave function given by the JWKB method is actually the leading term in the asymptotic expansion of (19) for large $|z_n(x)|$.

It is worth noting that when we do a numerical simulation of the Langer wave function (19), it may not converge to a prescribed precision near the two turning points, due to the vanishing of the classical momentum in the denominator. We shall replace it by its Taylor expansion around a turning point x_i

$$\psi_n(x) \simeq \sqrt{2m\omega_n} \left(\frac{1}{2\hbar m \left| \frac{d}{dx} V(x_i) \right|} \right)^{1/6} \text{Ai}(-z_n(x)). \tag{22}$$

Figures 2, 3, 4, and 5 now compare the exact wave function and its semiclassical approximation (19) for the first four modes of a one-dimensional Morse potential. We refer to [22] for the exact wave functions and energy eigenvalues for the Morse potential.

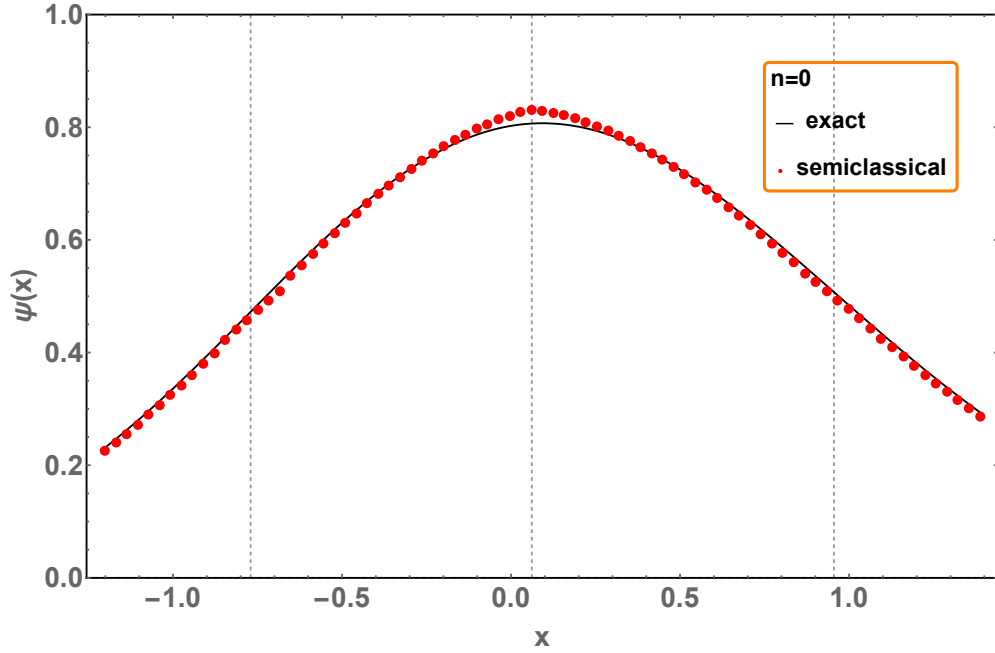


Figure 2. Exact wave function and its semiclassical approximation (19) for mode $n = 0$ of a one-dimensional Morse potential, $V(x) = D(e^{-2\beta x} - 2e^{-\beta x})$, with three vertical gridlines showing respectively x_1 , x_m , and x_2 .

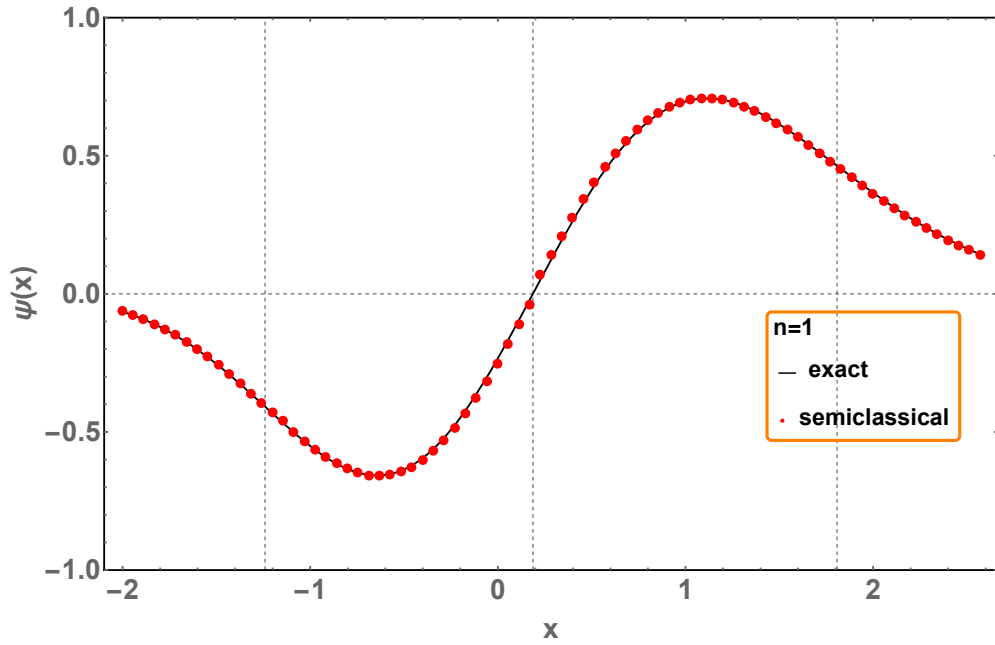


Figure 3. Exact wave function and its semiclassical approximation (19) as in figure 2 but for mode $n = 1$.

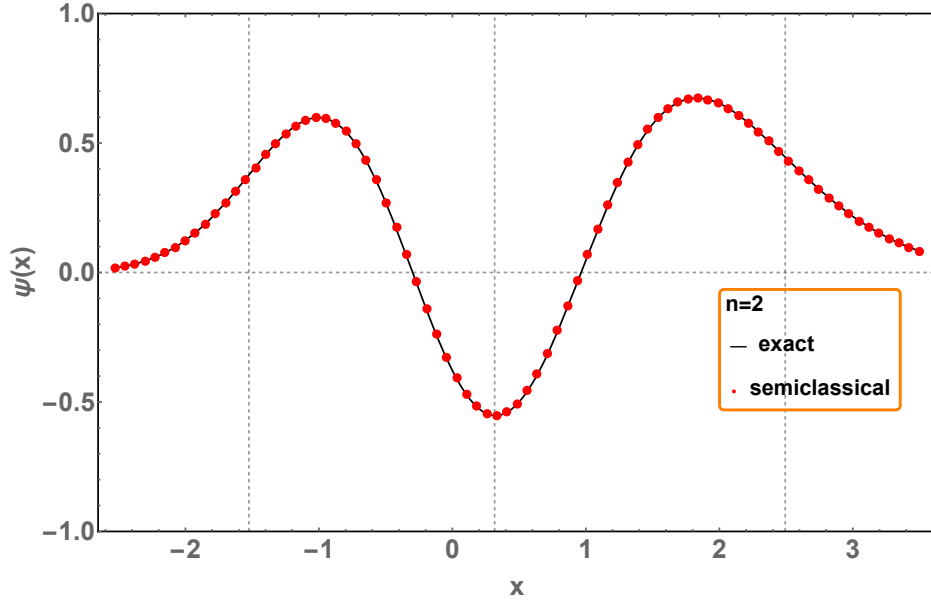


Figure 4. Exact wave function and its semiclassical approximation (19) as in figure 2 but for mode $n = 2$.

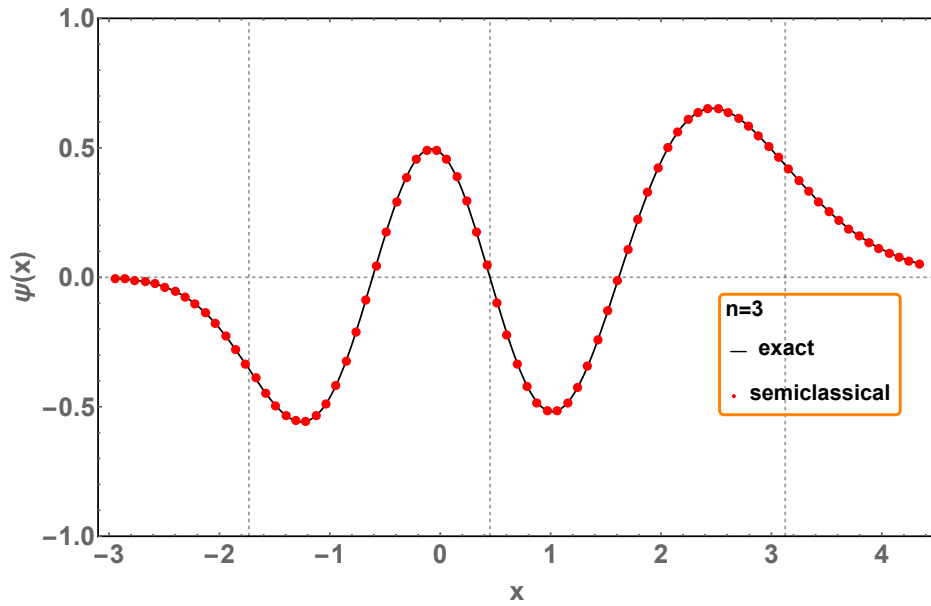


Figure 5. Exact wave function and its semiclassical approximation (19) as in figure 2 but for mode $n = 3$.

We can see that the semiclassical approximation matches well with the exact result in general. Nevertheless, the approximation does not work as well for the ground state as it does for the higher modes. For example, in figure 2, the matching point x_m of the

wave function is quite visible while figures 3, 4, and 5 are almost smooth curves. This is understandable since in the semiclassical regime, the classical action $S_1(x_2)$ (20), which increases with the energy, is very large compared to \hbar . We can also see that the number of nodes matches the quantum number n , as discussed earlier.

II.3. Semiclassical particle density of a non-interacting quantum gas of fermions in one dimension

In the TF model, the semiclassical particle density for a system of non-interacting spin-polarized fermions in a one-dimensional potential is given by (cf. for example [1])

$$n_{\text{TF}}(x) = \begin{cases} \frac{p_{\text{F}}(x)}{\pi\hbar}, & \text{in the classically allowed region} \\ 0, & \text{in the classically forbidden region,} \end{cases} \quad (23)$$

where $p_{\text{F}}(x)$ is the classical momentum at the Fermi energy level. We can see that the TF density, on top of having a cusp at the turning points, gives zero density in the classically forbidden region, where quantum effect must be taken into account for a better approximation of the exact density.

To provide a correction to the TF density, Ribeiro et al. [10] calculate the sum of the modulus square of the Langer wave functions and extract the leading contribution from it. The density of N occupied orbitals for a system of non-interacting fermions is given by

$$n(x) = \sum_{j=0}^{N-1} |\psi_j(x)|^2 = \sum_{k=-\infty}^{\infty} \int_{-1/2}^{N-1/2} d\lambda \frac{2m\omega_\lambda}{p_\lambda(x)} z_\lambda^{1/2}(x) \text{Ai}^2(-z_\lambda(x)) \exp(2\pi i k \lambda), \quad (24)$$

where in the last step, the Poisson summation formula (cf. Appendix 2 and [23]) is used to turn the sum into a sum of integrals. The authors [10] found an asymptotic approximation to the density in the semiclassical limit

$$n^{\text{sc}}(x) = \frac{p_{\text{F}}(x)}{\hbar} \left[\left(\sqrt{z} \text{Ai}^2(-z) + \frac{\text{Ai}'^2(-z)}{\sqrt{z}} \right) + \left(\frac{\hbar m \omega_{\text{F}}}{p_{\text{F}}^2(x)} \csc(\alpha_{\text{F}}(x)) - \frac{1}{2z^{3/2}} \right) \text{Ai}(-z) \text{Ai}'(-z) \right] \Big|_{z=z_{\text{F}}(x)}, \quad (25)$$

where the Fermi energy E_{F} is obtained by solving (5) for $n = N - 1/2$ (which is indeed the Fermi energy that normalizes the corresponding TF density (23) to N), and $\alpha_{\text{F}}(x)$ is given by

$$\alpha_{\text{F}}(x) = \sqrt{z_{\text{F}}(x)} \frac{\partial z_\lambda(x)}{\partial \lambda} \Big|_{\lambda=N-1/2}. \quad (26)$$

As pointed out in [10], equation (25) works for non-interacting fermions in a potential well with two turning points. Eventually, the external potential will be the effective potential which incorporates an interaction contribution and then allows for dealing with interacting fermions. The result is extremely accurate and is a correction to the TF density that is continuous to the forbidden region, as we can see in figure 6 for a system of two particles in a Morse potential.

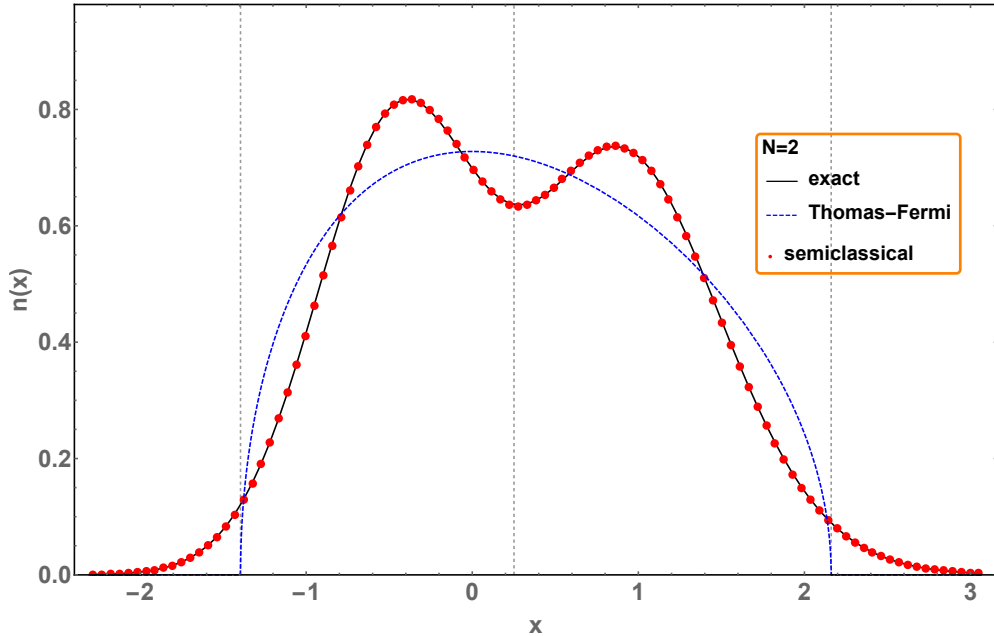


Figure 6. Exact density, TF density, and semiclassical density (25) for two particles in a one-dimensional Morse potential, $V(x) = D(e^{-2\beta x/2} - 2e^{-\beta x})$, with three vertical gridlines showing respectively x_1 , x_m , and x_2 .

II.4. Leading contribution to the particle density

Let $n_0(x)$ be the first term in the full expression (25) of the semiclassical density

$$n_0(x) = \frac{p_F(x)}{\hbar} \left[\sqrt{z} \text{Ai}^2(-z) + \frac{\text{Ai}'^2(-z)}{\sqrt{z}} \right] \Big|_{z=z_F(x)}. \quad (27)$$

It can also be written in terms of the functions F_m (see Appendix 1) as

$$n_0(x) = \frac{p_F(x)}{\hbar \sqrt{z_F(x)}} F_1(-z_F(x)). \quad (28)$$

With the relations (18) as well as the fact that $\frac{d}{dz}F_2(-z) = F_1(-z)$ (240), $n_0(x)$ can be written as

$$n_0(x) = \text{sgn}(x_m - x) \frac{d}{dx} F_2(-z_F(x)). \quad (29)$$

We can then, with ease, integrate $n_0(x)$ to get its contribution N_0 to the total particle number N . We find that

$$\begin{aligned} N_0 &= \int_{-\infty}^{\infty} dx n_0(x) \\ &= \int_{-\infty}^{x_m} dx \frac{d}{dx} F_2(-z_F(x)) - \int_{x_m}^{\infty} dx \frac{d}{dx} F_2(-z_F(x)) \\ &= 2F_2(-z_F(x_m)) - \underbrace{F_2(-z_F(\infty))}_0 - \underbrace{F_2(-z_F(-\infty))}_0 \\ &= 2F_2(-z_F(x_m)). \end{aligned} \quad (30)$$

The contribution at $\pm\infty$ is negligible since F_2 , as related to Airy function and its derivative, vanishes for large negative z_F , which is indeed the case at these two extremes.

By virtue of (15),

$$\begin{aligned} z_F(x_m) &= \left[\frac{3}{2\hbar} \int_{x_1}^{x_m} dx' \sqrt{2m(E_F - V(x'))} \right]^{\frac{2}{3}} \\ &= \frac{3}{4} \pi N, \end{aligned} \quad (31)$$

which increases with N . By an asymptotic expansion of F_2 (247) for large $z_F(x_m)$, we obtain

$$N_0 \stackrel{N \gg 1}{\simeq} 2 \frac{2}{3\pi} [z_F(x_m)]^{3/2}, \quad (32)$$

and hence

$$N_0 \stackrel{N \gg 1}{\simeq} N. \quad (33)$$

We find indeed that $n_0(x)$ is the dominant term in the full expression of the semiclassical density $n^{\text{sc}}(x)$. For large total numbers of particles, this leading term approaches the exact result. As we can see in figures 7 and 8, the density leading contribution $n_0(x)$ is comparable to the full contribution $n^{\text{sc}}(x)$ in its approximation to the exact density.

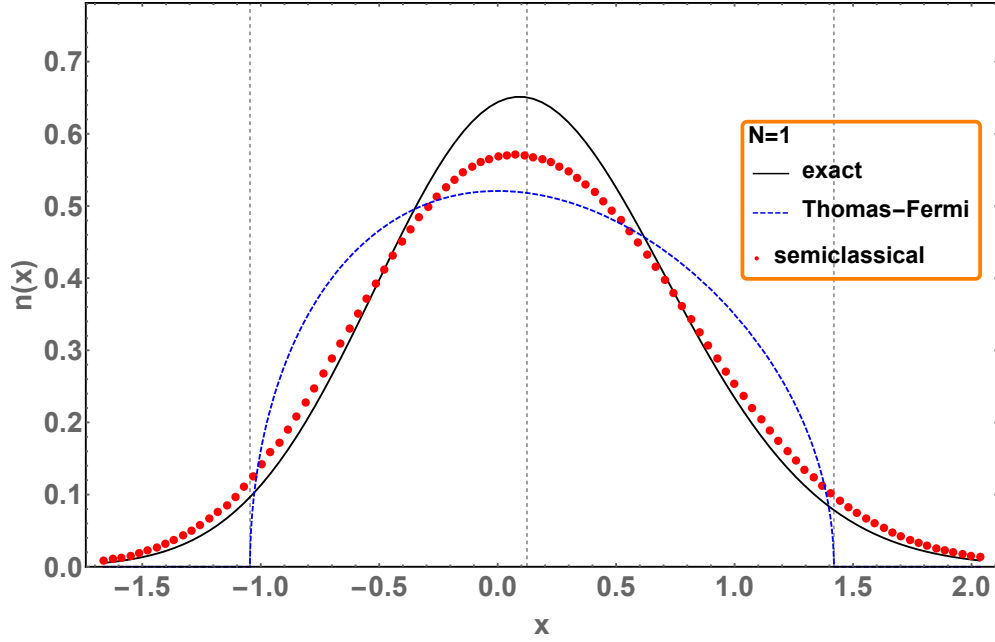


Figure 7. Exact density, TF density, and semiclassical density (27) for one particle in a one-dimensional Morse potential, $V(x) = D(e^{-2\beta x} - 2e^{-\beta x})$, with three vertical gridlines showing respectively x_1 , x_m , and x_2 .

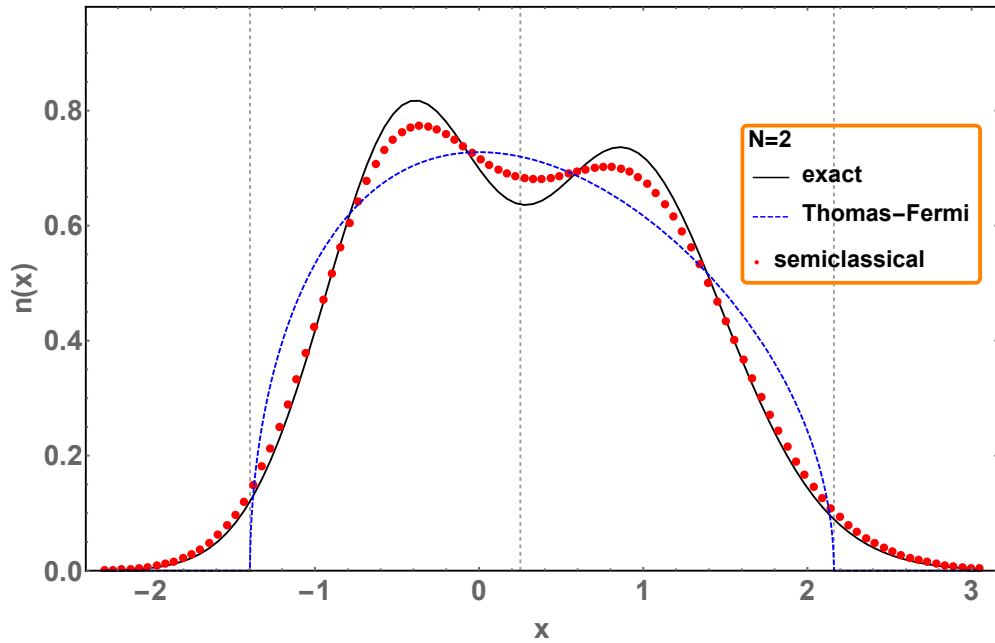


Figure 8. Exact density, TF density, and semiclassical density (27) as in figure 7 but for two particles.

In the present paper, we shall focus solely on the dominant term $n_0(x)$ of the particle density. For its re-derivation, the reader is referred to Appendix 4.

II.5. Normalization of the Langer wave function

As a final check of the normalization of the Langer wave function (19), we recover it from the leading contribution $n_0(x)$ to the density. The term $n_0(x)$ is derived from the term with $k = 0$ in the Poisson summation (24), cf. Appendix 4. Essentially, it is a replacement of a sum by an integral, i.e.

$$n(x) = \sum_{j=0}^N |\psi_j(x)|^2 \xrightarrow{\text{replace}} \int_{-1/2}^{N-1/2} d\nu |\psi_\nu(x)|^2. \quad (34)$$

It follows that we can retrieve the Langer wave function at the Fermi energy $\psi_F(x)$ by

$$|\psi_F(x)|^2 = |\psi_{N-1/2}(x)|^2 \simeq \frac{\partial}{\partial N} n_0(x). \quad (35)$$

By taking the derivative of

$$n_0(x) = \frac{p_F(x)}{\hbar \sqrt{z_F(x)}} F_1(-z_F(x)) \quad (36)$$

w.r.t N , we have

$$\frac{\partial}{\partial N} n_0(x) = \frac{\partial E_F}{\partial N} \left[\frac{\partial p_F(x)}{\partial E_F} \frac{F_1(-z_F(x))}{\hbar \sqrt{z_F(x)}} + \frac{p_F(x)}{\hbar} \frac{\partial z_F(x)}{\partial E_F} \left(\frac{\partial F_1(-z)}{\partial z} \frac{1}{\sqrt{z}} \right)_{z=z_F(x)} \right]. \quad (37)$$

By (21), we have

$$\frac{\partial E_F}{\partial N} = \hbar \omega_F. \quad (38)$$

Note also that

$$\frac{\partial}{\partial E_F} p_F(x) = \frac{m}{p_F(x)}. \quad (39)$$

We have hence, by (38), (39), and (243),

$$\frac{\partial}{\partial N} n_0(x) = \hbar \omega_F \left[\frac{m}{p_F(x)} \frac{F_1(-z_F(x))}{\hbar \sqrt{z_F(x)}} + \frac{p_F(x)}{\hbar} \frac{\partial z_F(x)}{\partial E_F} \left(-\frac{1}{4} \frac{F_{-2}(-z_F(x))}{(\sqrt{z_F(x)})^3} \right) \right]. \quad (40)$$

By (245), we can replace F_1 in the above equation by F_{-2} and F_0 and obtain

$$\begin{aligned} \frac{\partial}{\partial N} n_0(x) &= \frac{2m\omega_F \sqrt{z_F(x)}}{p_F(x)} F_0(-z_F(x)) \\ &+ \left[\frac{m\omega_F}{2p_F(x) \sqrt{z_F(x)}} F_{-2}(-z_F(x)) - \frac{1}{4} \omega_F p_F(x) \frac{\partial z_F(x)}{\partial E_F} \frac{F_{-2}(-z_F(x))}{\left(\sqrt{z_F(x)}\right)^3} \right]. \end{aligned} \quad (41)$$

By comparison with (19), we have

$$\frac{\partial}{\partial N} n_0(x) = |\psi_F(x)|^2 + [\dots]. \quad (42)$$

It can be proved by Taylor expansion that the correction term in the square brackets converges to zero when x approaches each of the turning points. In addition, when N increases, the Fermi energy E_F increases, and the left and right turning points are transitioned towards $\mp\infty$, respectively. Hence, as defined by (16) and (17), $z_F(x) \rightarrow \infty$ as $N \rightarrow \infty$ for all x . The correction term then vanishes in negative orders of $z_F(x)$. We recover the modulus square of the Langer wave function as the leading term in the derivative w.r.t N of $n_0(x)$. Since $n_0(x)$ has been shown to be normalized to N in the limit of large N , the Langer wave function (19) that we use to derive $n_0(x)$ is correctly normalized.

III. EXTENSION OF THE RESULT BY RIBEIRO *ET AL.* TO ISOTROPIC POTENTIALS IN HIGHER DIMENSIONS

III.1. Introduction

The essential point in the arguments of Ribeiro *et al.* [10] is the use of the Langer wave function (19), which is a semiclassical approximation that is continuous on the entire domain to the eigenfunction of the time-independent Schrödinger equation. Then, following the method set out by the authors, we can extract the leading contribution to the particle density of N occupied orbitals. It turns out that we can extend this method to two-dimensional and three-dimensional problems with isotropic potentials, since these can be reduced to one-dimensional problems by separation of variables. We consider the analog of the one-dimensional Langer wave function (19) for the radial motion in two and three dimensions, which eventually gives us the same form as in (27) for the dominant term in the semiclassical radial particle density (56) for each angular quantum number l . Great care must be taken in applying the JWKB method for radial motion as a centrifugal term has been introduced in the effective potential. Here we follow the prescription by Langer [11]. For two dimensions, the s-wave radial density (zero magnetic quantum number) requires special treatment as the centrifugal term becomes a centripetal one. We use the result by Berry and de Almeida [24] for the s-wave radial wave function near $s = 0$ and extract the leading contribution to the radial particle density, following the method by Ribeiro *et al.* [10]. For the two-dimensional Coulomb potential, which is highly singular near $s = 0$, the leading contribution to the density (114) that we have derived fails to converge to zero at $s = 0$. In this case, we choose to sum up manually the squared Langer wave functions for s-wave, which still approximate accurately the exact wave functions. In future works, we have to find a better approximation to arrive at the analog of formula (25) for s-wave, which is applicable to all potentials that blow up less rapidly than $1/s^2$ near $s = 0$. We illustrate the results of this section by the Coulomb and harmonic oscillator potentials in two and three dimensions.

III.2. Isotropic potentials in three dimensions

III.2.1. *Langer wave function for the radial motion and the corresponding radial particle density*

In the three-dimensional case where the potential energy depends only on the radius variable r in spherical coordinates, the wave function can be split into two parts

$$\psi_{n,l,m}(r, \theta, \phi) = R_{n,l}(r) Y_l^m(\theta, \phi), \quad (43)$$

where $Y_l^m(\theta, \phi)$ is the well-known spherical harmonics (see for example, [18]). Let $u_{n,l}(r) = R_{n,l}(r)r$, we obtain the so-called *radial Schrödinger equation*, which reads

$$\left\{ -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + V(r) + \frac{\hbar^2 l(l+1)}{2mr^2} - E \right\} u(r) = 0. \quad (44)$$

We can regard this as the Schrödinger equation for a one-dimensional equivalent problem with the effective potential $\tilde{V}(r) = V(r) + \frac{\hbar^2 l(l+1)}{2mr^2}$, but here the variable r goes from 0 to ∞ . Langer pointed out [11] that the semiclassical approximation can only be correctly applied after replacing $l(l+1)$ in the effective potential by $(l+1/2)^2$, explained in the following. He did this by considering the singular nature of the centrifugal term at $r=0$, which renders condition (6) no longer valid [5] (for a rigorous discussion, see also the review paper of semiclassical approximations in wave mechanics by Berry and Mount [25]). This is resolved by a change of variables that maps $(0, \infty)$ to $(-\infty, \infty)$.

Langer [11] suggested the following change from $(r, u(r))$ to $(x, \psi(x))$

$$\begin{aligned} r &= r_0 e^{x/r_0}, \\ u(r) &= e^{-x/2r_0} \psi(x), \end{aligned} \quad (45)$$

where r_0 is some length scale, which can be taken to be one in appropriate units. Now x also has the dimension of length and goes from $-\infty$ to ∞ . We obtain the equation

$$\left\{ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + [V(r_0 e^{x/r_0}) - E] e^{2x/r_0} + \frac{\hbar^2 (l+1/2)^2}{2mr_0^2} \right\} e^{-x/r_0} \psi(x) = 0. \quad (46)$$

We identify the constant term $-\frac{\hbar^2 (l+1/2)^2}{2mr_0^2}$ with the energy and $[V(r_0 e^{x/r_0}) - E] e^{2x/r_0}$ with the potential in the usual one-dimensional Schrödinger equation (4). The classical momentum for the x variable is hence given by

$$p(x) = \sqrt{2m \left\{ -\frac{\hbar^2 (l+1/2)^2}{2mr_0^2} - [V(r_0 e^{x/r_0}) - E] e^{2x/r_0} \right\}}. \quad (47)$$

We obtain the WKB quantization rule as in (5)

$$\pi\hbar(n_r + 1/2) = \int dx \sqrt{2m \left\{ -\frac{\hbar^2(l + 1/2)^2}{2mr_0^2} - [V(r_0 e^{x/r_0}) - E] e^{2x/r_0} \right\}}, \quad (48)$$

where $n_r = 0, 1, 2, \dots$ is the radial quantum number. The integral is taken over the range where the quantity under the square root sign is positive, i.e. in the classically allowed region. Changing the variable back to r , we have

$$\pi\hbar(n_r + 1/2) = \int dr \sqrt{2m \left\{ E - V(r) - \frac{\hbar^2(l + 1/2)^2}{2mr^2} \right\}}. \quad (49)$$

We notice that the change of variables thus carried out is equivalent to replacing $l(l + 1)$ in the centrifugal term by $(l + 1/2)^2$. The prescription works even for $l = 0$ in three dimensions (which requires special consideration in two dimensions, more on this later). It turns out that (49) gives the exact expressions for the energy eigenvalues of three-dimensional harmonic oscillator potential and Coulomb potential (cf. Appendix 5). However, it is shown in [24] (cited in [5]) that the potential $V(r)$ should not diverge faster than $\frac{1}{r^2}$ in the limit when $r \rightarrow 0$ for the Langer method to work.

Let $\tilde{\psi}(x) = e^{-x/r_0}\psi(x)$ and proceed as in [20], we obtain an Airy uniform approximation (see Appendix 3) to $\tilde{\psi}(x)$ satisfying equation (46):

$$\tilde{\psi}(x) = \frac{z(x)^{1/4}}{p(x)^{1/2}} \text{Ai}(-z(x)), \quad (50)$$

where $p(x)$ is given by equation (47), and $z(x)$ is defined as in [10] according to $p(x)$. We re-express z as a function of the r variable and obtain its expressions in different regions:

$$z(r) = \begin{cases} \left[\frac{3}{2\hbar} \int_{r_1}^r dr' \sqrt{2m \left(E - V(r') - \frac{\hbar^2(l+1/2)^2}{2mr'^2} \right)} \right]^{2/3}, & \text{for } r_1 < r < r_m \\ \left[\frac{3}{2\hbar} \int_r^{r_2} dr' \sqrt{2m \left(E - V(r') - \frac{\hbar^2(l+1/2)^2}{2mr'^2} \right)} \right]^{2/3}, & \text{for } r_m < r < r_2 \\ - \left[\frac{3}{2\hbar} \int_r^{r_1} dr' \sqrt{2m \left(V(r') + \frac{\hbar^2(l+1/2)^2}{2mr'^2} - E \right)} \right]^{2/3}, & \text{for } r < r_1 \\ - \left[\frac{3}{2\hbar} \int_{r_2}^r dr' \sqrt{2m \left(V(r') + \frac{\hbar^2(l+1/2)^2}{2mr'^2} - E \right)} \right]^{2/3}, & \text{for } r > r_2, \end{cases} \quad (51)$$

where r_1 , r_2 are the left and right turning points, respectively, and r_m is the mid-phase point where $z(r)$ is matched. This is equivalent to the case when the classical momentum is given by

$$p_{n_r,l}(r) = \sqrt{2m \left(E_{n_r,l} - V(r) - \frac{\hbar^2 (l + 1/2)^2}{2mr^2} \right)}. \quad (52)$$

Altogether, we have the approximation to the radial eigenfunctions with the normalization factor

$$u_{n_r,l}(r) = \sqrt{\frac{2m\omega_{n_r,l}}{p_{n_r,l}(r)}} z_{n_r,l}(r)^{1/4} \text{Ai}(-z_{n_r,l}(r)), \quad (53)$$

where $\omega_{n_r,l}$ is the classical frequency of one round-trip from one turning point of the effective potential to the other and back, given by

$$\omega_{n_r,l} = 2\pi \left[\int_{r_1}^{r_2} \frac{2dr}{p_{n_r,l}(r)/m} \right]^{-1}. \quad (54)$$

The energy eigenvalues $E_{n_r,l}$ are given by (49).

It is noted that for a fixed value of the angular quantum number l , the effective potential is fixed, and the semiclassical radial wave function (53) has the same form as the semiclassical wave function (19) in the one-dimensional case. Thus, in the same manner, we approximate the sum (which we call the radial particle density for the angular quantum number l)

$$\sum_{n_r=0}^{N-1} |u_{n_r,l}(r)|^2 \quad (55)$$

by

$$n_{N,l}(r) = \frac{p_{F,l}(r)}{\hbar} \left[\sqrt{z(r)} \text{Ai}^2(-z(r)) + \frac{\text{Ai}'^2(-z(r))}{\sqrt{z(r)}} \right] \Big|_{z=z_{F,l}(x)} \quad (56)$$

as we have the leading term (27) in the semiclassical density (25). The subscript F denotes the Fermi energy, obtained by solving (49) for a particular value of l and $n_r = N - 1/2$. The sum (55), nevertheless, is not the particle density for a practical system of non-interacting fermions yet since we have to take into account the spherical harmonics part of the wave function. We will illustrate how the density can be obtained for a certain total number of particles with the examples of harmonic oscillator potential and Coulomb potential in three dimensions.

III.2.2. TF density in three dimensions

For now, let us quickly review the result of the TF model in three dimensions. The particle density for spin-polarized fermions is given by [1]

$$n^{\text{TF}}(\mathbf{r}) = \frac{p_{\text{F}}(\mathbf{r})^3}{6\pi^2\hbar^3} \quad (57)$$

in the classically allowed region and zero elsewhere. $p_{\text{F}}(\mathbf{r})$ is the classical momentum at the Fermi energy and is given by

$$p_{\text{F}}(\mathbf{r}) = \sqrt{2m(E_{\text{F}} - V(\mathbf{r}))}, \quad (58)$$

where the Fermi energy E_{F} is chosen such that $n^{\text{TF}}(\mathbf{r})$ is normalized to the total number of particles N . Note that this E_{F} is in principle not the Fermi energy chosen for equation (56) for each angular quantum number. In the case of isotropic potential, the TF density is isotropic. The normalization condition in this case reads

$$\int_0^{\infty} 4\pi r^2 dr n^{\text{TF}}(r) = N. \quad (59)$$

We see here how the TF model is crude in describing the shell structure. It is not for all values of the total particle number that the density is isotropic even for isotropic external potential.

III.2.3. Three-dimensional harmonic oscillator potential

The exact solution to the three-dimensional harmonic oscillator problem can be found in various pieces of literature (cf. for example [26]). For the potential energy

$$V(r) = \frac{1}{2}m\omega^2 r^2, \quad (60)$$

the energy eigenvalue of each shell denoted by the principle quantum number n is given by

$$E_n = \left(n + \frac{3}{2}\right)\hbar\omega, \quad (61)$$

where

$$n = 2n_r + l. \quad (62)$$

Here, n_r and l are respectively the radial quantum number and the angular quantum number. For spin-polarized systems, the eigenvalue E_n comes with a degeneracy

$$j_n = \frac{(n+1)(n+2)}{2}. \quad (63)$$

Table I summarizes the orbitals corresponding to the four smallest values of the principal quantum number.

Table I. Orbitals of the four smallest values of the principal quantum number for a three-dimensional harmonic oscillator.

n	n_r	l	number of orbitals	j_n
0	0	0	1	1
1	0	1	3	3
2	1	0	1	6
	0	2	5	
3	1	1	3	10
	0	3	7	

By employing the result (56), we can deduce the density of fully filled shells by summing the contributions of all the orbitals corresponding to those shells, and group the sum according to the angular quantum number l .

For example, the first 3 shells $n = 0, 1, 2$ can accommodate at maximum $1 + 3 + 6 = 10$ electrons. The density of a system of 10 electrons is given by

$$\begin{aligned}
n^{10}(\mathbf{r}) &= \sum_{n_r=0}^1 \sum_{m=0}^0 \frac{|u_{n_r,0}(r)|^2}{r^2} |Y_0^m(\theta, \phi)|^2 \\
&+ \sum_{n_r=0}^0 \sum_{m=-1}^1 \frac{|u_{n_r,1}(r)|^2}{r^2} |Y_1^m(\theta, \phi)|^2 \\
&+ \sum_{n_r=0}^0 \sum_{m=-2}^2 \frac{|u_{n_r,2}(r)|^2}{r^2} |Y_2^m(\theta, \phi)|^2.
\end{aligned} \quad (64)$$

When a shell is fully filled, the density is isotropic as the spherical harmonics have the property [18]

$$\sum_{m=-l}^l |Y_l^m(\theta, \phi)|^2 = \frac{2l+1}{4\pi}. \quad (65)$$

Consequently, $n^{10}(\mathbf{r})$ becomes

$$n^{10}(\mathbf{r}) = \frac{1}{4\pi r^2} \left\{ \sum_{n_r=0}^1 |u_{n_r,0}(r)|^2 + 3 \sum_{n_r=0}^0 |u_{n_r,1}(r)|^2 + 5 \sum_{n_r=0}^0 |u_{n_r,2}(r)|^2 \right\}. \quad (66)$$

We shall replace each sum over n_r for each particular value of l by its semiclassical approximation $n_{N,l}$ as in (56). We obtain hence

$$n^{10}(r) = \frac{1}{4\pi r^2} [n_{2,0}(r) + 3n_{1,1}(r) + 5n_{1,2}(r)]. \quad (67)$$

In the same way, we get the density of systems of one electron

$$n^1(r) = \frac{1}{4\pi r^2} n_{1,0}(r), \quad (68)$$

and four electrons

$$n^4(r) = \frac{1}{4\pi r^2} [n_{1,0}(r) + 3n_{1,1}(r)]. \quad (69)$$

We can now compare the values of the density given by different methods, with the exact expression of the radial wave function $u_{n_r,l}$ given by (see [26])

$$u_{n_r,l}(r) = \frac{2^{n_r+l+1} \gamma^{l/2+3/4}}{\pi^{1/4}} \sqrt{\frac{n_r! (n_r+l)!}{(2n_r+2l+1)!}} r^{l+1} \exp(-\gamma r^2/2) L_{n_r}^{l+1/2}(\gamma r^2), \quad (70)$$

where $\gamma = \frac{m\omega}{\hbar}$ and L denotes the generalized Laguerre polynomial (see [27]).

In figures 9, 10 and 11, we compare the exact, semiclassical as well as the TF densities for $N = 1, 4, 10$ particles in a three-dimensional harmonic oscillator potential. Density for more fully filled shells can be generated in the like manner.

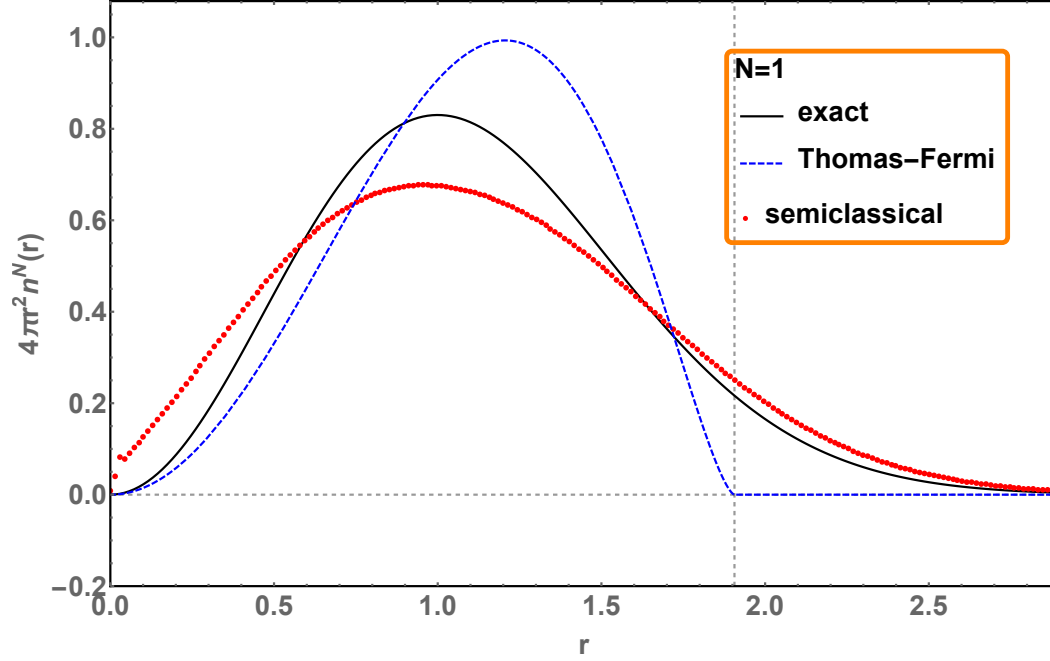


Figure 9. Exact density, TF density (57), and semiclassical density (68) for one particle in a three-dimensional harmonic oscillator potential, $V(r) = \frac{1}{2}m\omega^2 r^2$.

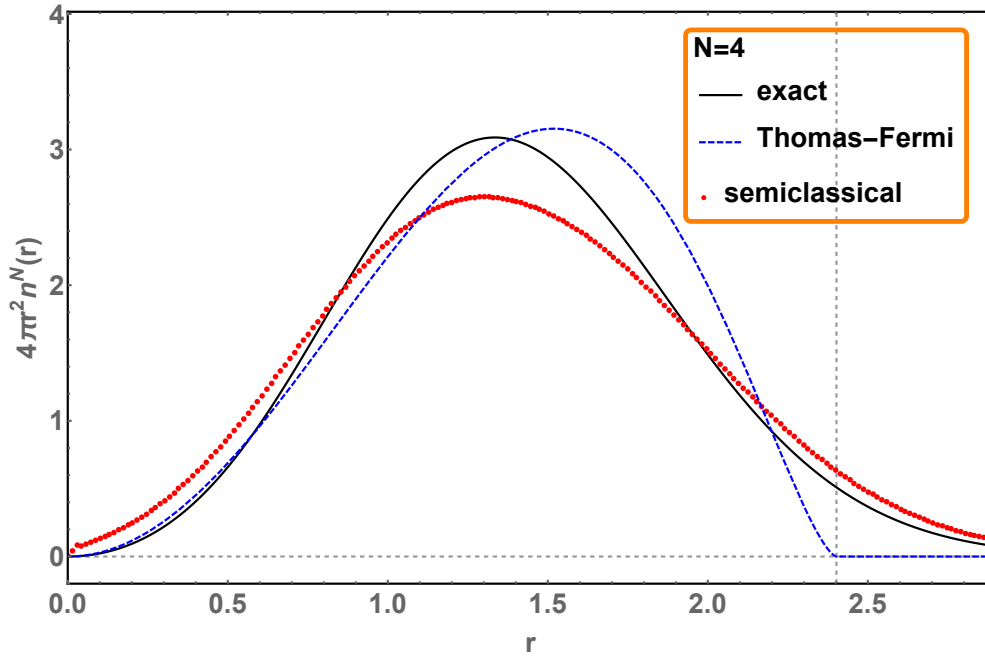


Figure 10. Exact density, TF density (57), and semiclassical density (69) for four particles in a three-dimensional harmonic oscillator potential, $V(r) = \frac{1}{2}m\omega^2 r^2$.

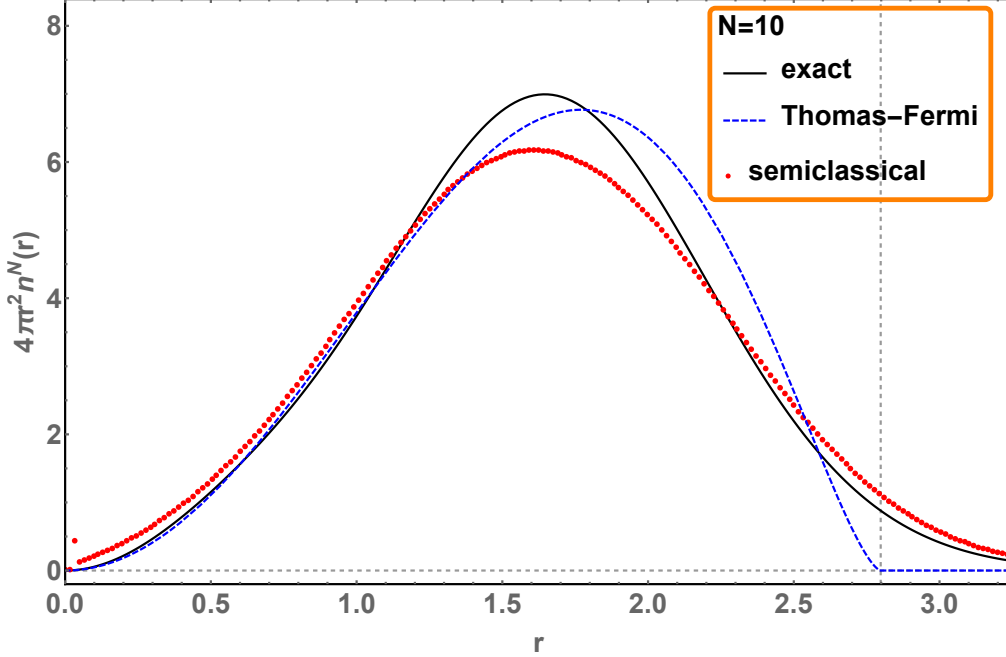


Figure 11. Exact density, TF density (57), and semiclassical density (67) for 10 particles in a three-dimensional harmonic oscillator potential, $V(r) = \frac{1}{2}m\omega^2 r^2$.

We observe that the leading term in the semiclassical density suggested by Ribeiro *et al.* [10] already gives an accurate approximation, which is continuous in the whole domain, to the exact density, while the TF version has a cusp at the turning point. We also observe that both the semiclassical density and the TF density approach the exact density as we increase the total number of particle. There is, however, some anomaly for the red dots near $r = 0$. This is error in numerical calculations as $p(r)$ and $z(r)$ tend both to infinity near $r = 0$, but this does not affect our result significantly.

III.2.4. Three-dimensional Coulomb potential

For the potential

$$V(r) = -\frac{e^2}{r}, \quad (71)$$

the exact radial wave function is given by (see [28] and [29])

$$u_{n_r, l}(r) = r \frac{2}{a^{3/2} n^2} \sqrt{\frac{(n-l-1)!}{(n+l)!}} \left(\frac{2r}{na}\right)^l e^{-r/na} L_{n-l-1}^{2l+1} \left(\frac{2r}{na}\right), \quad (72)$$

where $a = \frac{\hbar^2}{me^2}$, $n = n_r + l + 1$, and the energy eigenvalues are given by

$$E_n = -\frac{me^4}{2\hbar^2} \frac{1}{n^2}, \quad (73)$$

with a degeneracy

$$j_n = n^2 = \sum_{l=0}^{n-1} (2l + 1) \quad (74)$$

for spin-polarized systems.

Consider a system of N non-interacting spin-polarized electrons subject to the potential $V(r)$. We fill the electrons in the orbitals by the Aufbau rule, well-known in Chemistry (see [30]). The electron filling order is: 1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p,...

Table II. Aufbau rule for filling electrons in orbitals

	0	1	2	3	l
1	1s				
2	2s	2p			
3	3s	3p	3d		
4	4s	4p	4d	4f	
n					

As in the three-dimensional harmonic oscillator example, the particle density for the first four values of the total particle number with completely filled shells in the Coulomb potential is given by

$$n^1(r) = \frac{1}{4\pi r^2} n_{1,0}(r), \quad (75)$$

$$n^2(r) = \frac{1}{4\pi r^2} n_{2,0}(r), \quad (76)$$

$$n^5(r) = \frac{1}{4\pi r^2} [n_{2,0}(r) + 3n_{1,1}(r)], \quad (77)$$

$$n^6(r) = \frac{1}{4\pi r^2} [n_{3,0}(r) + 3n_{1,1}(r)], \quad (78)$$

where $n_{N,l}(r)$ is given by (56).

We compare the semiclassical, TF, and exact densities for these four values of the total particle number for the Coulomb potential in figures 12, 13, 14, and 15.

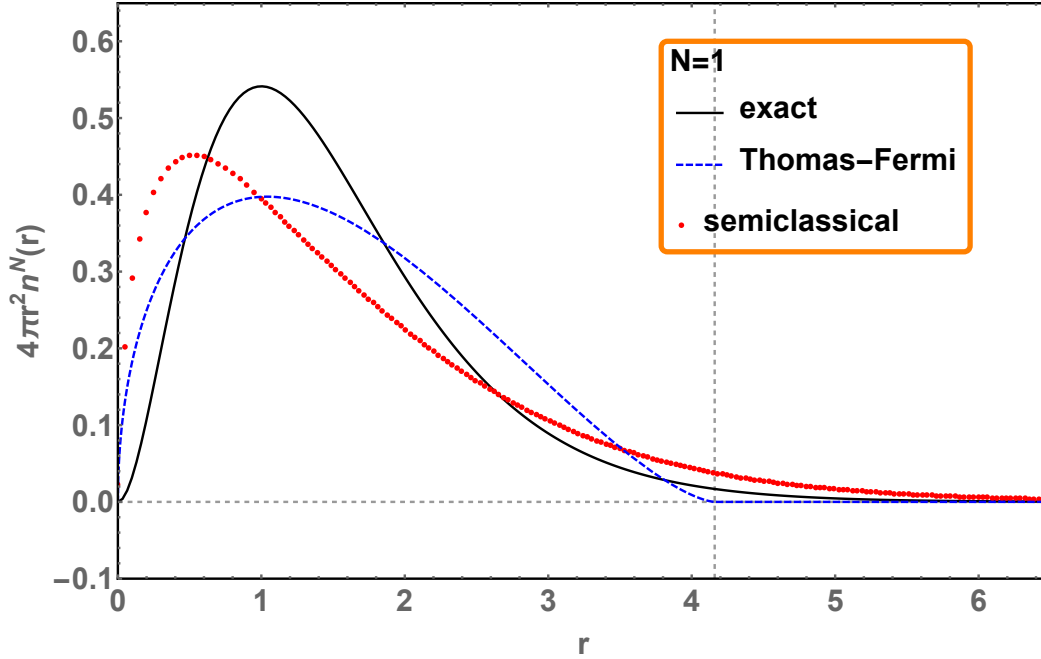


Figure 12. Exact density, TF density (57), and semiclassical density (75) for one particle in a three-dimensional Coulomb potential, $V(r) = -e^2/r$.

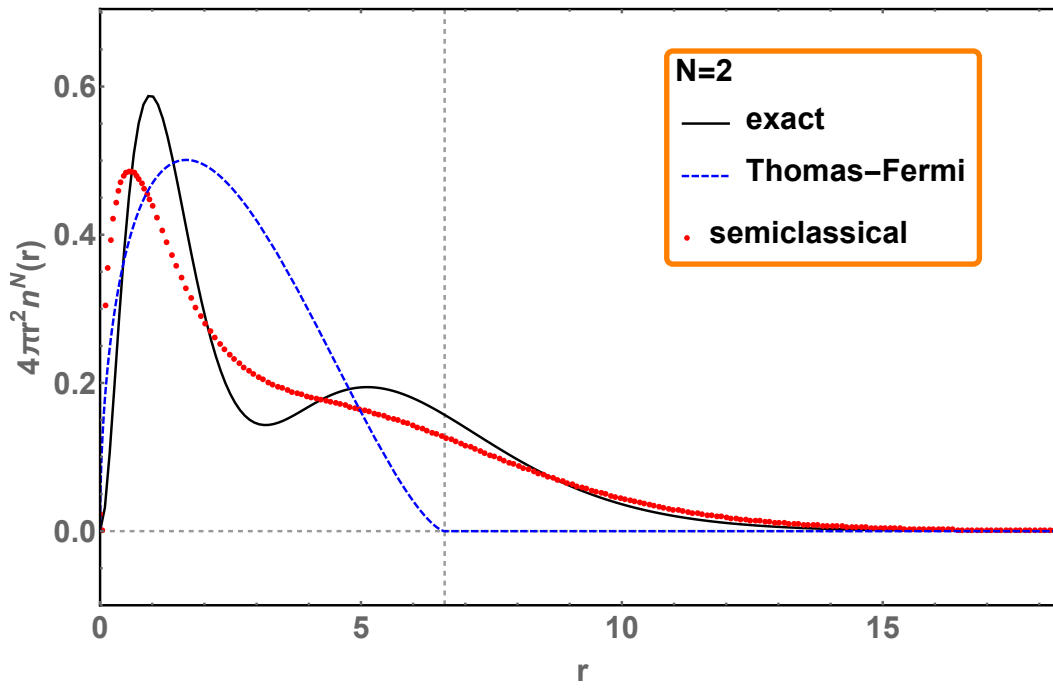


Figure 13. Exact density, TF density (57), and semiclassical density (76) for two particles in a three-dimensional Coulomb potential, $V(r) = -e^2/r$.

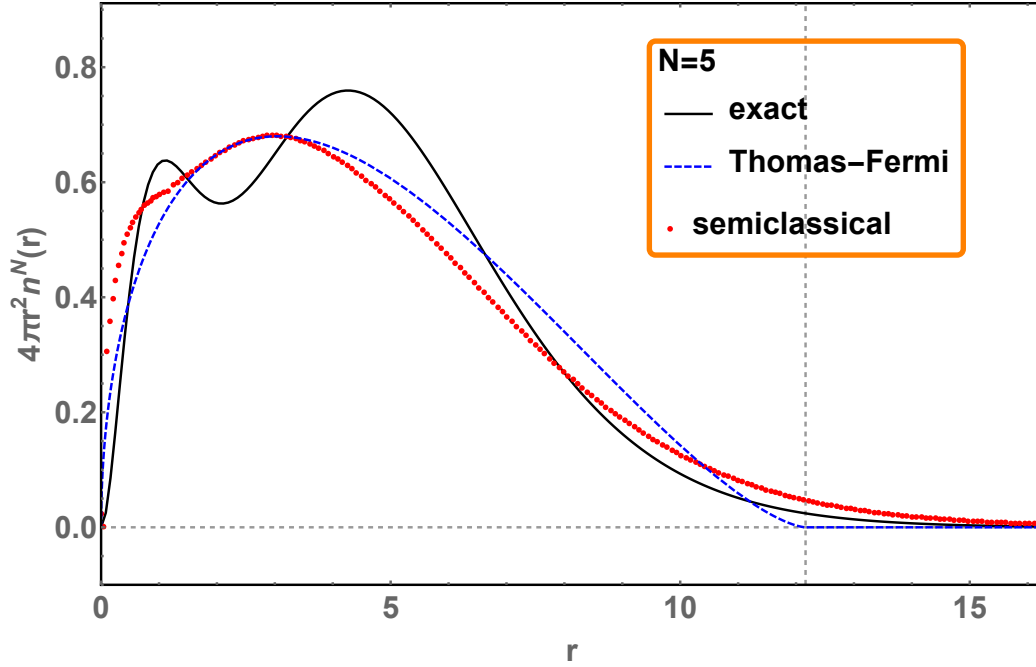


Figure 14. Exact density, TF density (57), and semiclassical density (77) for five particles in a three-dimensional Coulomb potential, $V(r) = -e^2/r$.

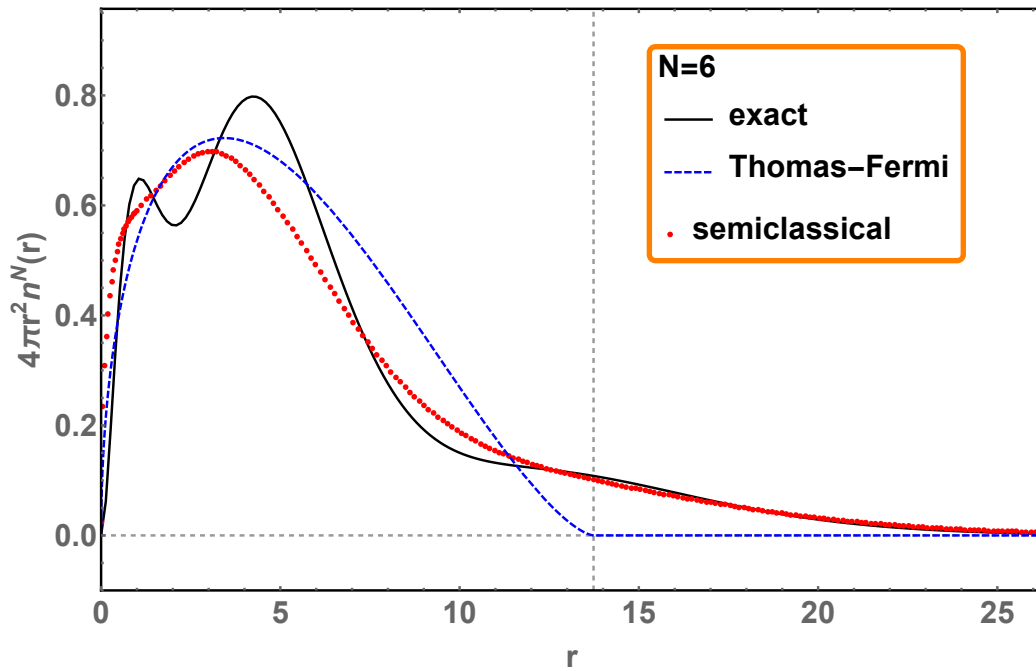


Figure 15. Exact density, TF density (57), and semiclassical density (78) for six particles in a three-dimensional Coulomb potential, $V(r) = -e^2/r$.

Again the semiclassical density gives quite an accurate approximation to the density and is a correction to the TF density, especially in the classically forbidden region.

III.3. Isotropic potentials in two dimensions

III.3.1. Semiclassical wave function for the radial motion

We proceed as in the three-dimensional case by separation of variables in polar coordinates,

$$\psi_{n,l}(s, \phi) = R_{n,l}(s) \frac{e^{il\phi}}{\sqrt{2\pi}}, \quad (79)$$

where n is the principle quantum number, and l is the magnetic quantum number, taking integer values. Let $u_{n,l}(s) = R_{n,l}(s) \sqrt{s}$. We have the radial wave equation for $u_{n,l}(s)$

$$-\frac{\hbar^2}{2m} \frac{d^2 u}{ds^2} + \left(V(s) + \frac{\hbar^2}{2ms^2} \left(l^2 - \frac{1}{4} \right) \right) u = Eu. \quad (80)$$

The normalization condition for $u(s)$ is

$$\int_0^\infty |u(s)|^2 ds = 1. \quad (81)$$

We also employ the same transformation of the s variable by Langer [11] as in the three-dimensional case. The effective potential $\tilde{V}(s) = V(s) + \frac{\hbar^2}{2ms^2} (l^2 - \frac{1}{4})$ should be replaced by

$$\tilde{V}(s) = V(s) + \frac{\hbar^2}{2ms^2} l^2. \quad (82)$$

This gives rise to the JWKB quantization rule for $l \neq 0$

$$\pi \hbar (n_s + 1/2) = \int_{s_1}^{s_2} ds \sqrt{2m \left\{ E - V(s) - \frac{\hbar^2 l^2}{2ms^2} \right\}}, \quad (83)$$

where the integral is taken from one turning point s_1 of the effective potential to another s_2 , and $n_s = 0, 1, 2, \dots$ is the radial quantum number. Again, for the method to work, $s^2 V(s) \rightarrow 0$ when $s \rightarrow 0$.

For $l \neq 0$, the semiclassical wave function in the entire domain is given up to a phase factor by

$$u_{n_s, l}(s) = \sqrt{\frac{2m\omega_{n_s, l}}{p_{n_s, l}(s)}} z_{n_s, l}(s)^{1/4} \text{Ai}(-z_{n_s, l}(s)), \quad (84)$$

with all the involved quantities defined as in the three dimensional case (see (53)).

However, the case $l = 0$ requires special consideration as the centrifugal term becomes a centripetal one and the left turning point for an attractive potential $V(s)$ is at $s = 0$ [5]. The treatment by Berry and Ozorio de Almeida [24] of this case is quite technical, so here we use their results without delving further into the detail. The first one is that equation (83) is still valid for $l = 0$ with the left turning point at $s = 0$.

The energy eigenvalues for harmonic oscillator and Coulomb potentials in two dimensions given by this JWKB quantization rule (derivations similar to Appendix 5) are found to be identical with the exact expressions (see the references in the discussion of the respective example shortly)

$$E_n = -\frac{Z^2 m e^4}{2\hbar^2} \frac{1}{\left(n - \frac{1}{2}\right)^2} = -\frac{Z^2 m e^4}{2\hbar^2} \frac{1}{\left((n_s + |l| + 1) - \frac{1}{2}\right)^2}, \text{ for Coulomb potential,} \quad (85)$$

and

$$E_n = \hbar\omega (n + 1) = \hbar\omega ((2n_s + |l|) + 1), \text{ for harmonic oscillator potential.} \quad (86)$$

The normalized semiclassical wave function for $l = 0$ near $s = 0$ is found to be [24]

$$u_{n_s, l=0}(s) = \sqrt{m\omega_{n_s}} \left(\frac{S_{n_s}(s)}{\hbar p_{n_s}(s)} \right)^{1/2} J_0 \left(\frac{S_{n_s}(s)}{\hbar} \right), \quad (87)$$

where

$$p_{n_s}(s) = \sqrt{2m(E_{n_s} - V(s))}, \quad (88)$$

$$S_{n_s}(s) = \int_0^s \sqrt{2m(E_{n_s} - V(s'))} ds', \quad (89)$$

and

$$\omega_{n_s} = \pi \left[\int_0^{s_2} \frac{m ds}{\sqrt{2m(E_{n_s} - V(s))}} \right]^{-1} = \hbar^{-1} \frac{\partial E_\lambda}{\partial \lambda} \Big|_{\lambda=n_s}. \quad (90)$$

For s near $s = s_2$, the semiclassical wave function is still given in the Airy form like in the case $l \neq 0$ ((84)), with the left turning point $s_1 = 0$.

We combine these two pieces of the semiclassical wave function near each turning point and match them at a mid-phase point s_m , where

$$\frac{1}{2} \pi \hbar (n_s + 1/2) = \int_0^{s_m} ds \sqrt{2m \{E_{n_s} - V(s)\}}. \quad (91)$$

Given that the number of nodes of the wave function is n_s , we add in a phase factor $e^{-in_s\pi}$ for $s < s_m$ as we have done earlier (see page 13). To summarize, we have

$$u_{n_s, l=0}(s) = \begin{cases} e^{-in_s\pi} \sqrt{m\omega_{n_s}} \left(\frac{S_{n_s}(s)/\hbar}{p_{n_s}(s)} \right)^{1/2} J_0 \left(\frac{S_{n_s}(s)}{\hbar} \right), & \text{for } s < s_m \\ \sqrt{\frac{2m\omega_{n_s}}{p_{n_s}(s)}} z_{n_s}(s)^{1/4} \text{Ai}(-z_{n_s}(s)), & \text{for } s > s_m. \end{cases} \quad (92)$$

The piecewise semiclassical radial wave function (92) is an accurate approximation to the exact wave function, as can be seen in figures 16, 17 and 18 below for the first three modes corresponding to $l = 0$ of a two-dimensional harmonic oscillator potential.

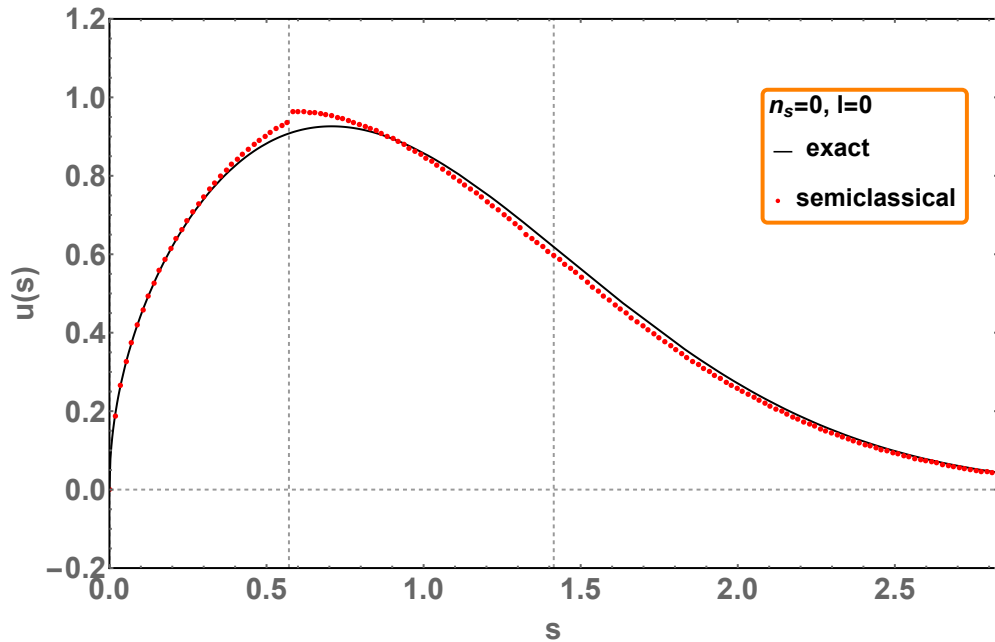


Figure 16. Exact wave function and its semiclassical approximation (92) for mode $n_s = 0, l = 0$ of a two-dimensional harmonic oscillator potential, $V(s) = \frac{1}{2}m\omega^2s^2$, with two vertical gridlines showing respectively s_m and s_2 .

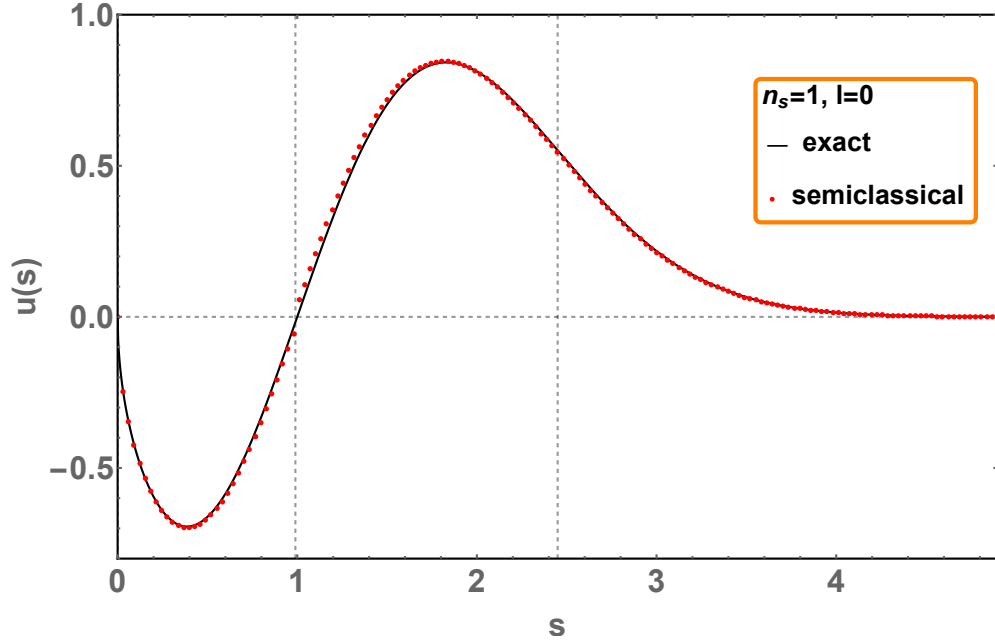


Figure 17. Exact wave function and its semiclassical approximation (92) as in figure 16 but for mode $n_s = 1, l = 0$.

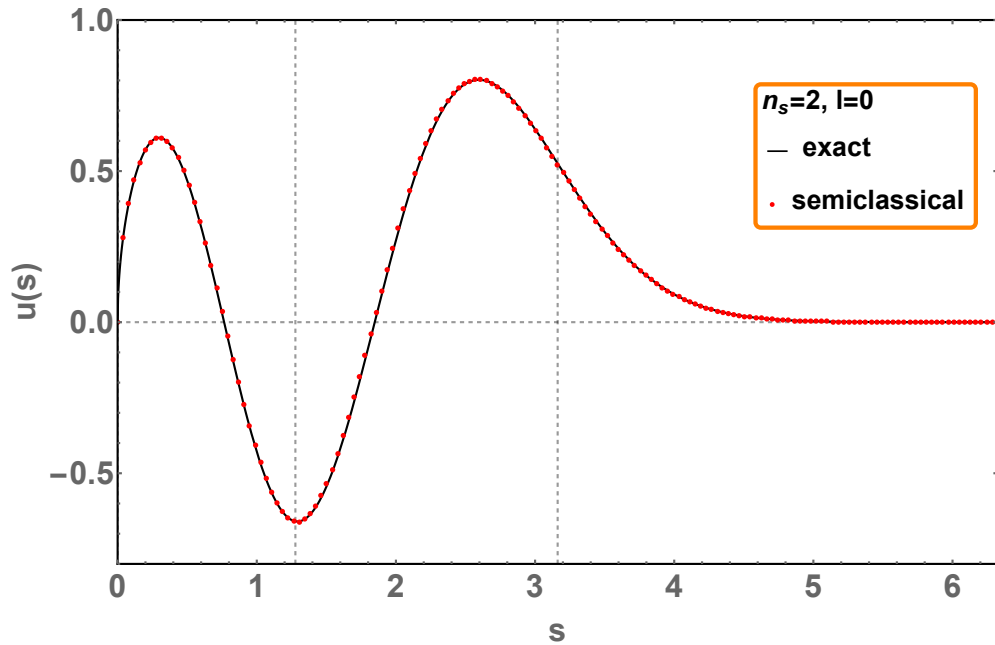


Figure 18. Exact wave function and its semiclassical approximation (92) as in figure 16 but for mode $n_s = 2, l = 0$.

For the moment, we do not see any obvious non-arbitrary way to patch the piecewise semi-

classical radial wave function (92) at the mid-phase point into a continuous function. However, the discontinuity at s_m in figure 16 is much less pronounced in figures 17 and 18 for higher modes, where the semiclassical approximation (92) fits almost perfectly with the exact result.

III.3.2. Radial particle density

We need to evaluate the sum (which we shall call *radial particle density*)

$$n_{N,l}(s) = \sum_{n_s=0}^{N-1} |u_{n_s,l}(s)|^2, \quad (93)$$

where $u_{n_s,l}(s)$ is given by (84) or (92) in order to find the particle density.

We know from the discussion on the three-dimensional case that for $l \neq 0$, and $l = 0$, $s > s_m$, since the semiclassical radial wave function is given in the Airy form, this sum can be approximated by

$$n_{N,l}(s) \simeq \frac{p_{F,l}(s)}{\hbar} \left[\sqrt{z_{F,l}(s)} \text{Ai}^2(-z_{F,l}(s)) + \frac{\text{Ai}'^2(-z_{F,l}(s))}{\sqrt{z_{F,l}(s)}} \right], \quad (94)$$

where the Fermi energy is $E_{N-1/2}$ for a particular value of l .

The semiclassical radial wave function for $l = 0$, $s < s_m$, however, is found to be in the Bessel form. Therefore, we need to find another closed form expression for a semiclassical approximation to the sum $n_{N,l=0}(s)$ when $s < s_m$, which we shall do by emulating the derivation in Appendix 4. We have

$$n_{N,l=0}(s) = \sum_{n_s=0}^{N-1} |u_{n_s,l=0}(s)|^2 = \frac{1}{\hbar} \sum_{n_s=0}^{N-1} \frac{m\omega_{n_s} S_{n_s}(s)}{p_{n_s}(s)} J_0^2\left(\frac{S_{n_s}(s)}{\hbar}\right), \text{ for } s < s_m. \quad (95)$$

This sum can be approximated by an integral, which is the first term in the Poisson summation formula (see Appendices 2 and 4).

$$n_0(s) = \frac{1}{\hbar} \int_{-1/2}^{N-1/2} d\lambda \frac{m\omega_\lambda S_\lambda(s)}{p_\lambda(s)} J_0^2\left(\frac{S_\lambda(s)}{\hbar}\right). \quad (96)$$

Changing the the intergration variable to p_λ , we have

$$n_0(s) = \frac{1}{\hbar} \int_{p_{-1/2}}^{p_{N-1/2}} dp_\lambda \frac{S_\lambda(s)}{\hbar} J_0^2\left(\frac{S_\lambda(s)}{\hbar}\right). \quad (97)$$

Let $f = \frac{p_\lambda}{S_\lambda}$. We have

$$\frac{dp_\lambda}{dS_\lambda} = f + S_\lambda \frac{df}{dS_\lambda}, \quad (98)$$

and $n_0(s)$ becomes

$$\begin{aligned} n_0(s) &= \int_{S_{-1/2}}^{S_{N-1/2}} \frac{dS_\lambda}{\hbar} \left(f + S_\lambda \frac{df}{dS_\lambda} \right) \frac{S_\lambda}{\hbar} J_0^2 \left(\frac{S_\lambda}{\hbar} \right) \\ &= \int_{S_{-1/2}}^{S_{N-1/2}} \frac{dS_\lambda}{\hbar} \frac{df}{dS_\lambda} \frac{S_\lambda^2}{\hbar} J_0^2 \left(\frac{S_\lambda}{\hbar} \right) + \int_{S_{-1/2}}^{S_{N-1/2}} \frac{dS_\lambda}{\hbar} f \frac{S_\lambda}{\hbar} J_0^2 \left(\frac{S_\lambda}{\hbar} \right) \\ &= n_0^1(s) + n_0^2(s), \end{aligned} \quad (99)$$

where we denote the two component integrals in the second last step by $n_0^1(s)$ and $n_0^2(s)$, respectively.

We shall find the leading contribution in the asymptotic approximation to $n_0(s)$ by integration by parts. We have

$$\begin{aligned} n_0^2(s) &= f \frac{1}{2} \left(\frac{S_\lambda}{\hbar} \right)^2 \left[J_0^2 \left(\frac{S_\lambda}{\hbar} \right) + J_1^2 \left(\frac{S_\lambda}{\hbar} \right) \right] \Big|_{S_{-1/2}}^{S_{N-1/2}} \\ &\quad - \int_{S_{-1/2}}^{S_{N-1/2}} dS_\lambda \frac{df}{dS_\lambda} \frac{1}{2} \left(\frac{S_\lambda}{\hbar} \right)^2 \left[J_0^2 \left(\frac{S_\lambda}{\hbar} \right) + J_1^2 \left(\frac{S_\lambda}{\hbar} \right) \right], \end{aligned} \quad (100)$$

where we use the fact that (see [29])

$$\int_0^x t J_0^2(t) dt = \frac{1}{2} x^2 [J_0^2(x) + J_1^2(x)]. \quad (101)$$

We have then

$$\begin{aligned} n_0(s) &= f \frac{1}{2} \left(\frac{S_\lambda}{\hbar} \right)^2 \left[J_0^2 \left(\frac{S_\lambda}{\hbar} \right) + J_1^2 \left(\frac{S_\lambda}{\hbar} \right) \right] \Big|_{S_{-1/2}}^{S_{N-1/2}} \\ &\quad + \int_{S_{-1/2}}^{S_{N-1/2}} dS_\lambda \frac{df}{dS_\lambda} \frac{1}{2} \left(\frac{S_\lambda}{\hbar} \right)^2 \left[J_0^2 \left(\frac{S_\lambda}{\hbar} \right) - J_1^2 \left(\frac{S_\lambda}{\hbar} \right) \right]. \end{aligned} \quad (102)$$

We denote the residual integral in the above equation by $n_0^3(s)$. Neglecting higher order contributions included in the lower limit of integration and $n_0^3(s)$, finally we obtain an asymptotic approximation to the radial density for $l = 0$, $s < s_m$

$$n_{N,l=0}(s) \simeq \frac{p_F(s)}{2} \frac{S_F(s)}{\hbar^2} \left[J_0^2 \left(\frac{S_F(s)}{\hbar} \right) + J_1^2 \left(\frac{S_F(s)}{\hbar} \right) \right], \quad (103)$$

where the Fermi energy is $E_{N-1/2}$. We shall integrate this density to convince ourselves that this is indeed the leading contribution to the sum $n_{N,l=0}(s)$ for $s < s_m$.

The integral of (103) up to s_m is

$$N_0 = \int_0^{s_m} ds \frac{p_F(s)}{2} \frac{S_F(s)}{\hbar^2} \left[J_0^2 \left(\frac{S_F(s)}{\hbar} \right) + J_1^2 \left(\frac{S_F(s)}{\hbar} \right) \right]. \quad (104)$$

A change of the integration variable gives

$$\begin{aligned} N_0 &= \int_{S_F(0)}^{S_F(s_m)} \frac{dS_F(s)}{2} \frac{S_F(s)}{\hbar^2} \left[J_0^2 \left(\frac{S_F(s)}{\hbar} \right) + J_1^2 \left(\frac{S_F(s)}{\hbar} \right) \right] \\ &= \frac{1}{2} \int_{x(0)}^{x(s_m)} x [J_0^2(x) + J_1^2(x)] dx, \end{aligned} \quad (105)$$

where $x(s) = S_F(s)$ and $x(0) = 0$.

We have

$$\int^x t J_1^2(t) dt = \frac{1}{2} x [x (J_0^2(x) + J_1^2(x)) - 2J_0(x) J_1(x)], \quad (106)$$

so

$$N_0 = \frac{1}{2} x^2 (J_0^2(x) + J_1^2(x)) \Big|_{x=S_F(s_m)/\hbar} - \frac{1}{2} x J_0(x) J_1(x) \Big|_{x=S_F(s_m)/\hbar}, \quad (107)$$

where (see (91))

$$S_F(s_m) = \frac{1}{2} \pi \hbar N. \quad (108)$$

For large particle number N , by an asymptotic expansion for large argument of the Bessel functions (see [31]), we have

$$\begin{aligned} N_0 &\simeq \frac{x}{\pi} \left[\cos^2 \left(x - \frac{\pi}{4} \right) + \cos^2 \left(x - \frac{\pi}{2} - \frac{\pi}{4} \right) \right] \Big|_{x=S_F(s_m)/\hbar} \\ &\quad - \frac{1}{\pi} \cos \left(x - \frac{\pi}{4} \right) \cos \left(x - \frac{\pi}{2} - \frac{\pi}{4} \right) \Big|_{x=S_F(s_m)/\hbar} \\ &\simeq \frac{N}{2}. \end{aligned} \quad (109)$$

This gives us half the total particle number, in addition to another $\frac{N}{2}$ from the integral $\int_{s_m}^{\infty} n_{N,l=0}(s) ds$. This shows that the semiclassical approximation to $n_{N,l=0}(s)$ is

$$n_{N,l=0}(s) \simeq \begin{cases} \frac{p_F(s)}{2} \frac{S_F(s)}{\hbar^2} \left[J_0^2 \left(\frac{S_F(s)}{\hbar} \right) + J_1^2 \left(\frac{S_F(s)}{\hbar} \right) \right], & \text{for } s < s_m, \\ \frac{p_F(s)}{\hbar} \left[\sqrt{z_F(s)} \text{Ai}^2(-z_F(s)) + \frac{\text{Ai}'^2(-z_F(s))}{\sqrt{z_F(s)}} \right], & \text{for } s > s_m. \end{cases} \quad (110)$$

However, there is a possible discontinuity at the matching point, as can be seen in figure 19 for the radial density $n_{N=2,l=0}(s)$ corresponding to the first two orbitals with $l=0$ of a two-dimensional harmonic oscillator potential.

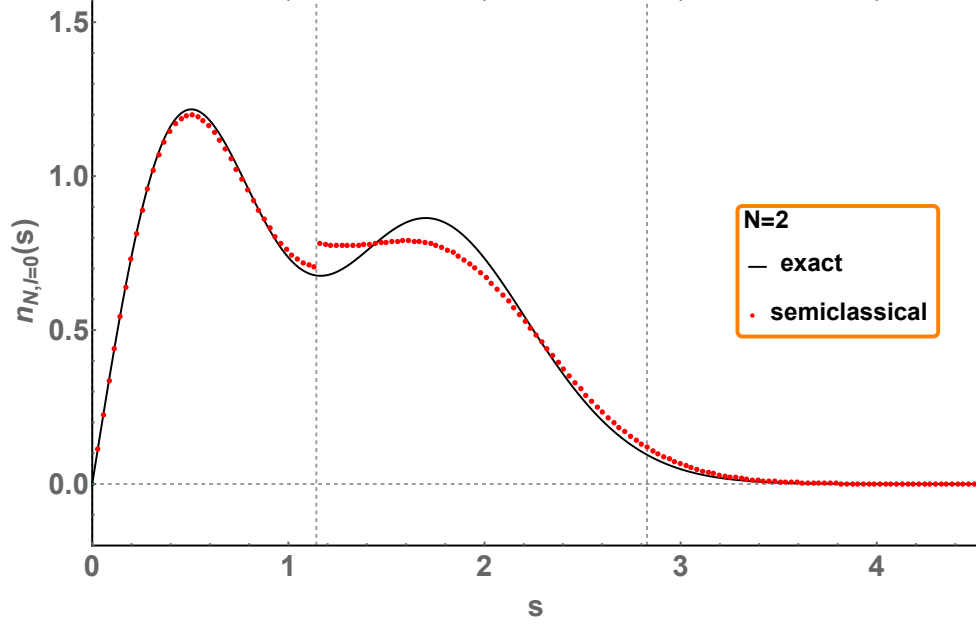


Figure 19. Exact radial density and semiclassical radial density 110 for the first two orbitals with $l = 0$ of a two-dimensional harmonic oscillator potential, $V(s) = \frac{1}{2}m\omega^2 s^2$.

This happens because the semiclassical wave function near each turning point is in a different form. What we have done so far is only considering the leading contribution to the semiclassical approximation of the sum $n_{N,l}(s)$. If we can extract higher order contribution, the semiclassical radial wave function will approach the exact result and therefore tends to be continuous at the mid-phase point. We shall do this by using the full expression of the semiclassical density as in (25) for $s > s_m$ and extracting higher contribution from the integral in (102).

Integrating by parts with the help of (101) and (106), we have

$$\begin{aligned}
 n_0^3(s) &= \int_{S_{-1/2}}^{S_{N-1/2}} dS_\lambda \frac{df}{dS_\lambda} \frac{1}{2} \left(\frac{S_\lambda}{\hbar} \right)^2 \left[J_0^2 \left(\frac{S_\lambda}{\hbar} \right) - J_1^2 \left(\frac{S_\lambda}{\hbar} \right) \right] \\
 &\simeq \frac{df}{dS_\lambda} \frac{S_\lambda}{2} \frac{S_\lambda}{\hbar} J_0 \left(\frac{S_\lambda}{\hbar} \right) J_1 \left(\frac{S_\lambda}{\hbar} \right) \Big|_{\lambda=N-1/2} + \dots
 \end{aligned} \tag{111}$$

As $S_\lambda(s)$ is given by (89), we have

$$\begin{aligned}
\frac{df}{dS_\lambda} &= \frac{1}{S_\lambda} \frac{dp_\lambda}{dS_\lambda} - \frac{p_\lambda}{S_\lambda^2} \\
&= \frac{1}{S_\lambda} \frac{dp_\lambda}{dE_\lambda} \left(\frac{dS_\lambda}{dE_\lambda} \right)^{-1} - \frac{p_\lambda}{S_\lambda^2} \\
&= \frac{1}{S_\lambda} \frac{m}{p_\lambda} \left[\int_0^s \frac{m}{p_\lambda(s')} ds' \right]^{-1} - \frac{p_\lambda}{S_\lambda^2}.
\end{aligned} \tag{112}$$

So,

$$n_0^3(s) \simeq \frac{1}{2\hbar} \left[\frac{S_\lambda}{p_\lambda} \left(\int_0^s \frac{ds'}{p_\lambda(s')} \right)^{-1} - p_\lambda \right] J_0 \left(\frac{S_\lambda}{\hbar} \right) J_1 \left(\frac{S_\lambda}{\hbar} \right) \Big|_{\lambda=N-1/2} + \dots \tag{113}$$

Hence, a better approximation to $n_{N,l=0}(s)$ than (110) is given by

$$\begin{aligned}
n_{N,l=0}(s) &\simeq \frac{p_F(s)}{2} \frac{S_F(s)}{\hbar^2} \left[J_0^2 \left(\frac{S_F(s)}{\hbar} \right) + J_1^2 \left(\frac{S_F(s)}{\hbar} \right) \right] \\
&\quad + \frac{1}{2\hbar} \left[\frac{S_F(s)}{p_F(s)} \left(\int_0^s \frac{ds'}{p_F(s')} \right)^{-1} - p_F(s) \right] J_0 \left(\frac{S_F(s)}{\hbar} \right) J_1 \left(\frac{S_F(s)}{\hbar} \right), \text{ for } s < s_m,
\end{aligned} \tag{114}$$

and

$$\begin{aligned}
n_{N,l=0}(s) &\simeq \frac{p_F(s)}{\hbar} \left[\left(\sqrt{z} \text{Ai}^2(-z) + \frac{\text{Ai}'^2(-z)}{\sqrt{z}} \right) \right. \\
&\quad \left. + \left(\frac{\hbar m \omega_F}{p_F^2(s)} \csc(\alpha_F(s)) - \frac{1}{2z^{3/2}} \right) \text{Ai}(-z) \text{Ai}'(-z) \right] \Big|_{z=z_F(s)}, \text{ for } s > s_m.
\end{aligned} \tag{115}$$

Now the discontinuity is less visible for the above-mentioned density

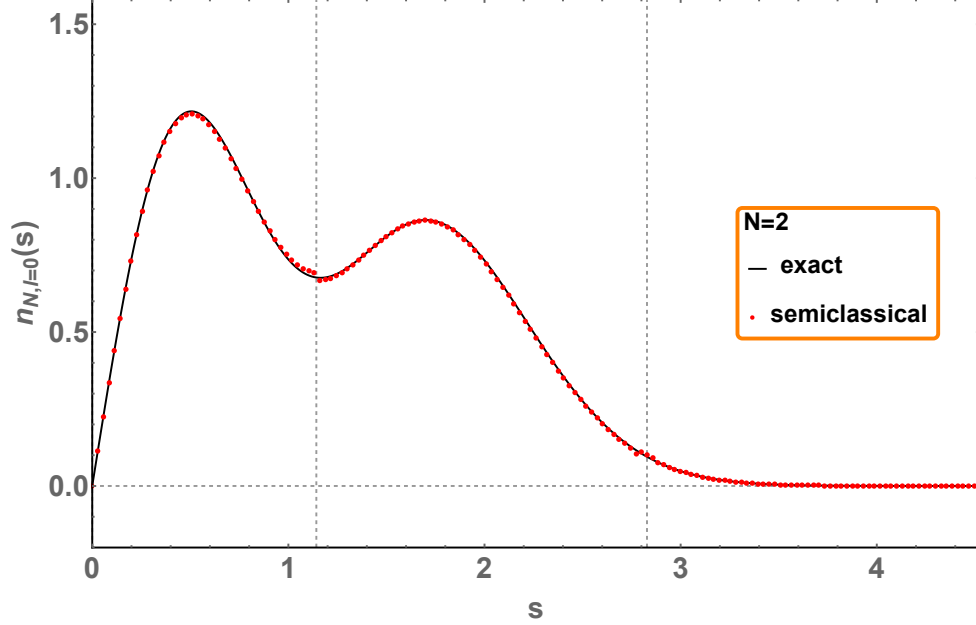


Figure 20. Exact radial density and semiclassical radial density, (114) and (115), for the first two orbitals with $l = 0$ of a two-dimensional harmonic oscillator potential, $V(s) = \frac{1}{2}m\omega^2 s^2$.

Now, we are in a position to find the density for some particular total numbers of particles. We illustrate this by the two-dimensional harmonic oscillator and Coulomb potentials.

III.3.3. TF density in two dimensions

The TF particle density for spin-polarized fermions in two dimensions is given by [1]

$$n^{\text{TF}}(\mathbf{r}) = \frac{p_{\text{F}}(\mathbf{r})^2}{4\pi\hbar^2} \quad (116)$$

in the classically allowed region and zero elsewhere. The classical momentum $p_{\text{F}}(\mathbf{r})$ is given by

$$p_{\text{F}}(\mathbf{r}) = \sqrt{2m(E_{\text{F}} - V(\mathbf{r}))}. \quad (117)$$

The Fermi energy E_{F} is chosen such that $n^{\text{TF}}(\mathbf{r})$ is normalized to the total particle number N . For isotropic potentials, the normalization condition reads

$$\int_0^{\infty} 2\pi s \, ds \, n^{\text{TF}}(s) = N. \quad (118)$$

III.3.4. Two-dimensional harmonic oscillator potential

The exact radial wave function for the two-dimensional potential

$$V(s) = \frac{1}{2}m\omega^2s^2 \quad (119)$$

is found to be (see [26])

$$u_{n_sl}(s) = \sqrt{2\gamma s} \sqrt{\frac{n_s!}{(n_s + |l|)!}} (\gamma s^2)^{|l|/2} \exp(-\gamma s^2/2) L_{n_s}^{|l|}(\gamma s^2), \quad (120)$$

where $\gamma = \frac{m\omega}{\hbar}$ and $n = 2n_s + |l|$. So for a particular value of $n = 0, 1, 2, 3, \dots$, l takes value $-n, -n + 2, -n + 4, \dots, n - 2, n$. For spin-polarized systems, the degeneracy of the energy eigenvalue E_n (86) is then

$$j_n = n + 1. \quad (121)$$

Table III. Orbitals corresponding to the first four values of the principal quantum number for the two-dimensional harmonic oscillator potential.

n	n_s	l	j_n
0	0	0	1
1	0	± 1	2
2	1	0	3
	0	± 2	
3	1	± 1	4
	0	± 3	

The orbitals corresponding to the first four values of the principal quantum number are tabulated in table IV. With $n_{N,l}$ given collectively by (114), (115), and (94), the particle density $n^N(s)$ for $N = 1, 3, 6, 10$ is given by

$$n^1(s) = \frac{1}{2\pi s} [n_{1,0}(s)], \quad (122)$$

$$n^3(s) = \frac{1}{2\pi s} [n_{1,0}(s) + 2n_{1,1}(s)], \quad (123)$$

$$n^6(s) = \frac{1}{2\pi s} [n_{2,0}(s) + 2n_{1,1}(s) + 2n_{1,2}(s)], \quad (124)$$

$$n^{10}(s) = \frac{1}{2\pi s} [n_{2,0}(s) + 2n_{2,1}(s) + 2n_{1,2}(s) + 2n_{1,3}(s)]. \quad (125)$$

Figures 21, 22, and 23 show the exact density, TF density, and semiclassical density for $N = 1, 3, 6$ particles in a two-dimensional harmonic oscillator potential. Except for a few cusps where we connect the particle density in Bessel and Airy forms or near the turning points where we choose to truncate the series expansion of the density, the semiclassical result correlates well with the exact result.

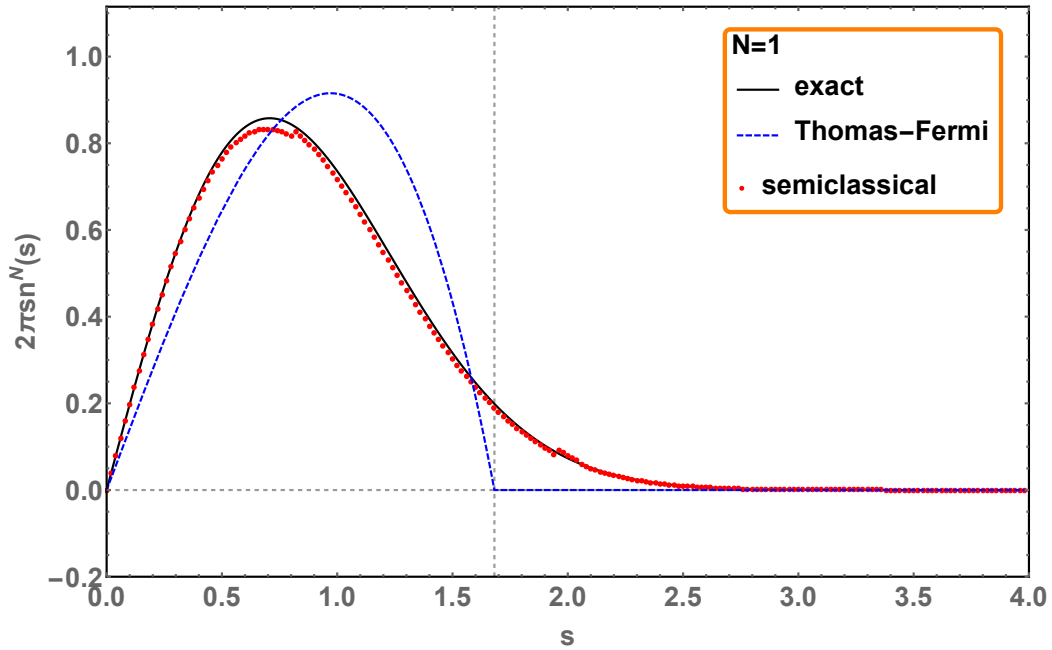


Figure 21. Exact density, TF density (116), and semiclassical density (122) for one particle in a two-dimensional harmonic oscillator potential, $V(s) = \frac{1}{2}m\omega^2 s^2$.

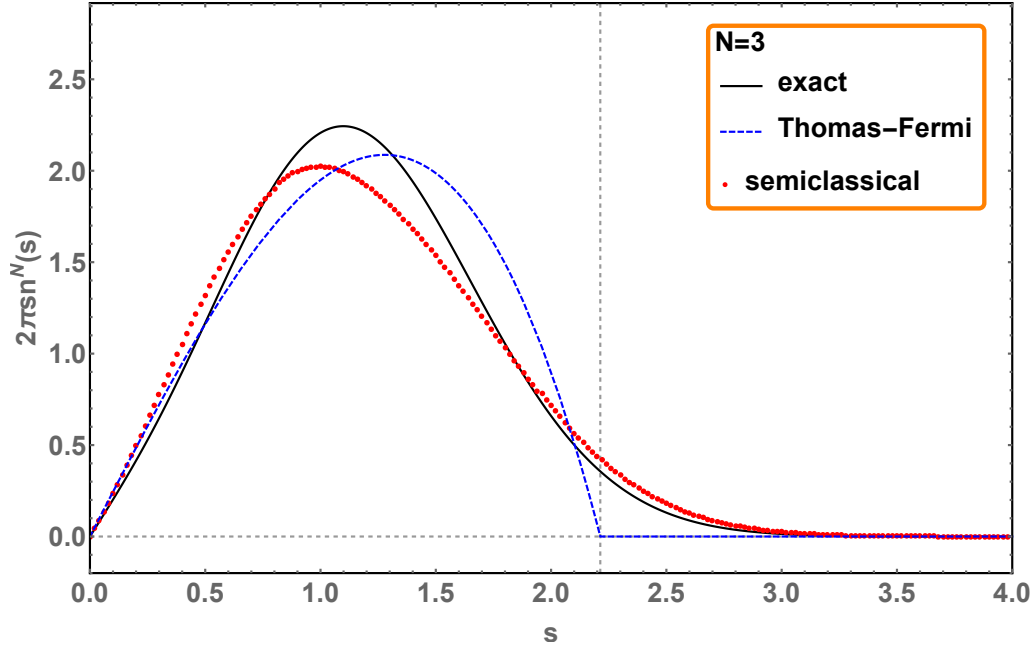


Figure 22. Exact density, TF density (116), and semiclassical density (123) for three particles in a two-dimensional harmonic oscillator potential, $V(s) = \frac{1}{2}m\omega^2 s^2$.

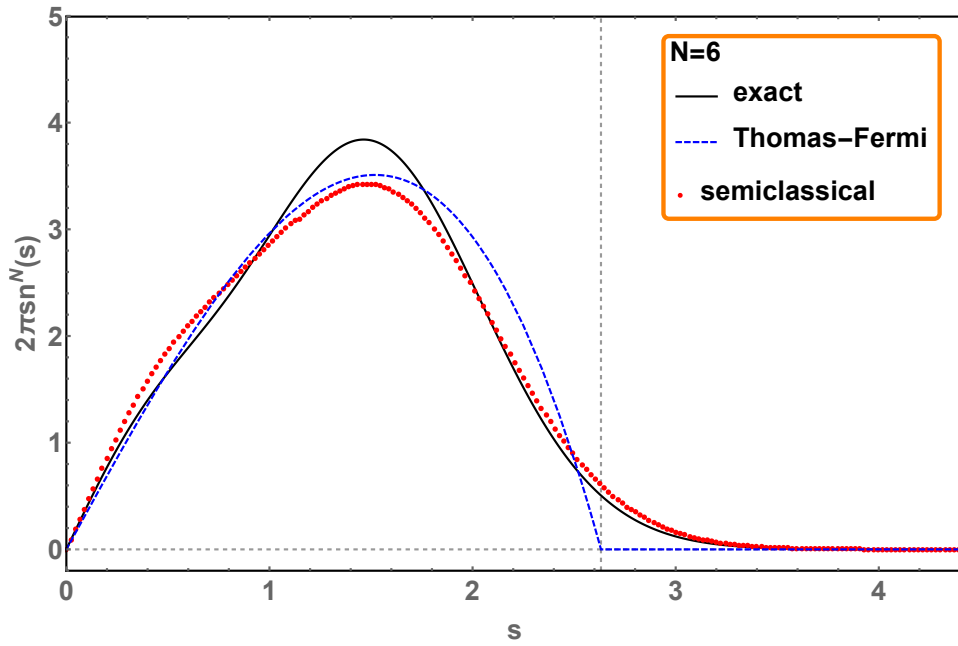


Figure 23. Exact density, TF density (116), and semiclassical density (124) for six particles in a two-dimensional harmonic oscillator potential, $V(s) = \frac{1}{2}m\omega^2 s^2$.

III.3.5. Two-dimensional Coulomb potential

The exact normalized radial wave function for the two-dimensional Coulomb potential

$$V(s) = -\frac{e^2}{s} \quad (126)$$

is found to be (see [32] or [33], but beware of the many misprints in the latter)

$$u_{n_s, l}(s) = \frac{1}{\left(n - \frac{1}{2}\right) \sqrt{a}} \sqrt{\frac{(n - |l| - 1)!}{(n + |l| - 1)!}} \times \left(\frac{2s}{\left(n - \frac{1}{2}\right) a}\right)^{|l|+1/2} e^{-s/(n-1/2)a} L_{n-|l|-1}^{2|l|} \left(\frac{2s}{\left(n - \frac{1}{2}\right) a}\right), \quad (127)$$

where $n = n_s + |l| + 1$ and $a = \frac{\hbar^2}{me^2}$. So, for a particular value of $n = 1, 2, 3, \dots$, $|l|$ can take value $0, 1, 2, \dots, n - 1$. The energy eigenvalues are given by (85).

For spin-polarized systems, the degeneracy of the energy eigenvalue E_n is

$$j_n = 2n - 1. \quad (128)$$

We tabulate the orbitals corresponding to the first three values of the principal quantum number for the two-dimensional Coulomb potential in table IV.

Table IV. Orbitals corresponding to the first three values of the principal quantum number for the two-dimensional Coulomb potential.

n	n_s	l	j_n
1	0	0	1
2	1	0	3
	0	± 1	
3	2	0	5
	1	± 1	
	0	± 2	

Denoting $n^N(s)$ as the semiclassical density for a system of N particles and $n_{N,l}(s)$ as the semiclassical approximation to the sum

$$\sum_{n_s=0}^{N-1} |u_{n_s, l}(s)|^2, \quad (129)$$

we have

$$n^1(s) = \frac{1}{2\pi s} n_{1,0}(s), \quad (130)$$

$$n^4(s) = \frac{1}{2\pi s} [n_{2,0}(s) + 2n_{1,1}(s)], \quad (131)$$

$$n^9(s) = \frac{1}{2\pi s} [n_{3,0}(s) + 2n_{2,1}(s) + 2n_{1,2}(s)]. \quad (132)$$

For the two-dimensional Coulomb potential, the effective potential has a singularity at $s = 0$. This makes the asymptotic approximation (114) to the radial density near $s = 0$ for $l = 0$, which is in Bessel form, no longer valid as it tends to a definite limit when $s \rightarrow 0$, while the correct behavior should be a rapid decrease to 0. Until we have a better way to extract the leading contribution to the radial density near $s = 0$, we shall sum the modulus square of the piecewise semiclassical wave functions (92) for the case $l = 0$. As we can see in figure 24 for mode $n_s = 2, l = 0$ of a two-dimensional Coulomb potential, the piecewise semiclassical wave function (92) is still valid as it tends to zero when $s \rightarrow 0$.

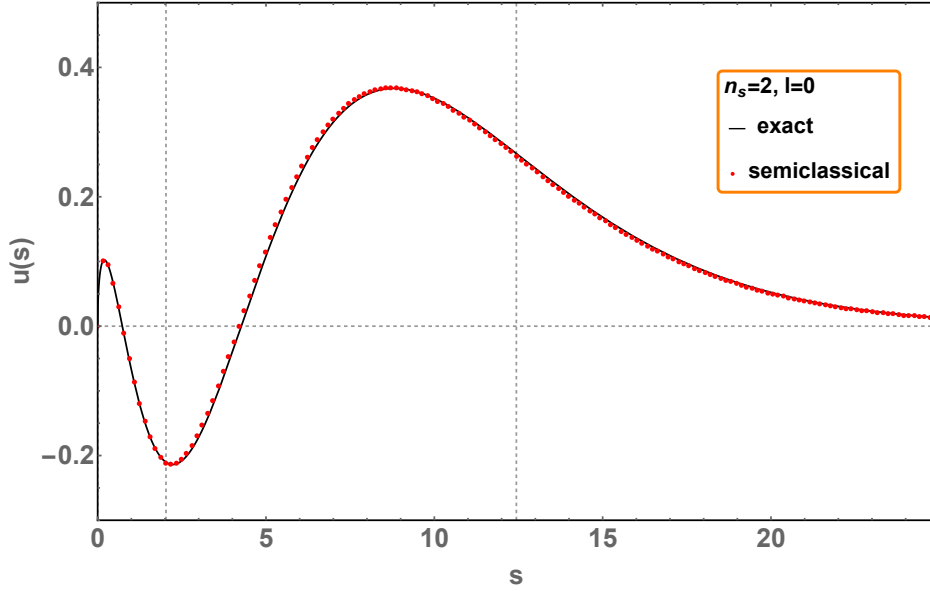


Figure 24. Exact wave function and its semiclassical approximation (92) for mode $n_s = 2, l = 0$ of a two-dimensional Coulomb potential, $V(s) = -e^2/s$, with two vertical gridlines showing s_m and s_2 respectively.

Figures 25, 26, and 27 compare the particle densities by various methods for $N = 1, 4, 9$ particles in a two-dimensional Coulomb potential.

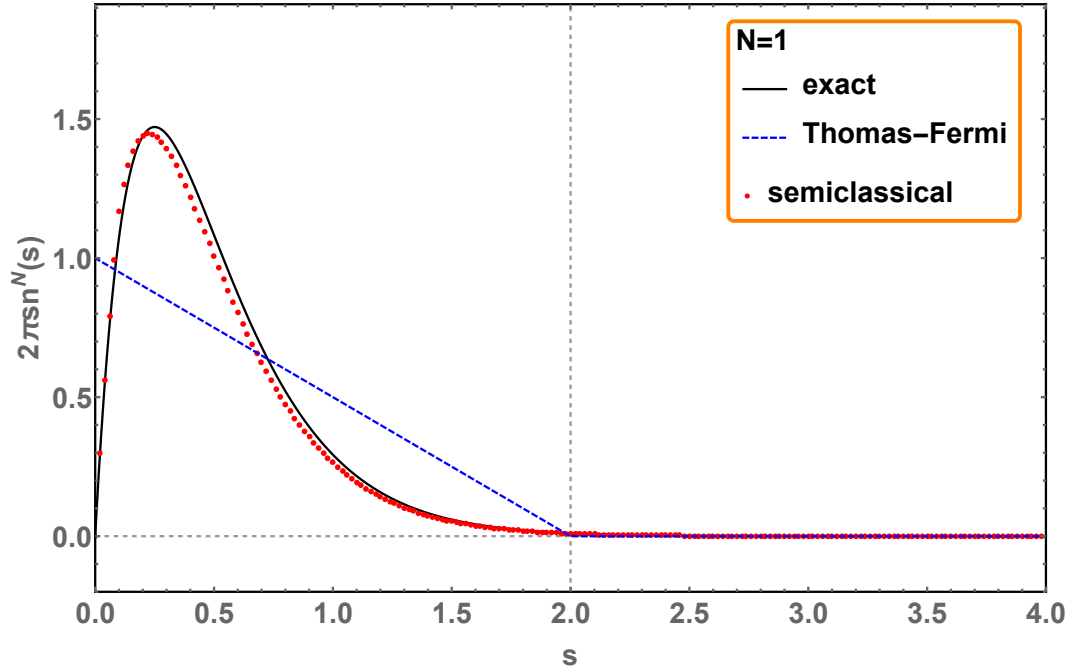


Figure 25. Exact density, TF density (116), and semiclassical density (130) for one particle in a two-dimensional Coulomb potential, $V(s) = -e^2/s$.

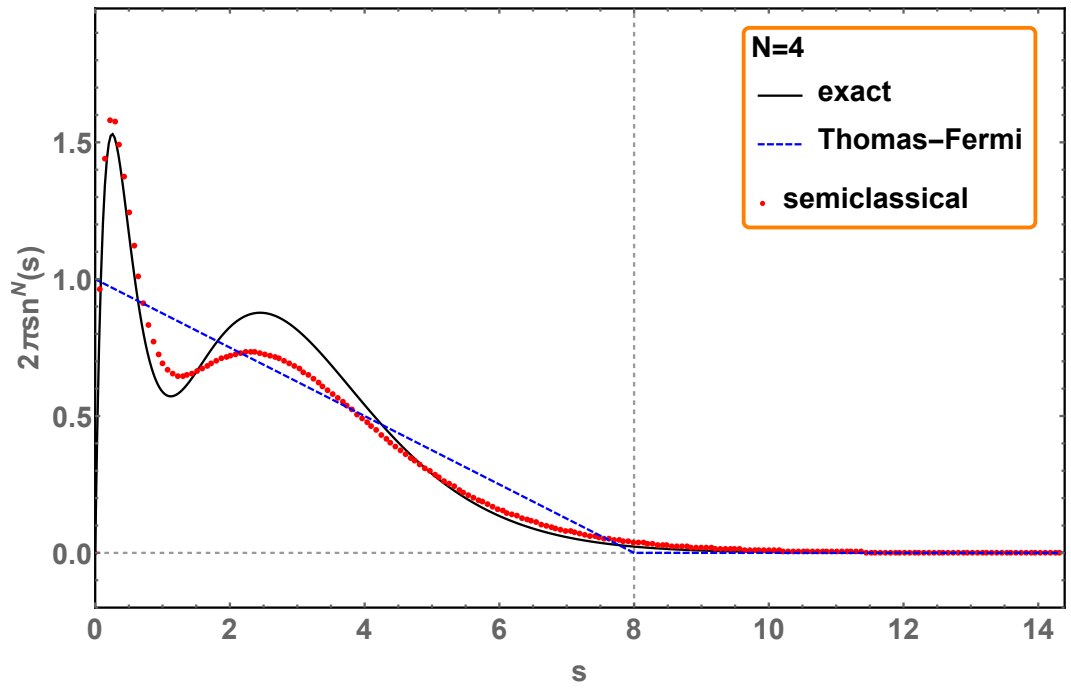


Figure 26. Exact density, TF density (116), and semiclassical density (131) for four particles in a two-dimensional Coulomb potential, $V(s) = -e^2/s$.

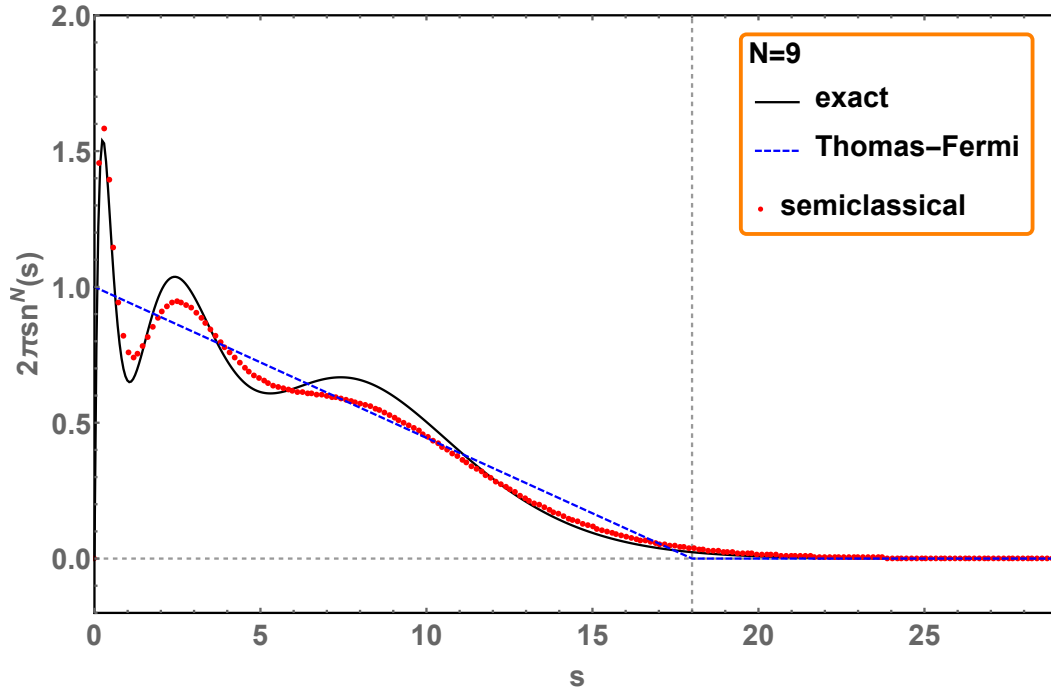


Figure 27. Exact density, TF density (116), and semiclassical density (132) for nine particles in a two-dimensional Coulomb potential, $V(s) = -e^2/s$.

The semiclassical density approximates the exact result very well. It especially catches the vanishing of the density near $s = 0$ where the TF density fails.

IV. A NEW APPROACH TO FINDING A SEMICLASSICAL PARTICLE DENSITY

IV.1. Introduction

In the previous sections, we have discussed the semiclassical density result by Ribeiro *et al.* [10] and how we can generalize it to isotropic potentials in higher dimensions. This generalization is possible because these problems can be reduced to a one-dimensional problem, where we know how to connect the semiclassical wave function from different turning points. In a more general setting, this is not as obvious. Moreover, the procedure does not come without limitations. We have only been able to find the closed form expression for the leading contribution to the density of fully filled shells. These are the cases when the density depends only on the distance from the origin. We even encounter the special case of $l = 0$ in two dimensions, where the semiclassical wave function near $s = 0$ is in a different form from its Airy form near the right turning point. We have not patched the two pieces of the semiclassical wave function into a continuous function in a satisfactory manner. With all these limitations, we want, therefore, a method that can be more easily generalized to higher dimensions.

This section is dedicated to that purpose. We propose a formula for particle density involving the propagator in the Feynman path integral formalism. With suitable approximations of the propagator and the integrals involved, we aim at deducing the same leading term in the particle density as given by (27). The propagator is well defined for higher dimensions, which perhaps gives us some insights into how we can resolve our connection problem and arrive at a method with a higher degree of generalization. Such a method may also prove useful in understanding the classical-quantum connection.

IV.2. Particle density

Suppose a single-particle Hamiltonian \hat{H} has the eigenstates denoted by $|\psi_k\rangle$ with the corresponding energy eigenvalues E_k . The eigenstates satisfy the completeness relation (see [34])

$$\sum_k |\psi_k\rangle \langle \psi_k| = \mathbb{1}. \quad (133)$$

The particle density at a point x of a system of N non-interacting fermions, described by the single-particle Hamiltonian \hat{H} is given by

$$n(x) = \sum_{k, E_k < \mu} |\psi_k(x)|^2, \quad (134)$$

where we sum all the orbitals with energy lower than the Fermi energy $\mu \equiv \mu(N)$. It follows that

$$\begin{aligned} n(x) &= \sum_k \eta(\mu - E_k) |\psi_k(x)|^2 \\ &= \sum_k \int_{-\infty}^{\mu} d\lambda \delta(\lambda - E_k) |\psi_k(x)|^2, \end{aligned} \quad (135)$$

where in the last step, we use the integral representation in terms of the Dirac delta function of the Heaviside step function

$$\eta(\mu - E_k) = \int_{-\infty}^{\mu} d\lambda \delta(\lambda - E_k). \quad (136)$$

With the integral representation of the Dirac delta function [31]

$$\delta(\lambda - E_k) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt \exp[i(\lambda - E_k)t/\hbar], \quad (137)$$

the density can be expressed as

$$\begin{aligned} n(x) &= \sum_k \int_{-\infty}^{\mu} d\lambda \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt \exp[i(\lambda - E_k)t/\hbar] |\psi_k(x)|^2 \\ &= \int_{-\infty}^{\mu} d\lambda \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dt \exp(i\lambda t/\hbar) \sum_k \exp(-iE_k t/\hbar) |\psi_k(x)|^2 \\ &= \int_{-\infty}^{\mu} d\lambda \frac{1}{2\pi\hbar} I(\lambda; x), \end{aligned} \quad (138)$$

where $I(\lambda; x)$ is given by

$$\begin{aligned} I(\lambda; x) &= \int_{-\infty}^{\infty} dt \exp(i\lambda t/\hbar) \sum_k \exp(-iE_k t/\hbar) |\psi_k(x)|^2 \\ &= 2\text{Re} \left\{ \int_0^{\infty} dt \exp(i\lambda t/\hbar) \sum_k \exp(-iE_k t/\hbar) |\psi_k(x)|^2 \right\}. \end{aligned} \quad (139)$$

For positive t , the sum

$$\sum_k \exp(-iE_k t/\hbar) |\psi_k(x)|^2$$

is the propagator $K(x, x; t) = \lim_{x' \rightarrow x} K(x', x; t)$ from the point x back to itself in time t (see [35]). So the density is given by

$$n(x) = \frac{1}{\pi\hbar} \text{Re} \int_{-\infty}^{\mu} d\lambda \int_0^{\infty} dt \exp(i\lambda t/\hbar) K(x, x; t). \quad (140)$$

The three-dimensional analog can be easily deduced

$$n(\mathbf{r}) = \frac{1}{\pi\hbar} \text{Re} \int_{-\infty}^{\mu} d\lambda \int_0^{\infty} dt \exp(i\lambda t/\hbar) K(\mathbf{r}, \mathbf{r}; t). \quad (141)$$

We might want to evaluate the integral over time t or both integrals, respectively, for the propagator $K(\mathbf{r}', \mathbf{r}; t)$ before taking the limit $\mathbf{r}' \rightarrow \mathbf{r}$.

IV.3. Quantum propagator: van Vleck-Gutzwiller formula

The propagator $K(\mathbf{r}', \mathbf{r}; t' - t)$ in quantum mechanics is defined as the transition amplitude between the state $|\mathbf{r}, t\rangle$ and $|\mathbf{r}', t'\rangle$. Assuming the Hamiltonian \hat{H} governing the time evolution has no explicit time dependence so that the unitary time evolution operator is $\exp(-i\hat{H}t/\hbar)$, we have

$$K(\mathbf{r}', \mathbf{r}; t' - t) = \langle \mathbf{r}', t' | \mathbf{r}, t \rangle = \langle \mathbf{r}' | \exp(-i\hat{H}(t' - t)/\hbar) | \mathbf{r} \rangle. \quad (142)$$

Inserting the completeness relation (133), we have

$$\begin{aligned} K(\mathbf{r}', \mathbf{r}; t' - t) &= \sum_k \langle \mathbf{r}' | \exp(-i\hat{H}(t' - t)/\hbar) | \psi_k \rangle \langle \psi_k | \mathbf{r} \rangle \\ &= \sum_k \exp(-iE_k(t' - t)/\hbar) \psi_k^*(\mathbf{r}') \psi_k(\mathbf{r}). \end{aligned} \quad (143)$$

This completes the proof for the particle density formula (141). By the completeness relation of the eigenstates of the position operator, the propagator satisfies the convolution relation

$$K(\mathbf{r}_2, \mathbf{r}_0; t_2 - t_0) = \int K(\mathbf{r}_2, \mathbf{r}_1; t_2 - t_1) K(\mathbf{r}_1, \mathbf{r}_0; t_1 - t_0) d\mathbf{r}_1. \quad (144)$$

This convolution relation is the key of the Feynman path integral formalism (see [35]), in which the propagator for a finite transition time can be found by dividing the time in small sections of length δt and integrating the product of the propagators for these short transitions over all possible intermediate positions. The path integral formalism provides an interesting link between classical and quantum mechanics. As we shall see shortly, the

propagator contains the classical action or the Hamilton principal function measured in \hbar in its phase factor.

Consider the propagator $K(\mathbf{r}_2, \mathbf{r}_1, \delta t)$ connecting two points \mathbf{r}_1 and \mathbf{r}_2 in an infinitesimal time δt . We have

$$\begin{aligned} K(\mathbf{r}_2, \mathbf{r}_1; \delta t) &= \langle \mathbf{r}_2 | \exp\left(-i\hat{H}\delta t/\hbar\right) | \mathbf{r}_1 \rangle \\ &= \int d\mathbf{p} \langle \mathbf{r}_2 | \mathbf{p} \rangle \langle \mathbf{p} | \exp\left(-i\hat{H}\delta t/\hbar\right) | \mathbf{r}_1 \rangle, \end{aligned} \quad (145)$$

where we invoke the completeness relation for the eigenstates $|\mathbf{p}\rangle$ of the momentum operator $\hat{\mathbf{p}}$. Assume the Hamiltonian is of the form $\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{r}})$. For a small time δt , we may keep the first term in the *Baker-Campbell-Hausdorff* series expansion of $\exp\left(-i\hat{H}\delta t/\hbar\right)$, see [36]. We have

$$\exp\left(-i\hat{H}\delta t/\hbar\right) \simeq \exp\left(-i\frac{\hat{\mathbf{p}}^2}{2m}\frac{\delta t}{\hbar}\right) \exp\left(-iV(\hat{\mathbf{r}})\frac{\delta t}{\hbar}\right). \quad (146)$$

As a result, we may replace the Hamiltonian operator by its classical counterpart

$$\begin{aligned} K(\mathbf{r}_2, \mathbf{r}_1; \delta t) &\simeq \int d\mathbf{p} \langle \mathbf{r}_2 | \mathbf{p} \rangle \langle \mathbf{p} | \mathbf{r}_1 \rangle \exp(-iH(\mathbf{p}, \mathbf{r})\delta t/\hbar) \\ &= \int d\mathbf{p} \langle \mathbf{r}_2 | \mathbf{p} \rangle \langle \mathbf{p} | \mathbf{r}_1 \rangle \exp\left(-i\frac{\mathbf{p}^2}{2m}\frac{\delta t}{\hbar}\right) \exp\left(-iV(\mathbf{r}_1)\frac{\delta t}{\hbar}\right). \end{aligned} \quad (147)$$

With the momentum eigenstate in position representation

$$\langle \mathbf{r}_2 | \mathbf{p} \rangle = \left(\frac{1}{\sqrt{2\pi\hbar}}\right)^3 \exp\left(i\frac{\mathbf{p} \cdot \mathbf{r}_2}{\hbar}\right), \quad (148)$$

we have

$$K(\mathbf{r}_2, \mathbf{r}_1; \delta t) \simeq \int d\mathbf{p} \left(\frac{1}{2\pi\hbar}\right)^3 \exp\left(i\frac{\mathbf{p} \cdot (\mathbf{r}_2 - \mathbf{r}_1)}{\hbar}\right) \exp\left(-i\frac{\mathbf{p}^2}{2m}\frac{\delta t}{\hbar}\right) \exp\left(-iV(\mathbf{r}_1)\frac{\delta t}{\hbar}\right). \quad (149)$$

The integral over \mathbf{p} can be done by completing the square and using the Gaussian integral. We obtain hence

$$K(\mathbf{r}_2, \mathbf{r}_1; \delta t) \simeq \left(\sqrt{\frac{m}{2\pi i\hbar\delta t}}\right)^3 \exp\left(i\frac{m}{2\hbar}\frac{(\mathbf{r}_2 - \mathbf{r}_1)^2}{\delta t} - iV(\mathbf{r}_1)\frac{\delta t}{\hbar}\right). \quad (150)$$

With the Lagrangian defined by

$$\mathcal{L}(\mathbf{r}, \dot{\mathbf{r}}) = \frac{m}{2}\dot{\mathbf{r}}^2 - V(\mathbf{r}), \quad (151)$$

we have

$$K(\mathbf{r}_2, \mathbf{r}_1; \delta t) \simeq \left(\sqrt{\frac{m}{2\pi i \hbar \delta t}} \right)^3 \exp\left(i \frac{\delta t}{\hbar} \mathcal{L}(\mathbf{r}_1, \dot{\mathbf{r}}_1) \right), \quad (152)$$

where

$$\dot{\mathbf{r}}_1 = \frac{\mathbf{r}_2 - \mathbf{r}_1}{\delta t}, \quad (153)$$

which is the velocity of the particle in time so small such that the trajectory is essentially that of a free particle.

For a path from \mathbf{r} to \mathbf{r}' in a finite transition time $t' - t$, we may divide the time in n sections of length δt with intermediate points (\mathbf{r}_j, t_j) where

$$\begin{aligned} \mathbf{r}_0 &= \mathbf{r}, \\ \mathbf{r}_n &= \mathbf{r}', \\ t_n - t_0 &= n \delta t = t' - t, \end{aligned} \quad (154)$$

By the convolution relation (144), the propagator between these two end points is given by

$$\begin{aligned} K(\mathbf{r}', \mathbf{r}; t' - t) &= \lim_{n \rightarrow \infty} \int \left(\sqrt{\frac{m}{2\pi i \hbar \delta t}} \right)^{3n} \exp\left(i \sum_{j=0}^{n-1} \delta t \mathcal{L}(\mathbf{r}_j, \dot{\mathbf{r}}_j) \right) d\mathbf{r}_1 d\mathbf{r}_2 \cdots d\mathbf{r}_{n-1} \\ &= \lim_{n \rightarrow \infty} \int \left(\sqrt{\frac{m}{2\pi i \hbar \delta t}} \right)^{3n} \exp\left(i \int_{t_0}^{t_n} dt \mathcal{L}(\mathbf{r}, \dot{\mathbf{r}}) \right) d\mathbf{r}_1 d\mathbf{r}_2 \cdots d\mathbf{r}_{n-1}. \end{aligned} \quad (155)$$

It may be written in a more compact form as

$$K(\mathbf{r}', \mathbf{r}; t' - t) = \int \mathcal{D}\mathbf{r} \exp\left(i \int_t^{t'} dt \mathcal{L}(\mathbf{r}, \dot{\mathbf{r}}) \right), \quad (156)$$

where the integral $\int \mathcal{D}\mathbf{r}$ is called the path integral. The measure $\mathcal{D}\mathbf{r}$ is defined as

$$\mathcal{D}\mathbf{r} = \lim_{n \rightarrow \infty} \left(\sqrt{\frac{m}{2\pi i \hbar \delta t}} \right)^{3n} d\mathbf{r}_1 d\mathbf{r}_2 \cdots d\mathbf{r}_{n-1}. \quad (157)$$

As we can see in formula (156), the propagator is proportional to a phase factor containing the quantity called the *classical action* or the *Hamilton principal function* R , defined by

$$R(\mathbf{r}', \mathbf{r}; t' - t) = \int_t^{t'} dt \mathcal{L}(\mathbf{r}, \dot{\mathbf{r}}), \quad (158)$$

where $\mathbf{r}(t)$ is the trajectory along a certain path. However, in (156), we include all possible paths along which the motion can be carried out between (\mathbf{r}, t) and (\mathbf{r}', t') . This is what is meant by path integral; we integrate over all paths.

In the semiclassical limit, the time, the position, the mass, etc. are so large that the Hamilton principal function is very large compared to \hbar . The phase factor oscillates very rapidly even for a small variation in the path. This leads to cancellation of the phases, except for those paths that are stationary. Along these paths, the Hamilton principal function is nearly a constant, and these are nothing different from the classical orbits. So, the most contribution to the propagator comes from these classical paths

$$K(\mathbf{r}', \mathbf{r}; t' - t) = \sum_{\text{class. paths } j} \mathcal{A}_j \exp\left(\frac{i}{\hbar} R_j(\mathbf{r}', \mathbf{r}; t' - t)\right), \quad (159)$$

with some amplitude \mathcal{A}_j .

van Vleck and Gutzwiller (see [37, 38] and also [5, 13]) found a semiclassical approximation to the propagator in D dimension

$$K_{\text{sc}}(\mathbf{r}', \mathbf{r}; t' - t) = \sum_{\text{class. paths}} (2\pi i \hbar)^{-D/2} \sqrt{|\det C|} \exp\left[\frac{i}{\hbar} R(\mathbf{r}', \mathbf{r}; t' - t) - \frac{i\kappa\pi}{2}\right], \quad (160)$$

where the matrix C is defined by

$$C_{ij}(\mathbf{r}', \mathbf{r}; t' - t) = -\frac{\partial^2 R}{\partial r_i \partial r'_j} \quad (i, j = 1, 2, \dots, D), \quad (161)$$

and κ is obtained by counting the number of times the determinant of C changes sign along the classical path from t to t' .

For small time $t' - t$, we usually have exactly one classical trajectory that connect (\mathbf{r}, t) and (\mathbf{r}', t') . However, there may be more than one classical trajectory for large time $t' - t$.

The formula (160) turns out to be exact for potentials in quadratic form ([5, 13]). It also has an advantage in specifying correctly the phase of the propagator, as we shall see for the one-dimensional harmonic oscillator potential.

IV.4. Short-time approximation

In the present work, we are interested in the propagator connecting a point with itself in a certain time period. In general, we have different orbits for such kinds of motion. As it turns out, in our method, only one particular orbit already gives us a good estimation for the particle density. We shall see this when considering the example of a symmetric linear potential.

The particular orbit that we are using is illustrated in figure 28 for a typical one-dimensional potential well. The particle starts out in the direction of the potential's gradient up to a certain Fermi energy $E(t)$ and then retreats back to the original position, which occurs in a total time period of t .

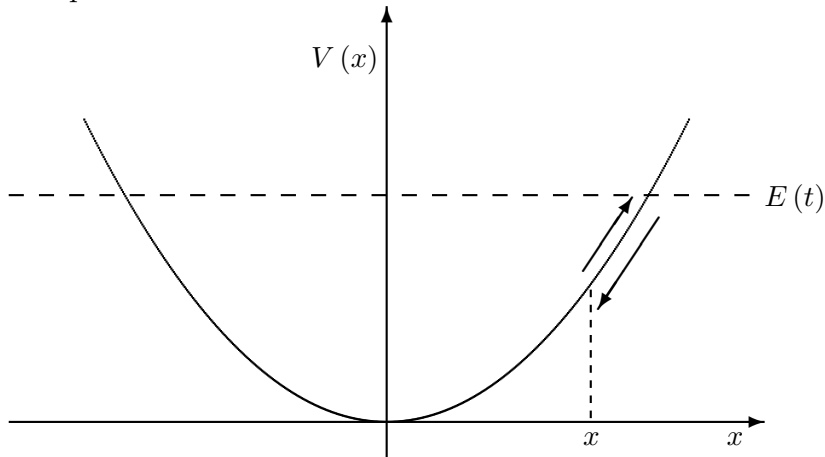


Figure 28. Classical orbit in short-time approximation from a point x back to itself in time t in a harmonic oscillator potential $V(x)$, with $E(t)$ indicating the Fermi energy, which depends on time t .

We can easily imagine a similar trajectory in higher dimensions. There is always a direction parallel to the gradient of a general potential well, and such a trajectory is always possible for small time. This is why we call *short-time approximation*.

The short-time approximation also shows up in another interesting way, as we shall see in the discussion of a one-dimensional harmonic oscillator. It is when the determinant of C generally changes sign for large values of t . In the formula (140), we integrate over t from 0 to ∞ . However, as it turns out, all what large t does is to add extra phases to the integral over small enough t . This shall result in some sort of energy quantization, which links the discussion to the JWKB method.

IV.5. Symmetric linear potential

IV.5.1. Stationary states

We consider a symmetric linear potential given by

$$V(x) = f|x|, \tag{162}$$

where f is a positive constant. We want to solve the eigenvalue problem corresponding to this potential

$$\frac{d^2}{dx^2}\psi(x) = \frac{2m(V(x) - E)}{\hbar^2}\psi(x). \quad (163)$$

In the region $x > 0$, (163) becomes

$$\frac{d^2}{dx^2}\psi(x) = \frac{2m(fx - E)}{\hbar^2}\psi(x). \quad (164)$$

Let $z = \alpha \frac{2m(fx - E)}{\hbar^2}$, where α is a constant, to be found subsequently. We have then

$$\left(\alpha \frac{2mf}{\hbar^2}\right)^2 \frac{d^2}{dz^2}\psi(z) = \frac{z}{\alpha}\psi(z). \quad (165)$$

We choose α so that

$$\begin{aligned} 1 &= \alpha \left(\alpha \frac{2mf}{\hbar^2}\right)^2 \\ \Leftrightarrow \alpha &= \left(\frac{\hbar^2}{2mf}\right)^{2/3}, \end{aligned} \quad (166)$$

and (165) assumes the form of the *Airy differential equation* (cf. [20])

$$\frac{d^2}{dz^2}\psi(z) = z\psi(z), \quad (167)$$

of which the only physically meaningful solution is the Airy function, which vanishes at $\pm\infty$,

$$\psi(z) = a\text{Ai}(z). \quad (168)$$

Since

$$\begin{aligned} z &= \left(\frac{\hbar^2}{2mf}\right)^{2/3} \frac{2m(fx - E)}{\hbar^2} \\ &= \left(\frac{2mf}{\hbar^2}\right)^{1/3} (x - E/f), \end{aligned} \quad (169)$$

we have

$$\psi(x) \equiv \psi_1(x) = a\text{Ai}\left[\left(\frac{2mf}{\hbar^2}\right)^{1/3} (x - E/f)\right] \text{ for } x > 0. \quad (170)$$

By the same argument, we prove that

$$\psi(x) \equiv \psi_2(x) = b\text{Ai}\left[-\left(\frac{2mf}{\hbar^2}\right)^{1/3} (x + E/f)\right] \text{ for } x < 0. \quad (171)$$

In the above equations, a and b are two normalization factors. By the continuity of the wave function and its derivative w.r.t x at $x = 0$, we have

$$(a - b) \text{Ai}\left[-\left(\frac{2mf}{\hbar^2}\right)^{1/3} E/f\right] = 0, \quad (172)$$

and

$$(a + b) \text{Ai}' \left[- \left(\frac{2mf}{\hbar^2} \right)^{1/3} E/f \right] = 0. \quad (173)$$

These two equations resolve to two scenarios

$$\begin{cases} a = b; \text{Ai}' \left[- \left(\frac{2mf}{\hbar^2} \right)^{1/3} E/f \right] = 0, \\ a = -b; \text{Ai} \left[- \left(\frac{2mf}{\hbar^2} \right)^{1/3} E/f \right] = 0. \end{cases} \quad (174)$$

These correspond in fact to two classes of the eigenfunctions, *symmetric* and *antisymmetric*.

In summary, the eigenfunctions are given by

$$\psi_n(x) = \begin{cases} a \text{Ai} \left[\left(\frac{2mf}{\hbar^2} \right)^{1/3} (x - E_n/f) \right] & \text{for } x > 0, \\ \pm \psi(-x) & \text{for } x < 0. \end{cases} \quad (175)$$

The normalization constant is found to be

$$a = \left(\frac{2mf}{\hbar^2} \right)^{1/6} \left(\frac{1}{2F_1 \left[- \left(\frac{2mf}{\hbar^2} \right)^{1/3} E_n/f \right]} \right)^{1/2}, \quad (176)$$

where F_1 is a function in the family F_m (see Appendix 1). For the two classes of eigenfunctions, the eigenvalues E_n are given by

$$\begin{cases} \text{Ai}' \left[- \left(\frac{2mf}{\hbar^2} \right)^{1/3} E_n/f \right] = 0 & \text{for even } n, \\ \text{Ai} \left[- \left(\frac{2mf}{\hbar^2} \right)^{1/3} E_n/f \right] = 0 & \text{for odd } n, \end{cases} \quad (177)$$

or jointly by

$$F_2 \left[- \left(\frac{2mf}{\hbar^2} \right)^{1/3} E_n/f \right] = 0. \quad (178)$$

The numerical values of the first 20 energy eigenvalues are given in table V as multiples of $f \left(\frac{2mf}{\hbar^2} \right)^{-1/3}$ [31].

Table V. The first 20 energy eigenvalues for the symmetric linear potential as multiples of $f \left(\frac{2mf}{\hbar^2} \right)^{-1/3}$.

even n	E_n	odd n	E_n
0	1.018	1	2.338
2	3.248	3	4.087
4	4.820	5	5.520
6	6.163	7	6.786
8	7.372	9	7.944
10	8.488	11	9.022
12	9.535	13	10.040
14	10.527	15	11.008
16	11.475	17	11.936
18	12.384	19	12.828

IV.5.2. Exact particle density

The exact particle density of N occupied orbitals is obtained by summing the modulus square of the eigenfunctions of the first N states

$$n(x) = \sum_{n=0}^{N-1} \left(\frac{2mf}{\hbar^2} \right)^{1/3} \left(\frac{1}{2F_1 \left[- \left(\frac{2mf}{\hbar^2} \right)^{1/3} E_n/f \right]} \right) \text{Ai}^2 \left[\left(\frac{2mf}{\hbar^2} \right)^{1/3} (x - E_n/f) \right]. \quad (179)$$

IV.5.3. Particle density given by the propagator method

We prove that the density given by this method is the same as the dominant term of that given by Ribeiro *et al.*'s method [10]. By the propagator method, the density is given by

$$n(x) = \frac{1}{\pi\hbar} \text{Re} \int_{-\infty}^{\mu} d\lambda \int_0^{\infty} dT \exp(i\lambda T/\hbar) K(x, x; T). \quad (180)$$

The propagator $K(x, x; T)$ given by the van Vleck-Gutzwiller formula under short-time approximation is found to be (see Appendix 6)

$$K(x, x; T) \simeq \sqrt{\frac{m}{2\pi i\hbar T}} \exp \left\{ -\frac{ifT|x|}{\hbar} - \frac{if^2 T^3}{24\hbar m} \right\}. \quad (181)$$

We have, by substituting this into (180) and simplifying the notation by taking the derivative w.r.t. μ

$$\begin{aligned}
\frac{\partial}{\partial \mu} n(x) &\simeq \frac{1}{\pi \hbar} \operatorname{Re} \int_0^\infty dT \sqrt{\frac{m}{2\pi i \hbar T}} \exp \left\{ \frac{i}{\hbar} (\mu - f|x|) T - \frac{if^2 T^3}{24 \hbar m} \right\} \\
&= \frac{1}{\pi \hbar} \operatorname{Re} \int_0^\infty dT \sqrt{\frac{m}{2\pi \hbar T}} \exp \left\{ \frac{i}{\hbar} (\mu - f|x|) T - \frac{if^2 T^3}{24 \hbar m} - \frac{i\pi}{4} \right\} \\
&= \frac{1}{\pi \hbar} \int_0^\infty dT \sqrt{\frac{m}{2\pi \hbar T}} \cos \left\{ \frac{f^2 T^3}{24 \hbar m} - \frac{1}{\hbar} (\mu - f|x|) T + \frac{\pi}{4} \right\}.
\end{aligned} \tag{182}$$

We observe that the integral will give us the square of the Airy function, following its integral representation [20]

$$\operatorname{Ai}^2(x) = \frac{1}{2\pi^{3/2}} \int_0^\infty \frac{1}{\sqrt{t}} \cos \left(t^3/12 + tx + \frac{\pi}{4} \right) dt. \tag{183}$$

By a change of variable $T = \left(\frac{2\hbar m}{f^2} \right)^{1/3} t$, we have

$$\begin{aligned}
&\frac{\partial}{\partial \mu} n(x) \\
&\simeq \frac{1}{\pi \hbar} \int_0^\infty dT \sqrt{\frac{m}{2\pi \hbar T}} \cos \left\{ \frac{f^2 T^3}{24 \hbar m} - \frac{1}{\hbar} (\mu - f|x|) T + \frac{\pi}{4} \right\} \\
&= \frac{1}{\pi \hbar} \left(\frac{2\hbar m}{f^2} \right)^{1/6} \left(\frac{m}{2\pi \hbar} \right)^{1/2} \int_0^\infty dt \frac{1}{\sqrt{t}} \cos \left\{ \frac{t^3}{12} - \frac{\mu - f|x|}{\hbar} \left(\frac{2\hbar m}{f^2} \right)^{1/3} t + \frac{\pi}{4} \right\} \\
&= \left(\frac{4m^2}{f\hbar^4} \right)^{1/3} \operatorname{Ai}^2 \left[-\frac{(\mu - f|x|)}{\hbar} \left(\frac{2\hbar m}{f^2} \right)^{1/3} \right].
\end{aligned} \tag{184}$$

We obtain hence

$$n(x) = \int_{-\infty}^\mu \left(\frac{4m^2}{f\hbar^4} \right)^{1/3} \operatorname{Ai}^2 \left[-\frac{(\lambda - f|x|)}{\hbar} \left(\frac{2\hbar m}{f^2} \right)^{1/3} \right] d\lambda. \tag{185}$$

By a change of variable $z = \frac{(\lambda - f|x|)}{\hbar} \left(\frac{2\hbar m}{f^2} \right)^{1/3}$, we have

$$\begin{aligned}
n(x) &\simeq \int_{-\infty}^\mu \left(\frac{4m^2}{f\hbar^4} \right)^{1/3} \hbar \left(\frac{f^2}{2\hbar m} \right)^{1/3} \operatorname{Ai}^2[-z] dz \\
&= \left(\frac{2mf}{\hbar^2} \right)^{1/3} \int_{-\infty}^{z_F(x)} \operatorname{Ai}^2[-z] dz \\
&= \left(\frac{2mf}{\hbar^2} \right)^{1/3} \int_{-\infty}^{z_F(x)} F_0[-z] dz \\
&= \left(\frac{2mf}{\hbar^2} \right)^{1/3} F_1(-z_F(x)),
\end{aligned} \tag{186}$$

where the integrand in the second last step is the function $F_0(-z)$, whose anti-derivative is $F_1(-z)$, see Appendix 1.

IV.5.4. Particle density given by Ribeiro et al.'s method

We start out by calculating the abbreviated action for a point $x > 0$, but $x < x_2$, where x_2 is the right turning point for the Fermi energy E_F . The result as given by (13) is found to be

$$S(x) = \frac{p_F^3(x)}{3mf}, \quad (187)$$

where $p_F(x)$ is the classical momentum at the Fermi level. Similar derivations show that for a general point x , the absolute value of $z_F(x)$ is given by

$$\begin{aligned} |z_F(x)| &= \left[\frac{3}{2\hbar} \frac{|p_F|^3(x)}{3mf} \right]^{2/3} \\ &= \left[\frac{1}{2\hbar mf} \right]^{2/3} |p_F|^2(x). \end{aligned} \quad (188)$$

As can be inferred from the earlier discussion, $p_F(x)$ always has the same phase as $\sqrt{z_F(x)}$. Hence, the dominant term in the density given by this method is found to be (27)

$$n_0(x) = \left(\frac{2mf}{\hbar^2} \right)^{1/3} F_1(-z_F(x)), \quad (189)$$

which is exactly the result (186) found by the propagator method if we choose the same Fermi energy $E_F = E_{N-1/2}$ for a system of N non-interacting fermions. E_n for the semiclassical methods are given by the JWKB quantization rule which resolves into

$$E_n = \frac{1}{2m} \left(\frac{3mf\pi\hbar(n+1/2)}{2} \right)^{2/3}. \quad (190)$$

Figure 29 compares the particle densities given by various methods. The semiclassical density (186) correlates quite accurately with the exact result. This is a first example to confirm the validity of the proposed method of finding the particle density via the quantum propagator. This also shows that we may greatly simplify the problem of finding the propagator by considering only one particular orbit associated with short transition time. Even so, the particle density we found is already quite accurate. Of course, we need further investigations to arrive at the general picture. In the next section, we consider the example of a one-dimensional harmonic oscillator, where we know its propagator exactly. We shall see how by using suitable approximations, we can relate the present method and the JWKB method.

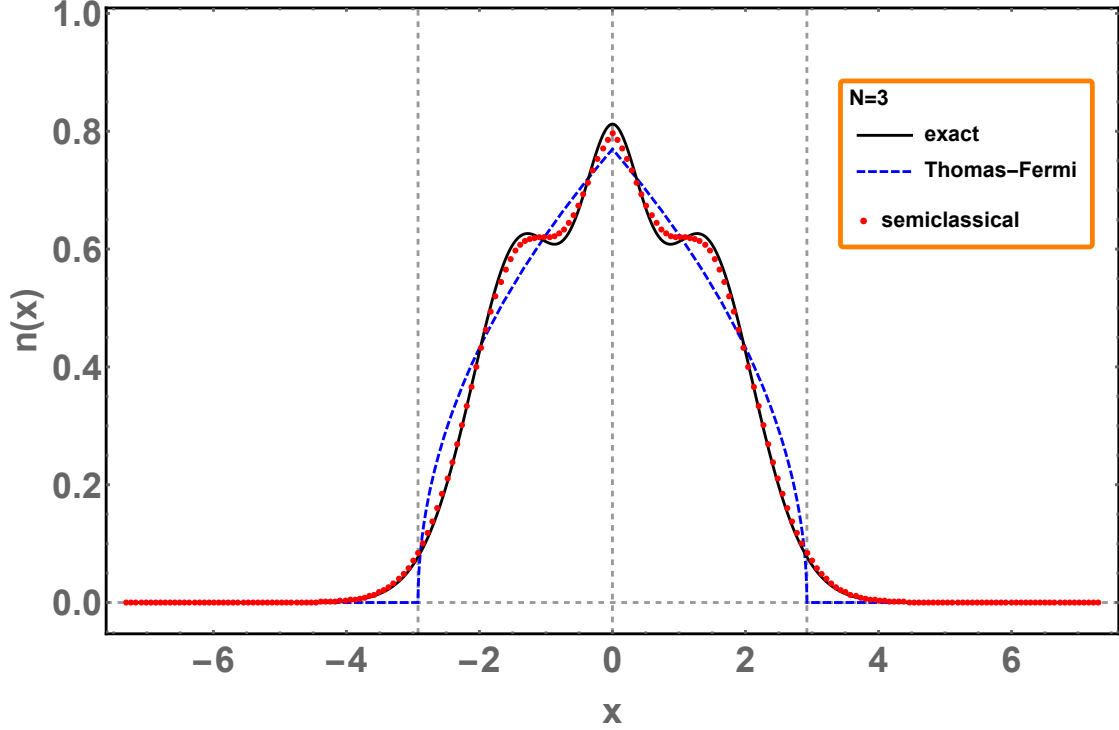


Figure 29. Exact density, TF density, and semiclassical density (186) for three particles in a one-dimensional symmetric linear potential, $V(x) = f|x|$.

IV.6. One-dimensional harmonic oscillator potential

For the Hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2, \quad (191)$$

the propagator from a point x back to itself in some time t is given by (see Appendix 7)

$$K(x, x; t) = \sqrt{\frac{m\omega}{2\pi i\hbar |\sin(\omega t)|}} \exp \left\{ -\frac{im\omega x^2}{\hbar} \tan\left(\frac{\omega t}{2}\right) - \frac{i\kappa\pi}{2} \right\}, \quad (192)$$

where

$$\kappa = \left[\frac{\omega t}{\pi} \right]. \quad (193)$$

The density according to formula (140) is given by

$$n(x) = \frac{\text{Re}}{\pi\hbar} \int^\mu d\lambda \int_0^\infty dt \sqrt{\frac{m\omega}{2\pi i\hbar |\sin(\omega t)|}} \exp \left\{ -\frac{im\omega x^2}{\hbar} \tan\left(\frac{\omega t}{2}\right) + \frac{i\lambda t}{\hbar} - \frac{i\kappa\pi}{2} \right\}. \quad (194)$$

Denote

$$I_\lambda(x) = \int_0^\infty dt \sqrt{\frac{m\omega}{2\pi i \hbar |\sin(\omega t)|}} \exp \left\{ -\frac{im\omega x^2}{\hbar} \tan\left(\frac{\omega t}{2}\right) + \frac{i\lambda t}{\hbar} - \frac{i\kappa\pi}{2} \right\}. \quad (195)$$

We divide the domain of integration into sections of length $\frac{2\pi}{\omega}$,

$$I_\lambda(x) = \sum_{j=0}^{\infty} \int_{2j\pi/\omega}^{2(j+1)\pi/\omega} dt \sqrt{\frac{m\omega}{2\pi i \hbar |\sin(\omega t)|}} \exp \left\{ -\frac{im\omega x^2}{\hbar} \tan\left(\frac{\omega t}{2}\right) + \frac{i\lambda t}{\hbar} - \frac{i\kappa\pi}{2} \right\}. \quad (196)$$

Let

$$I_\lambda^0(x) = \int_0^{2\pi/\omega} dt \sqrt{\frac{m\omega}{2\pi i \hbar |\sin(\omega t)|}} \exp \left\{ -\frac{im\omega x^2}{\hbar} \tan\left(\frac{\omega t}{2}\right) + \frac{i\lambda t}{\hbar} - \frac{i\kappa\pi}{2} \right\}. \quad (197)$$

By changing the integration variable and taking into account the correct κ for integrals over the sections, we deduce

$$I_\lambda(x) = I_\lambda^0(x) \sum_{j=0}^{\infty} \exp\left(\frac{i\lambda}{\hbar} \frac{2j\pi}{\omega}\right) \exp(-ij\pi). \quad (198)$$

The sum on the right-hand side does not converge in the usual sense. We shall see that not this but the same sum over all integer j can be evaluated by the Poisson summation formula. This sum arises when we take the real part of $I_\lambda(x)$ with the evaluated expression of $I_\lambda^0(x)$ substituted in. Our focus now is on the evaluation of $I_\lambda^0(x)$.

Let

$$\begin{aligned} f(t) &= -m\omega x^2 \tan\left(\frac{\omega t}{2}\right) + \lambda t, \\ g(t) &= \left(\frac{m\omega}{2\pi i \hbar |\sin(\omega t)|}\right)^{1/2}. \end{aligned} \quad (199)$$

We have

$$I_\lambda^0(x) = I_1(x) + I_2(x), \quad (200)$$

where

$$\begin{aligned} I_1(x) &= \int_0^{\pi/\omega} dt g(t) \exp\left(\frac{i}{\hbar} f(t)\right), \\ I_2(x) &= \int_{\pi/\omega}^{2\pi/\omega} dt g(t) \exp\left(\frac{i}{\hbar} f(t) - \frac{i\pi}{2}\right). \end{aligned} \quad (201)$$

We shall consider two separate cases of the values of λ and x : the classically forbidden region ($\lambda < V(x)$), and the classically allowed region ($\lambda > V(x)$).

IV.6.1. *Classically forbidden region*

Now, we treat the case $\lambda < V(x)$. Let

$$\rho(t) = -\frac{1}{\hbar}f(t) = -\frac{1}{\hbar} \left(\lambda t - m\omega x^2 \tan\left(\frac{\omega t}{2}\right) \right). \quad (202)$$

For $\lambda < V(x)$, $\rho(t)$ is an increasing function on the range $[0, \pi/\omega)$, which permits us to make the change of variable

$$\rho(t) = \xi(u(t)) = \frac{u^3}{12} + uz, \quad (203)$$

where z is a positive constant to be determined. The functions $\rho(t)$ and $\xi(u)$ are both analytic for $|t| \in [0, \pi/\omega)$ and $z \in \mathbb{C}$ respectively, so if they agree on $|t| \in [0, \pi/\omega)$ for a given choice of the analytic function $u(t)$, they agree on the entire open domain of analyticity. It is generally difficult to invert the relation to express t as a function of u . We shall choose instead to truncate the power series of t in orders of u . By inspection, we notice that $u = 0$ when $t = 0$. Therefore, in general we have

$$t \simeq \frac{dt(0)}{du}u + \dots \quad (204)$$

for small values of u . Since the phases of the integrands of $I_1(x)$ and $I_2(x)$ are rapidly oscillatory in the semiclassical limit, the dominant contribution to these integrals comes from the vicinity of $t = 0$, which justifies the truncation.

To determine $\frac{dt(0)}{du}$, we compare the first derivatives of $\rho(t)$ and $\xi(u(t))$ at $t = 0$. From

$$\begin{aligned} \rho'(t) &= \frac{1}{\hbar} \left(\frac{V(x)}{\cos^2(\omega t/2)} - \lambda \right), \\ \xi'(u(t)) &= \left(\frac{u^2}{4} + z \right) \frac{du}{dt}, \end{aligned} \quad (205)$$

we deduce that

$$\frac{dt(0)}{du} = \frac{z\hbar}{V(x) - \lambda}. \quad (206)$$

Therefore,

$$\begin{aligned}
& I_1(x) \\
&= \int_0^\infty du \frac{dt}{du} \left(\frac{m\omega}{2\pi i \hbar |\sin(\omega t)|} \right)^{1/2} \exp \left[-i \left(\frac{u^3}{12} + uz \right) \right] \\
&\simeq \int_0^\infty du \left(\frac{z\hbar}{V(x) - \lambda} \right)^{1/2} \left(\frac{m}{2\pi\hbar} \right)^{1/2} \frac{1}{\sqrt{u}} \exp \left[-i \left(\frac{u^3}{12} + uz + \frac{\pi}{4} \right) \right] \\
&\simeq \left(\frac{mz}{2\pi(V(x) - \lambda)} \right)^{1/2} \int_0^\infty \frac{du}{\sqrt{u}} \left[\cos \left(\frac{u^3}{12} + uz + \frac{\pi}{4} \right) - i \sin \left(\frac{u^3}{12} + uz + \frac{\pi}{4} \right) \right] \\
&= \pi \left(\frac{2mz}{(V(x) - \lambda)} \right)^{1/2} [\text{Ai}^2(z) - i \text{Ai}(z) \text{Bi}(z)],
\end{aligned} \tag{207}$$

where we use the integral representations of $\text{Ai}^2(z)$ (183) and of $\text{Ai}(z) \text{Bi}(z)$ [20].

To find z , we compare $\rho(t)$ and $\xi(u(t))$ where they are stationary on the domain of analyticity. We have $\rho'(t)$ and $\xi'(u(t))$ vanish when

$$\begin{aligned}
t &= \pm i t_0, \\
u &= \pm i 2\sqrt{z},
\end{aligned} \tag{208}$$

where t_0 is the positive solution of

$$\cosh^2 \left(\frac{\omega t_0}{2} \right) = \frac{V(x)}{\lambda} > 1. \tag{209}$$

The stationary values of $\rho(t)$ and $\xi(u(t))$ are then

$$\begin{aligned}
\xi &= \pm i \frac{4}{3} z^{3/2}, \\
\rho &= \pm \frac{i}{\hbar} \left(m\omega x^2 \tanh \left(\frac{\omega t_0}{2} \right) - \lambda t_0 \right).
\end{aligned} \tag{210}$$

We deduce that

$$z = \left[\frac{3}{4\hbar} \left(m\omega x^2 \tanh \left(\frac{\omega t_0}{2} \right) - \lambda t_0 \right) \right]^{2/3} > 0. \tag{211}$$

As for $I_2(x)$, we have after some changes of variable

$$\begin{aligned}
& I_2(x) \\
&= \int_{\pi/\omega}^{2\pi/\omega} dt \left(\frac{m\omega}{2\pi i \hbar |\sin(\omega t)|} \right)^{1/2} \exp \left[\frac{i}{\hbar} \left(\lambda t - m\omega x^2 \tan \left(\frac{\omega t}{2} \right) \right) - \frac{i\pi}{2} \right] \\
&= \int_{-\pi/\omega}^0 dt \left(\frac{m\omega}{2\pi i \hbar |\sin(\omega t)|} \right)^{1/2} \exp \left[\frac{i}{\hbar} \left(\lambda t - m\omega x^2 \tan \left(\frac{\omega t}{2} \right) \right) \right] \exp \left(\frac{i\lambda 2\pi}{\hbar\omega} - \frac{i\pi}{2} \right) \\
&= - \int_0^{\pi/\omega} dt \left(\frac{m\omega}{2\pi i \hbar |\sin(\omega t)|} \right)^{1/2} \exp \left[-\frac{i}{\hbar} \left(\lambda t - m\omega x^2 \tan \left(\frac{\omega t}{2} \right) \right) + \frac{i\pi}{4} \right] \exp \left(\frac{i\lambda 2\pi}{\hbar\omega} \right) \\
&= -I_1^*(x) \exp \left(\frac{i\lambda 2\pi}{\hbar\omega} \right).
\end{aligned} \tag{212}$$

With (207), we have

$$I_2(x) \simeq -\pi \left(\frac{2mz}{V(x) - \lambda} \right)^{1/2} [\text{Ai}^2(z) + i\text{Ai}(z) \text{Bi}(z)] \exp \left(\frac{i\lambda 2\pi}{\hbar\omega} \right). \tag{213}$$

Altogether, for $\lambda < V(x)$,

$$\begin{aligned}
I_\lambda^0(x) &\simeq \pi \left(\frac{2mz}{V(x) - \lambda} \right)^{1/2} [\text{Ai}^2(z) - i\text{Ai}(z) \text{Bi}(z)] \\
&\quad - \pi \left(\frac{2mz}{V(x) - \lambda} \right)^{1/2} [\text{Ai}^2(z) + i\text{Ai}(z) \text{Bi}(z)] \exp \left(\frac{i\lambda 2\pi}{\hbar\omega} \right) \\
&= \pi \left(\frac{2mz}{V(x) - \lambda} \right)^{1/2} \text{Ai}^2(z) \left[1 - \exp \left(\frac{i\lambda 2\pi}{\hbar\omega} \right) \right] \\
&\quad - i\pi \left(\frac{2mz}{V(x) - \lambda} \right)^{1/2} \text{Ai}(z) \text{Bi}(z) \left[1 + \exp \left(\frac{i\lambda 2\pi}{\hbar\omega} \right) \right].
\end{aligned} \tag{214}$$

IV.6.2. Classically allowed region

When $\lambda > V(x)$, the graph of $\rho(t)$ on the range $[0, \pi/\omega)$ now has a convex shape. This suggests the change of variable

$$\rho(t) = \xi(u(t)) = \frac{u^3}{12} - uz, \tag{215}$$

for a positive constant z to be determined. Following the same method as for the classically forbidden region, we expand t in orders of u for small values of u ,

$$t \simeq \frac{dt(0)}{du} u + \dots \tag{216}$$

We have

$$\begin{aligned}\rho'(t) &= \frac{1}{\hbar} \left(\frac{V(x)}{\cos^2(\omega t/2)} - \lambda \right), \\ \xi'(u(t)) &= \left(\frac{u^2}{4} - z \right) \frac{du}{dt}.\end{aligned}\tag{217}$$

Therefore,

$$\frac{dt(0)}{du} = \frac{z\hbar}{\lambda - V(x)},\tag{218}$$

and

$$\begin{aligned}I_1(x) &= \int_0^\infty du \frac{dt}{du} \left(\frac{m\omega}{2\pi i \hbar |\sin(\omega t)|} \right)^{1/2} \exp \left[-i \left(\frac{u^3}{12} - uz \right) \right] \\ &\simeq \int_0^\infty du \left(\frac{z\hbar}{\lambda - V(x)} \right)^{1/2} \left(\frac{m}{2\pi\hbar} \right)^{1/2} \frac{1}{\sqrt{u}} \exp \left[-i \left(\frac{u^3}{12} - uz + \frac{\pi}{4} \right) \right] \\ &\simeq \left(\frac{mz}{2\pi(\lambda - V(x))} \right)^{1/2} \int_0^\infty \frac{du}{\sqrt{u}} \left[\cos \left(\frac{u^3}{12} - uz + \pi/4 \right) - i \sin \left(\frac{u^3}{12} - uz + \frac{\pi}{4} \right) \right] \\ &= \pi \left(\frac{2mz}{\lambda - V(x)} \right)^{1/2} [\text{Ai}^2(-z) - i \text{Ai}(-z) \text{Bi}(-z)].\end{aligned}\tag{219}$$

It follows that

$$I_2(x) \simeq -\pi \left(\frac{2mz}{\lambda - V(x)} \right)^{1/2} [\text{Ai}^2(-z) + i \text{Ai}(-z) \text{Bi}(-z)] \exp \left(\frac{i\lambda 2\pi}{\hbar\omega} \right).\tag{220}$$

As a result, for $\lambda > V(x)$,

$$\begin{aligned}I_\lambda^0(x) &= \pi \left(\frac{2mz}{\lambda - V(x)} \right)^{1/2} \text{Ai}^2(-z) \left[1 - \exp \left(\frac{i\lambda 2\pi}{\hbar\omega} \right) \right] \\ &\quad - i\pi \left(\frac{2mz}{\lambda - V(x)} \right)^{1/2} \text{Ai}(-z) \text{Bi}(-z) \left[1 + \exp \left(\frac{i\lambda 2\pi}{\hbar\omega} \right) \right].\end{aligned}\tag{221}$$

The constant z in this case is also obtained by comparing the stationary values of $\rho(t)$ and $\xi(u(t))$. We have vanishing first derivatives at

$$\begin{aligned}t &= \pm t_1, \\ u &= \pm 2\sqrt{z},\end{aligned}\tag{222}$$

where t_0 is the smallest positive solution to

$$\cos^2 \left(\frac{\omega t_1}{2} \right) = \frac{V(x)}{\lambda} < 1.\tag{223}$$

The stationary values of $\rho(t)$ and $\xi(t)$ are given by

$$\begin{aligned}\xi &= \pm \frac{4}{3} z^{3/2}, \\ \rho &= \pm \frac{1}{\hbar} \left(\lambda t_1 - m\omega x^2 \tan\left(\frac{\omega t_1}{2}\right) \right).\end{aligned}\tag{224}$$

We deduce that

$$z = \left[\frac{3}{4\hbar} \left(\lambda t_1 - m\omega x^2 \tan\left(\frac{\omega t_1}{2}\right) \right) \right]^{2/3} > 0.\tag{225}$$

In summary

$$\begin{aligned}I_\lambda^0(x) &\simeq \frac{2m\pi z^{1/2}}{|p_\lambda(x)|} \text{Ai}^2(\pm z) \left[1 - \exp\left(\frac{i\lambda 2\pi}{\hbar\omega}\right) \right] \\ &\quad - i \frac{2m\pi z^{1/2}}{|p_\lambda(x)|} \text{Ai}(\pm z) \text{Bi}(\pm z) \left[1 + \exp\left(\frac{i\lambda 2\pi}{\hbar\omega}\right) \right],\end{aligned}\tag{226}$$

where plus sign corresponds to the classically forbidden region and z is given by (225) and (211) for the respective regions.

IV.6.3. Particle density

We are now in a position to calculate $\text{Re}(I_\lambda(x))$ and the particle density. We have

$$\begin{aligned}\text{Re}(I_\lambda(x)) &= \frac{1}{2} I_\lambda^0(x) \sum_{j=0}^{\infty} \exp\left(\frac{i\lambda 2j\pi}{\hbar\omega}\right) \exp(-ij\pi) \\ &\quad + \frac{1}{2} I_\lambda^0(x)^* \sum_{j=0}^{\infty} \exp\left(-\frac{i\lambda 2j\pi}{\hbar\omega}\right) \exp(ij\pi).\end{aligned}\tag{227}$$

We substitute (226) in (227) and pay attention in grouping the terms so that we have the sum of the phases over all integer j . We obtain eventually

$$\begin{aligned}\text{Re}(I_\lambda(x)) &\simeq \frac{m\pi z^{1/2}}{|p_\lambda(x)|} \text{Ai}^2(\pm z) \left[1 - \exp\left(\frac{i\lambda 2\pi}{\hbar\omega}\right) \right] \sum_{j=-\infty}^{\infty} \exp\left(\frac{i\lambda 2j\pi}{\hbar\omega}\right) \exp(-ij\pi) \\ &\quad - i \frac{m\pi z^{1/2}}{|p_\lambda(x)|} \text{Ai}(\pm z) \text{Bi}(\pm z) \left[1 + \exp\left(\frac{i\lambda 2\pi}{\hbar\omega}\right) \right] \sum_{j=-\infty}^{\infty} \exp\left(\frac{i\lambda 2j\pi}{\hbar\omega}\right) \exp(-ij\pi).\end{aligned}\tag{228}$$

We apply the Poisson summation formula (see Appendix 2) to evaluate the last sum, which can be separated into sums over even and odd j .

$$\begin{aligned}
\sum_{j=-\infty}^{\infty} (-1)^j \exp\left(\frac{i\lambda}{\hbar\omega} 2\pi j\right) &= \sum_{l=-\infty}^{\infty} \exp\left(\frac{i\lambda}{\hbar\omega} 4\pi l\right) \\
&\quad - \sum_{l=-\infty}^{\infty} \exp\left(\frac{i\lambda}{\hbar\omega} 4\pi(l+1/2)\right) \\
&= \left[1 - \exp\left(\frac{i2\pi\lambda}{\hbar\omega}\right)\right] \sum_{l=-\infty}^{\infty} \exp\left(\frac{i2\lambda}{\hbar\omega} 2\pi l\right) \\
&= \left[1 - \exp\left(\frac{i2\pi\lambda}{\hbar\omega}\right)\right] \sum_{l=-\infty}^{\infty} \delta\left(\frac{2\lambda}{\hbar\omega} - l\right) \\
&= 2 \sum_{k=-\infty}^{\infty} \delta\left(\frac{2\lambda}{\hbar\omega} - (2k+1)\right),
\end{aligned} \tag{229}$$

where the coefficient before the sum in the second last step is zero for even l . Substituting this into (228) gives

$$\operatorname{Re}(I_\lambda(x)) \simeq \frac{4m\pi z^{1/2}}{|p_\lambda(x)|} \operatorname{Ai}^2(\pm z) \sum_{k=-\infty}^{\infty} \delta\left(\frac{2\lambda}{\hbar\omega} - (2k+1)\right). \tag{230}$$

The density is found to be

$$\begin{aligned}
n(x) &\simeq \int_0^\mu \frac{d\lambda}{\pi\hbar} \frac{4m\pi z^{1/2}}{|p_\lambda(x)|} \operatorname{Ai}^2(\pm z) \sum_{k=-\infty}^{\infty} \delta\left(\frac{2\lambda}{\hbar\omega} - (2k+1)\right) \\
&= \int_0^{\frac{2\mu}{\hbar\omega}} d\nu \frac{2m\omega z^{1/2}}{|p_\lambda(x)|} \operatorname{Ai}^2(\pm z) \sum_{k=-\infty}^{\infty} \delta(\nu - (2k+1)),
\end{aligned} \tag{231}$$

where we employ the change of the integration variable $\nu = \frac{2\lambda}{\hbar\omega}$. Finally,

$$n(x) \simeq \sum_{\lambda=\hbar\omega(n+1/2)}^{\mu} \frac{2m\omega z^{1/2}}{|p_\lambda(x)|} \operatorname{Ai}^2(\pm z) \tag{232}$$

where we sum over the mode energies from 0 to the Fermi energy μ .

We identify the expression inside the sum to be the probability density for each mode. We compare this with the Langer wave function as in equation (19),

$$|\psi(x)|^2 = \frac{2m\omega |z|^{1/2}}{|p|} \operatorname{Ai}^2(-z) \tag{233}$$

One will find that these are exactly the same by working out the exact expressions of $z(x)$ defined in the discussion on the Langer wave function for the one-dimensional harmonic oscillator. The particle density (232) is nothing but (24).

Now, suppose we do not take into account the integrals over all the small sections of length $2\pi/\omega$ in evaluating $I_\lambda(x)$ (196). Instead of a sum of integrals in the final result (231), we shall only have one term, and the density is an integral in place of a sum (232). This gives rise to the dominant term in the particle density (see Appendix 4). In other words, a sum has been approximated by an integral.

CONCLUSIONS AND FUTURE WORKS

IV.7. Conclusions

The semiclassical particle density (25) by [10] in one dimension has been adapted to find the semiclassical particle density for non-interacting fermions in two and three dimensional potentials in terms of the radial particle density ((56), (94), (114), and (115)) for each angular quantum number or magnetic quantum number. The formula (140) for particle density in one dimension involving the quantum propagator, applied to two concrete examples, gives the same result by [10] with the propagator approximated by the van Vleck-Gutzwiller formula (160) and the short-time approximation.

We have discussed the Langer wave function (19), which is an accurate approximation to the exact solution of the one-dimensional time-independent Schrödinger equation. We have also observed how we can connect the Langer wave function from various turning points. The case of two turning points has been presented. The Langer wave function is valid in the entire position space including the turning points, as illustrated in figures 2, 3, 4, and 5. With the Langer wave function, a good approximation to the particle density in the case of non-interacting fermion gas is obtainable by just summing the respective orbitals; with [10], we know that the semiclassical density can be expressed in a closed form formula (25), the dominant term (27) of which we have checked and also rederived with a method based on the quantum propagator for two examples in one dimension.

We have also extended the results by [10] to isotropic potentials in higher dimensions, following the line of thought in the one-dimensional counterpart. The semiclassical radial wave function (53) has turned out to be of the same form as in the one-dimensional case, with the external potential replaced by an effective potential with a non-zero centrifugal term. The anomaly for zero magnetic quantum number in two dimensions where the centrifugal

term vanishes has also been treated. We have demonstrated how from the semiclassical radial wave function, we arrive at the semiclassical particle density of non-interacting fermions in higher dimensions for completely filled shells. An attempt to extract the leading contribution to the radial particle density from the sum of the modulus square of the semiclassical wave functions has been made for the case of zero magnetic quantum number near $s = 0$ in two dimensions. The result is accurate for the harmonic oscillator potential, but fails for the Coulomb potential, where we choose to sum the semiclassical radial wave functions (92) to find the radial particle density for zero magnetic moment.

We move on to discuss another method to get a semiclassical particle density of non-interacting fermions via the quantum propagator. We aim at getting a better intuition of which physical approximations lead to the existing result by Ribeiro *et al.*'s method and possibly a more general method for higher dimensions, which can resolve the “connection issue”. The potential choice for the semiclassical propagator is the Van Vleck-Gutzwiller's formula. The new method's formula for particle density has been tested on two examples: a symmetric linear potential and a harmonic oscillator potential in one dimension. As it turns out, we do not usually need many classical orbits in the van Vleck-Gutzwiller's formula. The typical orbit that exists for small transition time normally gives a good approximation to the particle density. We have shown through explicit consideration of these two examples that we indeed get the same result as by Ribeiro *et al.*'s method. The discussion of the latter example also shows a connection of the present method with the JWKB approximation. Based on the intuition gained in these concrete examples, we can now consider the general case, for any one-dimensional potentials with two turning points and regular potentials that vanish less rapidly than the inverse square law in two and three dimensions.

IV.8. Future works

For a future follow-up, we can keep investigate the process of extracting the leading contribution to the radial particle density from the sum of the modulus square of the semiclassical radial wave functions, in Airy form or Bessel form. Various results can also be used to modify the several functionals in the density functional theory.

As for the new method, we can continue working on various concrete examples in one dimension to gain more intuition, which proves valuable as we move on. The results for

the concrete examples are derived from the knowledge of the explicit form of the quantum propagator. To be able to consider the general case, we have to discuss the general properties of the involved quantities like the Hamilton principal function, the propagator, and possibly the Green function, which was the topic of various earlier works. It is likely that the proposed method can be placed in a more general framework of the research on the classical-quantum connection.

APPENDICES

1. F_m functions (see [1])

a. Expressions of F_m for some definite values of m

$$F_{-2}(z) = 2 [z\text{Ai}^2(z) + \text{Ai}'^2(z)] \quad (234)$$

$$F_{-1}(z) = -2\text{Ai}(z) \text{Ai}'(z), \quad (235)$$

$$F_0(z) = \text{Ai}^2(z), \quad (236)$$

$$F_1(z) = -z\text{Ai}^2(z) + \text{Ai}'^2(z), \quad (237)$$

$$F_2(z) = \frac{2}{3} \left[z^2\text{Ai}^2(z) - \frac{1}{2}\text{Ai}(z) \text{Ai}'(z) - z\text{Ai}'^2(z) \right]. \quad (238)$$

b. Recurrence formulas

For m integer,

$$\left(m - \frac{1}{2}\right) F_m(-z) = \frac{1}{4}F_{m-3}(-z) + zF_{m-1}(-z), \quad (239)$$

$$\frac{\partial}{\partial z} F_m(-z) = F_{m-1}(-z). \quad (240)$$

Substituting (240) into (239) gives

$$\underbrace{\left(m - \frac{1}{2} - z \frac{\partial}{\partial z}\right)}_{-z^{\frac{1}{2}+m} \frac{\partial}{\partial z} z^{\frac{1}{2}-m}} F_m(-z) = \frac{1}{4}F_{m-3}(-z). \quad (241)$$

As a consequence,

$$\frac{\partial}{\partial z} \frac{F_m(-z)}{z^{m-\frac{1}{2}}} = -\frac{1}{4} \frac{F_{m-3}(-z)}{z^{m+\frac{1}{2}}}. \quad (242)$$

It follows that

$$\frac{\partial}{\partial z} \frac{F_1(-z)}{\sqrt{z}} = -\frac{1}{4} \frac{F_{-2}(-z)}{(\sqrt{z})^3}. \quad (243)$$

(239) gives for $m = 1$:

$$\frac{1}{2}F_1(-z) = \frac{1}{4}F_{-2}(-z) + zF_0(-z), \quad (244)$$

or

$$\frac{F_1(-z)}{\sqrt{z}} = \frac{1}{2} \frac{F_{-2}(-z)}{\sqrt{z}} + 2\sqrt{z}F_0(-z). \quad (245)$$

c. *Asymptotic behavior of F_m*

$$F_1(-z)|_{z \gg 1} \sim \frac{\sqrt{z}}{\pi}, \quad (246)$$

$$F_2(-z)|_{z \gg 1} \sim \frac{1}{2\pi} \frac{1}{3} z^{\frac{3}{2}} = \frac{2}{3\pi} z^{\frac{3}{2}}. \quad (247)$$

2. Poisson summation formula

We have the Poisson identity (see for example, [23]):

$$\sum_{k=-\infty}^{\infty} \delta(x - k) = \sum_{j=-\infty}^{\infty} e^{i2\pi jx}. \quad (248)$$

Suppose we have a sum $\sum_{k=0}^{N-1} f_k$. We can rewrite the sum as an integral

$$\sum_{k=0}^{N-1} f_k = \int_{-1/2}^{N-1/2} d\nu f(\nu) \sum_{k=-\infty}^{\infty} \delta(\nu - k), \quad (249)$$

where $f(\nu)$ is a continuous extension of f_ν . Note that we add the sum of the Dirac delta distributions to restrict ν to take integer values. Applying Poisson identity (248), we have

$$\begin{aligned} \sum_{k=0}^{N-1} f_k &= \int_{-1/2}^{N-1/2} d\nu f(\nu) \sum_{j=-\infty}^{\infty} e^{i2\pi j\nu} \\ &= \int_{-1/2}^{N-1/2} d\nu f(\nu) + \dots, \end{aligned} \quad (250)$$

with the correction terms corresponding to $j \neq 0$.

3. Airy uniform approximation to the one-dimensional time-independent Schrödinger equation

Consider the one-dimensional Schrödinger equation (or the radial Schrödinger equation in the three-dimensional case) in the form

$$-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} u(r) + V(r) u(r) = E u(r). \quad (251)$$

The equation can be written as

$$\frac{d^2}{dr^2} u(r) + \frac{p(r)^2}{\hbar^2} u(r) = 0, \quad (252)$$

where the classical momentum $p(r)$ is given by

$$p(r)^2 = 2m(E - V(r)). \quad (253)$$

We make the following transforms of both the dependent and independent variables by

$$\begin{aligned} z &= z(r), \\ u &= \rho(z) \phi(z). \end{aligned}$$

This change of variables gives us a differential equation for $\rho(z)$.

$$\begin{aligned} \rho'' + \left[2 \frac{d}{dz} \ln \phi - \frac{d^2 r}{dz^2} \frac{dz}{dr} \right] \rho' \\ + \left[\frac{1}{\phi} \frac{d^2 \phi}{dz^2} - \frac{d^2 r}{dz^2} \frac{dz}{dr} \left(\frac{d}{dz} \ln \phi \right) + \frac{p^2(r)}{\hbar^2} \left(\frac{dz}{dr} \right)^{-2} \right] \rho = 0. \end{aligned} \quad (254)$$

By putting

$$\phi = \left(\frac{dz}{dr} \right)^{-1/2} = \left(\frac{dr}{dz} \right)^{1/2} \quad (255)$$

such that the term associated with the first derivative of ρ in equation (254) vanishes, we obtain an equation where the quantity $\{z, r\}$ appears

$$\{z, r\} = \frac{z'''}{z'} - \frac{3}{2} \left(\frac{z''}{z'} \right)^2,$$

where z' , z'' , and z''' are the successive derivatives of z as a function of r . The equation reads

$$\rho'' + \left[\frac{p(r)^2}{\hbar^2 z'^2(r)} - \frac{1}{z'^2(r)} \{z, r\} \right] \rho = 0. \quad (256)$$

In the semiclassical approximation, we assume that \hbar tends formally towards 0 so that we could neglect the term $\{z, r\}$. The equation becomes

$$\rho'' + \frac{p(r)^2}{\hbar^2 z'^2(r)} \rho = 0. \quad (257)$$

The general method to proceed further consists in choosing the form of the function

$$\xi(z) = \frac{p^2(r)}{\hbar^2 z'^2(r)} \quad (258)$$

such that we know the solution of equation (257). By (255) the approximate solution to the Schrödinger equation is

$$u(r) = \left(\frac{dz}{dr} \right)^{-1/2} \rho(z).$$

The JWKB method consists in choosing

$$\xi(z) = 1$$

The integration of equation (258) gives us

$$z(r) = \begin{cases} \frac{1}{\hbar} \int_{r_t}^r |p(r')| dr', & \text{if } p^2(r) > 0, \\ \frac{i}{\hbar} \int_{r_t}^r |p(r')| dr', & \text{if } p^2(r) < 0. \end{cases} \quad (259)$$

In (259) r_t is one zero of the momentum $p(r)$ or turning point. The obtained solution is the known JWKB solution

$$u(r) = \frac{1}{\sqrt{|p(r)|}} \exp(\pm iz(r)). \quad (260)$$

As for the Airy uniform approximation, we choose $\xi(z) = z$. Suppose we have a potential with one turning point, where the classically allowed region is to the right of this turning point. This choice resolves into

$$z(r) = \begin{cases} \left[\frac{3}{2\hbar} \int_{r_t}^r p(r) dr \right]^{2/3}, & \text{for the classically allowed region,} \\ - \left[\frac{3}{2\hbar} \int_r^{r_t} |p(r)| dr \right]^{2/3}, & \text{for the classically forbidden region.} \end{cases} \quad (261)$$

We have then the approximate solution to the one-dimensional Schrödinger equation

$$u(r) \sim \left[\hbar^2 \frac{z(r)}{p^2(r)} \right]^{1/4} \text{Ai}(-z(r)). \quad (262)$$

The derivation above is in no way new. Here we adopt the representation in [20]. Similar derivations may be found in various texts.

4. Rederivation of equations (10) and (12) in Ribeiro *et al.*'s paper

a. Equation (10)

We start with the notice that in writing down equation (9), the authors have assigned $m = 1$. This may be convenient, but can also be confusing as we cannot keep track of the dimension of the two sides of an equation. We shall restore m to be a parameter denoting the mass of the fermion and rewrite the term corresponding to $k = 0$ (always in reference to the authors' paper):

$$n_0(x) = 2m \int_{-1/2}^{N-1/2} d\lambda \frac{\omega_\lambda \sqrt{z_\lambda(x)}}{p_\lambda(x)} \text{Ai}^2[-z_\lambda(x)]. \quad (263)$$

As suggested by the authors, we first carry out a change of variable from λ to $p_\lambda(x)$. In what follows x is treated as a parameter, so we can forget about it for the moment and agree that $p_\lambda(x)$, E_λ , and $z_\lambda(x)$ depend on the same variable λ , by the means of which we can always write any one of p , E , and z as a function of another. For example, $p_\lambda(x)$ by right is a function of x with a parameter dependence λ , but since we treat x as a parameter, we can easily write $p_\lambda(x) = p(z)$.

Given $p_\lambda(x) = \sqrt{2m(E_\lambda - V(x))}$, we have

$$\frac{\partial p_\lambda}{\partial \lambda} = \frac{2m \frac{\partial E_\lambda}{\partial \lambda}}{2p_\lambda} = \frac{m\hbar\omega_\lambda}{p_\lambda}, \quad (264)$$

where ω_λ is defined as

$$\omega_\lambda = \hbar^{-1} \frac{\partial E_\lambda}{\partial \lambda}. \quad (265)$$

So the integral becomes

$$\begin{aligned} n_0(x) &= 2m \int_{p_{-1/2}}^{p_{N-1/2}} dp_\lambda(x) \frac{p_\lambda(x) \omega_\lambda \sqrt{z_\lambda(x)}}{m\hbar\omega_\lambda p_\lambda(x)} \text{Ai}^2[-z_\lambda(x)] \\ &= 2\hbar^{-1} \int_{p_{-1/2}}^{p_{N-1/2}} dp_\lambda(x) \sqrt{z_\lambda(x)} \text{Ai}^2[-z_\lambda(x)]. \end{aligned} \quad (266)$$

We change next the variable from $p_\lambda(x)$ to $z_\lambda(x)$. With $f(z) = \frac{p(z)}{\sqrt{z}}$ as defined in the paper, we have

$$\begin{aligned} dp &= \frac{\partial p}{\partial z} dz = \frac{\partial (f\sqrt{z})}{\partial z} dz \\ &= \left(f' \sqrt{z} + \frac{f}{2\sqrt{z}} \right) dz. \end{aligned} \quad (267)$$

As a result, we have

$$\begin{aligned}
n_0(x) &= 2\hbar^{-1} \int_{z_{-1/2}}^{z_{N-1/2}} dz \left(f' \sqrt{z} + \frac{f}{2\sqrt{z}} \right) \sqrt{z} \text{Ai}^2[-z] \\
&= 2\hbar^{-1} \int_{z_{-1/2}}^{z_{N-1/2}} dz f'(z) z \text{Ai}^2[-z] + \hbar^{-1} \int_{z_{-1/2}}^{z_{N-1/2}} dz f(z) \text{Ai}^2[-z].
\end{aligned} \tag{268}$$

We focus now on the second term and denote it as $B = \hbar^{-1} \int_{z_{-1/2}}^{z_{N-1/2}} dz f \text{Ai}^2[-z]$. We notice that

$$\text{Ai}^2[-z] = \frac{d}{dz} [F_1(-z)]. \tag{269}$$

An integration by part gives us

$$\begin{aligned}
B &= \hbar^{-1} \left[f(z) F_1(-z) \Big|_{z=z_{N-1/2}} - f(z) F_1(-z) \Big|_{z=z_{-1/2}} \right] \\
&\quad - \hbar^{-1} \int_{z_{-1/2}}^{z_{N-1/2}} dz \frac{\partial f}{\partial z} F_1(-z).
\end{aligned} \tag{270}$$

Now

$$\begin{aligned}
n_0(x) &= \hbar^{-1} \left[f(z) F_1(-z) \Big|_{z=z_{N-1/2}} - f(z) F_1(-z) \Big|_{z=z_{-1/2}} \right] \\
&\quad + 2\hbar^{-1} \int_{z_{-1/2}}^{z_{N-1/2}} dz f'(z) z \text{Ai}^2[-z] - \hbar^{-1} \int_{z_{-1/2}}^{z_{N-1/2}} dz \frac{\partial f}{\partial z} F_1(-z) \\
&= \hbar^{-1} \left[f(z) F_1(-z) \Big|_{z=z_{N-1/2}} - f(z) F_1(-z) \Big|_{z=z_{-1/2}} \right] \\
&\quad + \hbar^{-1} \int_{z_{-1/2}}^{z_{N-1/2}} dz f'(z) [2z \text{Ai}^2[-z] - F_1(-z)].
\end{aligned} \tag{271}$$

We notice that

$$F_1(-z) = \sqrt{z} g_+(z), \tag{272}$$

and

$$\begin{aligned}
2z \text{Ai}^2[-z] - F_1(-z) &= 2z \text{Ai}^2[-z] - [z \text{Ai}^2[-z] + \text{Ai}'^2[-z]] \\
&= z \text{Ai}^2[-z] - \text{Ai}'^2[-z] \\
&= \sqrt{z} g_-(z),
\end{aligned} \tag{273}$$

where $g_{\pm}(z) = z^{1/2} \text{Ai}^2(-z) \pm z^{-1/2} \text{Ai}'^2(-z)$ is defined in Ribeiro *et al.*'s paper. So altogether, we have

$$n_0(x) \sim \hbar^{-1} p_{\text{F}}(x) g_+[z_{\text{F}}(x)] + \hbar^{-1} \int_{z_{-1/2}}^{z_{N-1/2}} dz \sqrt{z} \frac{\partial f}{\partial z} g_-(z). \tag{274}$$

It seems that the authors have missed a factor of \hbar^{-1} in the second term. Integrating by parts the second term and ignoring the contribution from the lower bound of the integral, we have

$$n_0(x) \sim \hbar^{-1} p_F(x) g_+[z_F(x)] + \hbar^{-1} \left. \frac{\partial f}{\partial z} \right|_{E_F, x} A_0(z_F), \quad (275)$$

where $A_0(z) = -\frac{1}{2}F_{-1}(-z) = \text{Ai}(-z) \text{Ai}'(-z)$. The justification of the negligence of the terms associated with the lower bound is the normalization of the leading contribution to N in the semiclassical limit, as can be seen in II.4.

b. Equation (12)

Still treating x as a parameter and denoting now $\frac{\partial}{\partial \lambda}$ as a prime, we have

$$\begin{aligned} \frac{\partial f}{\partial z} &= \frac{f'}{z'} = \frac{(p/\sqrt{z})'}{z'} \\ &= \frac{1}{z'} \frac{p' \sqrt{z} - p \frac{1}{2\sqrt{z}} z'}{z} \\ &= \frac{p'}{\sqrt{z} z'} - \frac{p}{2z^{3/2}}. \end{aligned} \quad (276)$$

After substituting p' as in (264) into the above equation, we have

$$\left. \frac{\partial f}{\partial z} \right|_{E_F, x} = \frac{1}{\sqrt{z_F(x)} \left. \frac{\partial z_\lambda(x)}{\partial \lambda} \right|_{\lambda=N-1/2}} \frac{m\hbar\omega_F}{p_F(x)} - \frac{p_F(x)}{2z_F^{3/2}}. \quad (277)$$

There may be a problem with the definition of $\alpha_F(x)$ in the paper. $\alpha_F(x)$ appears as the argument of csc in the particle density, so it should be dimensionless. If any α is to be defined, it should be

$$\alpha_F(x) = \sqrt{z_F(x)} \left. \frac{\partial z_\lambda(x)}{\partial \lambda} \right|_{\lambda=N-1/2}, \quad (278)$$

thereby giving

$$\left. \frac{\partial f}{\partial z} \right|_{E_F, x} = \frac{m\hbar\omega_F}{p_F(x) \alpha_F(x)} - \frac{p_F(x)}{2z_F^{3/2}}. \quad (279)$$

The term n_0 is then given by

$$n_0(x) \sim \hbar^{-1} p_F(x) g_+[z_F(x)] + \left(\frac{m\omega_F}{p_F(x) \alpha_F(x)} - \frac{p_F(x)}{2\hbar z_F^{3/2}} \right) A_0(z_F). \quad (280)$$

We could not rederive the term n_1 for the moment, so we quote the result here

$$n_1(x) = \frac{m\omega_F}{p_F(x)} \left(\text{csc}(\alpha_F(x)) - \frac{1}{\alpha_F(x)} \right) A_0(z_F(x)). \quad (281)$$

The sum of the two terms n_0 and n_1 gives us the full semiclassical approximation to the particle density

$$\begin{aligned}
n^{sc}(x) &= \hbar^{-1} p_F(x) g_+[z_F(x)] + \left(\frac{m\omega_F}{p_F(x)} \csc(\alpha_F(x)) - \frac{p_F(x)}{2\hbar z_F^{3/2}} \right) A_0(z_F) \\
&= \frac{p_F(x)}{\hbar} \left[\sqrt{z} \text{Ai}^2(-z) + \frac{\text{Ai}'^2(-z)}{\sqrt{z}} \right. \\
&\quad \left. + \left(\frac{\hbar m\omega_F}{p_F^2(x)} \csc(\alpha_F(x)) - \frac{1}{2z^{3/2}} \right) \text{Ai}(-z) \text{Ai}'(-z) \right] \Big|_{z=z_F(x)}.
\end{aligned} \tag{282}$$

5. Energy eigenvalues of the harmonic oscillator and Coulomb potentials in three dimensions given by the JWKB quantization rule

As has been discussed in III.2, Langer [11] noticed that the correct JWKB quantization for a three-dimensional isotropic potential should be obtained by replacing the centrifugal term $\frac{\hbar^2 l(l+1)}{2mr^2}$ of the effective potential by $\frac{\hbar^2 (l+1/2)^2}{2mr^2}$. The JWKB quantization rule then reads

$$\int_{r_1}^{r_2} dr \sqrt{2m \left\{ E - V(r) - \frac{\hbar^2 (l+1/2)^2}{2mr^2} \right\}} = \pi \hbar (n_r + 1/2), \quad (283)$$

where the integral is taken between the two turning points r_1 and r_2 , i.e. the two zeros of the term under the square root sign, and n_r is the radial quantum number. Here, we derive from (283) the energy eigenvalues for the three-dimensional harmonic oscillator and Coulomb potential problems.

In what follows, we use extensively the integral

$$\int_{-\pi}^{\pi} \frac{d\alpha}{1 + \epsilon \sin(\alpha)} = \frac{2\pi}{\sqrt{1 - \epsilon^2}}, \quad \text{for } |\epsilon| < 1. \quad (284)$$

Let $u(\alpha) = \tan(\alpha/2)$. In the range $(-\pi, \pi)$, $u(\alpha)$ is a monotonic function. Therefore, $\alpha = 2 \arctan(u)$. We have hence

$$d\alpha = \frac{2}{1 + u^2} du. \quad (285)$$

We also have

$$\begin{aligned} \sin(\alpha) &= 2 \tan\left(\frac{\alpha}{2}\right) \cos^2\left(\frac{\alpha}{2}\right) \\ &= \frac{2u}{1 + u^2}. \end{aligned} \quad (286)$$

The left-hand side of (284) now becomes

$$\begin{aligned} \int_{-\infty}^{\infty} \frac{1}{1 + \frac{2\epsilon u}{1+u^2}} \frac{2}{1+u^2} du &= \int_{-\infty}^{\infty} \frac{2du}{u^2 + 2\epsilon u + 1} \\ &= \int_{-\infty}^{\infty} \frac{2du}{(u + \epsilon)^2 + (1 - \epsilon^2)} \end{aligned} \quad (287)$$

By a change of variable $t = \frac{u+\epsilon}{\sqrt{1-\epsilon^2}}$, the integral becomes

$$\begin{aligned} \int_{-\infty}^{\infty} \frac{2\sqrt{1-\epsilon^2} dt}{(1-\epsilon^2)(t^2+1)} &= \frac{2}{\sqrt{1-\epsilon^2}} \int_{-\infty}^{\infty} \frac{dt}{t^2+1} \\ &= \frac{2}{\sqrt{1-\epsilon^2}} [\arctan(t)] \Big|_{-\infty}^{\infty} \\ &= \frac{2\pi}{\sqrt{1-\epsilon^2}}. \end{aligned} \quad (288)$$

Hence, (284) is proven.

a. *Three-dimensional harmonic oscillator*

With the potential $V(r) = \frac{1}{2}m\omega^2 r^2$, the left-hand side of (283) becomes

$$\begin{aligned}
& \int_{r_1}^{r_2} dr \sqrt{2m \left[E - \frac{1}{2}m\omega^2 r^2 - \frac{\hbar^2 (l+1/2)^2}{2mr^2} \right]} \\
&= \int_{r_1}^{r_2} \frac{dr}{r} \sqrt{2m \left[Er^2 - \frac{1}{2}m\omega^2 r^4 - \frac{\hbar^2 (l+1/2)^2}{2m} \right]} \\
&= m\omega \int_{r_1}^{r_2} \frac{dr}{r} \sqrt{(r_2^2 - r^2)(r^2 - r_1^2)}.
\end{aligned} \tag{289}$$

The last step follows from the fact that r_1 and r_2 are the two zeros of the integrand with $r_2 > r_1$. Let

$$r^2 = \frac{r_1^2 + r_2^2}{2} + \frac{r_2^2 - r_1^2}{2} \sin \alpha, \text{ for } \alpha \in (-\pi/2, \pi/2). \tag{290}$$

This implies

$$2rdr = \frac{r_2^2 - r_1^2}{2} \cos(\alpha) d\alpha, \tag{291}$$

and

$$\begin{aligned}
\sqrt{(r_2^2 - r^2)(r^2 - r_1^2)} &= \sqrt{\left(\frac{r_2^2 - r_1^2}{2}\right)^2 (1 - \sin \alpha)(1 + \sin \alpha)} \\
&= \left(\frac{r_2^2 - r_1^2}{2}\right) \cos \alpha.
\end{aligned} \tag{292}$$

The integral (289) now becomes

$$\begin{aligned}
& m\omega \int_{-\pi/2}^{\pi/2} d\alpha \frac{r_2^2 - r_1^2}{4} \cos \alpha \left(\frac{r_2^2 - r_1^2}{2}\right) \cos \alpha \frac{1}{\frac{r_2^2 + r_1^2}{2} + \frac{r_2^2 - r_1^2}{2} \sin \alpha} \\
&= \frac{m\omega}{4} \frac{(r_2^2 - r_1^2)^2}{r_2^2 + r_1^2} \int_{-\pi/2}^{\pi/2} d\alpha \frac{\cos^2(\alpha)}{1 + \epsilon \sin \alpha} \\
&= \frac{m\omega}{4} (r_2^2 + r_1^2) \epsilon^2 \int_{-\pi/2}^{\pi/2} d\alpha \frac{\cos^2(\alpha)}{1 + \epsilon \sin \alpha},
\end{aligned} \tag{293}$$

where

$$\epsilon = \frac{r_2^2 - r_1^2}{r_2^2 + r_1^2} < 1. \tag{294}$$

Consider now the integral

$$\int_{-\pi/2}^{\pi/2} d\alpha \frac{\cos^2(\alpha)}{1 + \epsilon \sin \alpha} = \int_{-\pi/2}^0 d\alpha \frac{\cos^2(\alpha)}{1 + \epsilon \sin \alpha} + \int_0^{\pi/2} d\alpha \frac{\cos^2(\alpha)}{1 + \epsilon \sin \alpha}. \tag{295}$$

By changing the variable $\alpha \rightarrow -\pi - \alpha$ for the first integral and $\alpha \rightarrow \pi - \alpha$ for the second integral on the right-hand side, we obtain

$$\begin{aligned}
& 2 \int_{-\pi/2}^{\pi/2} d\alpha \frac{\cos^2(\alpha)}{1 + \epsilon \sin \alpha} \\
&= \int_{-\pi/2}^{\pi/2} d\alpha \frac{\cos^2(\alpha)}{1 + \epsilon \sin \alpha} + \int_{-\pi}^{-\pi/2} d\alpha \frac{\cos^2(\alpha)}{1 + \epsilon \sin \alpha} + \int_{\pi/2}^{\pi} d\alpha \frac{\cos^2(\alpha)}{1 + \epsilon \sin \alpha} \\
&= \int_{\pi}^{\pi} d\alpha \frac{\cos^2(\alpha)}{1 + \epsilon \sin \alpha} \\
&= \frac{1}{\epsilon^2} \int_{\pi}^{\pi} d\alpha \left[\frac{\epsilon^2 - 1}{1 + \epsilon \sin \alpha} + \frac{1 - \epsilon^2 \sin^2(\alpha)}{1 + \epsilon \sin \alpha} \right] \tag{296} \\
&= \frac{\epsilon^2 - 1}{\epsilon^2} \int_{\pi}^{\pi} d\alpha \frac{1}{1 + \epsilon \sin \alpha} + \frac{1}{\epsilon^2} \int_{\pi}^{\pi} d\alpha (1 - \epsilon \sin(\alpha)) \\
&= \frac{\epsilon^2 - 1}{\epsilon^2} \frac{2\pi}{\sqrt{1 - \epsilon^2}} + \frac{1}{\epsilon^2} [\alpha + \epsilon \cos \alpha] \Big|_{-\pi}^{\pi} \\
&= \frac{\epsilon^2 - 1}{\epsilon^2} \frac{2\pi}{\sqrt{1 - \epsilon^2}} + \frac{2\pi}{\epsilon^2}.
\end{aligned}$$

Now, r_1^2 and r_2^2 are solutions to

$$(m\omega)^2 x^2 - 2mEx + \hbar^2 (l + 1/2)^2 = 0, \tag{297}$$

so

$$r_{1,2}^2 = \frac{mE \mp \sqrt{[(mE)^2 - (m\omega)^2 \hbar^2 (l + 1/2)^2]}}{(m\omega)^2}. \tag{298}$$

Note that for the harmonic oscillator potential, the energy eigenvalues are positive, as a result of the Sturm-Liouville theorem. As a result,

$$r_2^2 + r_1^2 = \frac{2mE}{(m\omega)^2}, \tag{299}$$

$$r_2^2 - r_1^2 = \frac{2\sqrt{[(mE)^2 - (m\omega)^2 \hbar^2 (l + 1/2)^2]}}{(m\omega)^2}. \tag{300}$$

We have then

$$\begin{aligned}
\epsilon &= \frac{r_2^2 - r_1^2}{r_2^2 + r_1^2} \\
&= \frac{\sqrt{[(mE)^2 - (m\omega)^2 \hbar^2 (l + 1/2)^2]}}{mE} \\
\Rightarrow \epsilon^2 &= \frac{(mE)^2 - (m\omega)^2 \hbar^2 (l + 1/2)^2}{(mE)^2} \\
\Rightarrow 1 - \epsilon^2 &= \frac{(m\omega)^2 \hbar^2 (l + 1/2)^2}{(mE)^2} \\
\Rightarrow \sqrt{1 - \epsilon^2} &= \frac{\hbar\omega (l + 1/2)}{E}.
\end{aligned} \tag{301}$$

By virtue of (296) and (301), the integral (293) becomes

$$\begin{aligned}
&\frac{m\omega}{4} (r_2^2 + r_1^2) \epsilon^2 \int_{-\pi/2}^{\pi/2} d\alpha \frac{\cos^2(\alpha)}{1 + \epsilon \sin \alpha} \\
&= \frac{m\omega}{4} (r_2^2 + r_1^2) \pi \left[1 - \sqrt{1 - \epsilon^2} \right] \\
&= \frac{m\omega}{4} \frac{2mE}{(m\omega)^2} \pi \left[1 - \frac{\hbar\omega (l + 1/2)}{E} \right] \\
&= \frac{\pi}{2\omega} [E - \hbar\omega (l + 1/2)].
\end{aligned} \tag{302}$$

The JWKB quantization rule now reads

$$\frac{\pi}{2\omega} [E - \hbar\omega (l + 1/2)] = \pi \hbar (n_r + 1/2). \tag{303}$$

Whence, we obtain the correct energy eigenvalues for the three-dimensional harmonic oscillator problem

$$E_n = \hbar\omega (n + 3/2), \tag{304}$$

where

$$n = 2n_r + l. \tag{305}$$

b. Three-dimensional Coulomb potential

The Coulomb potential is given by

$$V(r) = -Z \frac{e^2}{r^2}, \tag{306}$$

where Z is the number of elementary positive charges at the center of the potential field, and e is the elementary charge with suitable unit.

For the Coulomb potential problem, the left-hand side of (283) becomes

$$\begin{aligned} & \int_{r_1}^{r_2} \frac{dr}{r} \sqrt{2mEr^2 + 2mZe^2r - \hbar^2(l+1/2)^2} \\ &= \sqrt{-2mE} \int_{r_1}^{r_2} \frac{dr}{r} \sqrt{(r-r_1)(r_2-r)}, \end{aligned} \quad (307)$$

where $E < 0$ as the potential is unbounded below. We proceed as in the harmonic oscillator example and let

$$r = \frac{r_1 + r_2}{2} + \frac{r_2 - r_1}{2} \sin \alpha, \text{ for } \alpha \in \left(-\frac{\pi}{2}, \frac{\pi}{2}\right). \quad (308)$$

It follows that

$$dr = d\alpha \frac{r_2 - r_1}{2} \cos \alpha,$$

and

$$\sqrt{(r-r_1)(r_2-r)} = \frac{r_2 - r_1}{2} \cos \alpha. \quad (309)$$

The integral (307) becomes

$$\begin{aligned} & \sqrt{-2mE} \int_{-\pi/2}^{\pi/2} d\alpha \frac{(r_2 - r_1) \cos \alpha}{(r_1 + r_2) + (r_2 - r_1) \sin \alpha} \frac{r_2 - r_1}{2} \cos \alpha \\ &= (r_1 + r_2) \frac{\sqrt{-2mE}}{2} \epsilon^2 \int_{-\pi/2}^{\pi/2} d\alpha \frac{\cos^2 \alpha}{1 + \epsilon \sin \alpha}, \end{aligned} \quad (310)$$

where

$$\epsilon = \frac{r_2 - r_1}{r_1 + r_2}. \quad (311)$$

With the result for the integral over α (296) in the previous subsection, the integral (310) now becomes

$$(r_1 + r_2) \frac{\sqrt{-2mE}}{2} \pi \left(1 - \sqrt{1 - \epsilon^2}\right). \quad (312)$$

Now, r_1 and r_2 solve

$$x^2 + \frac{Ze^2}{E}x - \frac{\hbar^2(l+1/2)^2}{2mE} = 0, \quad (313)$$

so

$$r_{2,1} = \frac{-Ze^2/E \pm \sqrt{(Ze^2/E)^2 + 2\hbar^2(l+1/2)^2/mE}}{2}. \quad (314)$$

Consequently,

$$\begin{aligned} r_2 + r_1 &= -\frac{Ze^2}{E}, \\ r_2 - r_1 &= \sqrt{(Ze^2/E)^2 + 2\hbar^2(l+1/2)^2/mE}. \end{aligned} \quad (315)$$

We obtain the value of ϵ as defined in (311)

$$\begin{aligned}\epsilon &= \frac{\sqrt{(Ze^2/E)^2 + 2\hbar^2(l+1/2)^2/mE}}{-Ze^2/E} \\ \Rightarrow \sqrt{1-\epsilon^2} &= \sqrt{-\frac{2E}{m} \frac{\hbar(l+1/2)}{Ze^2}}.\end{aligned}\tag{316}$$

With (312), (315), and (316), the JWKB quantization equation for the Coulomb potential problem reads

$$\begin{aligned}-\frac{Ze^2}{E} \frac{\sqrt{-2mE}}{2} \pi \left(1 - \sqrt{-\frac{2E}{m} \frac{\hbar(l+1/2)}{Ze^2}} \right) &= \pi \hbar (n_r + 1/2), \\ \pi Ze^2 \sqrt{\frac{-m}{2E}} - \pi \hbar (l + 1/2) &= \pi \hbar (n_r + 1/2), \\ \sqrt{\frac{-m}{2E}} &= \frac{\hbar(n_r + l + 1)}{Ze^2}.\end{aligned}\tag{317}$$

We obtain the correct expression for the energy eigenvalues of the Coulomb potential

$$E = -\frac{Z^2 me^4}{2\hbar^2} \frac{1}{(n_r + l + 1)^2},\tag{318}$$

where

$$\frac{Z^2 me^4}{2\hbar^2}$$

is the Rydberg constant.

6. Semiclassical propagator for a symmetric linear potential in one dimension

Consider a particle initially at point $x_0 > 0$ in a symmetric linear potential well $V(x) = f|x|$. In order to apply the van Vleck-Gutzwiller formula (160), we have to find the Hamilton principal function for the trajectory in short-time approximation. We consider an end point x_1 which is arbitrary close to x_0 such that $x_1 < x_0$. The reason for this choice is because no matter how small the time duration T of the trip is, we can always find a trajectory from x_0 along the gradient of the potential and backward to point x_1 . We eventually take the coinciding point limit $x_1 \rightarrow x_0$.

On the right branch of the potential, the equation of motion in Newtonian mechanics is

$$\begin{aligned} m \frac{d^2 x}{dt^2} &= -f \\ \implies v(t) &= -\frac{f}{m}t + v_0 \\ \implies x(t) &= -\frac{f}{2m}t^2 + v_0 t + x_0, \end{aligned} \quad (319)$$

where x_0 and v_0 are respectively the initial position and velocity of the particle. By construction, $v_0 > 0$.

The time T when the particle reaches the point x_1 now satisfies

$$-\frac{f}{2m}T^2 + v_0 T + x_0 = x_1, \quad (320)$$

which resolves into

$$T = \frac{mv_0}{f} + \sqrt{\left(\frac{mv_0}{f}\right)^2 + \frac{2m(x_0 - x_1)}{f}}. \quad (321)$$

Inverting this gives v_0 in terms of T

$$v_0 = -\frac{(x_0 - x_1)}{T} + \frac{fT}{2m}. \quad (322)$$

Now the Hamilton principal function along this path is given by

$$\begin{aligned} R(x_1, x_0; T) &= \int_0^T \left[\frac{m}{2}v^2(t) - fx(t) \right] dt \\ &= \frac{f^2}{2m}T^3 - fv_0T^2 + \left(\frac{m}{2}v_0^2 - fx_0 \right) T \\ &= -\frac{f^2}{24m}T^3 - \frac{f(x_0 + x_1)}{2}T + \frac{m(x_0 - x_1)^2}{2T}, \end{aligned} \quad (323)$$

where in the last step, we substitute the expression (322) of v_0 in terms of T . We have now

$$C = -\frac{\partial^2 R}{\partial x_0 \partial x_1} = \frac{m}{T}. \quad (324)$$

So the semiclassical propagator is given by

$$K(x_1, x_0; T) \simeq \sqrt{\frac{m}{2\pi i \hbar T}} \exp\left(-\frac{if^2}{24\hbar m} T^3 - \frac{if(x_0 + x_1)}{2\hbar} T + \frac{im(x_0 - x_1)^2}{2\hbar T}\right). \quad (325)$$

Taking the coinciding point limit gives

$$K(x_0, x_0; T) \simeq \sqrt{\frac{m}{2\pi i \hbar T}} \exp\left(-\frac{if^2}{24\hbar m} T^3 - \frac{ifx_0}{\hbar} T\right). \quad (326)$$

Similar argument for $x_0 < 0$ gives finally for a general point x ,

$$K(x, x; T) \simeq \sqrt{\frac{m}{2\pi i \hbar T}} \exp\left(-\frac{if^2}{24\hbar m} T^3 - \frac{if|x|}{\hbar} T\right). \quad (327)$$

7. Semiclassical propagator for a harmonic oscillator potential in one dimension

We have the equation of motion of a particle in a one-dimensional harmonic oscillator potential $V(x) = \frac{1}{2}m\omega^2x^2$

$$m\ddot{x} = -m\omega^2x, \quad (328)$$

whose solution is given by

$$x(t) = A \cos(\omega t) + B \sin(\omega t). \quad (329)$$

Consider the initial conditions $x(0) = x_0$, $v(0) = v_0$, where we assume $v_0x_0 > 0$. Assume for now $x_0 > 0$, we have

$$\begin{aligned} A &= x_0, \\ B &= \frac{v_0}{\omega}. \end{aligned} \quad (330)$$

So the trajectory is given by

$$x(t) = x_0 \cos(\omega t) + \frac{v_0}{\omega} \sin(\omega t), \quad (331)$$

with velocity

$$\dot{x}(t) = -\omega x_0 \sin(\omega t) + v_0 \cos(\omega t). \quad (332)$$

The particle reaches a point $x_1 < x_0$ arbitrarily close to x_0 at a time T satisfying

$$x_0 \cos(\omega T) + \frac{v_0}{\omega} \sin(\omega T) = x_1. \quad (333)$$

Let $0 \leq \alpha \leq \pi/2$ satisfy

$$\begin{aligned} \sin \alpha &= \frac{x_0}{\sqrt{x_0^2 + v_0^2/\omega^2}}, \\ \cos \alpha &= \frac{v_0/\omega}{\sqrt{x_0^2 + v_0^2/\omega^2}}. \end{aligned} \quad (334)$$

Equation (333) becomes

$$\sin(\omega T + \alpha) = \frac{x_1}{\sqrt{x_0^2 + v_0^2/\omega^2}} < 1, \quad (335)$$

and we shall choose the smallest positive T satisfying the above equation. Inverting relation (333) gives

$$v_0 = \frac{\omega}{\sin(\omega T)} (x_1 - x_0 \cos(\omega T)). \quad (336)$$

Now the Hamilton principal function is given by

$$R(x_1, x_0; T) = \int_0^T \left[\frac{m}{2} \dot{x}^2(t) - \frac{m}{2} \omega^2 x^2(t) \right] dt. \quad (337)$$

An integration by parts gives

$$R(x_1, x_0; T) = \frac{m}{2} \dot{x}(t) x(t) \Big|_0^T - \int_0^T \left[\frac{m}{2} \ddot{x}(t) x(t) + \frac{m}{2} \omega^2 x^2(t) \right] dt. \quad (338)$$

Since $x(t)$ is the classical trajectory, satisfying (328), the integral in the last equation vanishes, and we are left with the boundary terms. Substituting (331) and (332) for $x(t)$ and $\dot{x}(t)$ into (338) gives

$$R(x_1, x_0; T) = -\frac{m\omega}{2} \left[\frac{2x_0 v_0}{\omega} \sin^2(\omega T) + \left(x_0^2 - \frac{v_0^2}{\omega^2} \right) \sin(\omega T) \cos(\omega T) \right]. \quad (339)$$

Finally, substituting the inverted relation (336) of v_0 in terms of T into (339) gives

$$R(x_1, x_0; T) = \frac{m\omega}{2 \sin(\omega T)} \left[(x_0^2 + x_1^2) \cos(\omega T) - 2x_0 x_1 \right]. \quad (340)$$

By the same token, we have the same expression for the Hamilton principal function for $x_0 < 0$, and $x_1 > x_0$ arbitrarily close to x_0 .

We have then

$$C = -\frac{\partial^2 R}{\partial x_0 \partial x_1} = \frac{m\omega}{\sin(\omega T)}, \quad (341)$$

and the semiclassical propagator is given by

$$K(x_1, x_0; T) = \sqrt{\frac{m\omega}{2\pi i \hbar |\sin(\omega T)|}} \exp \left\{ \frac{i m \omega}{2 \hbar \sin(\omega T)} \left[(x_0^2 + x_1^2) \cos(\omega T) - 2x_0 x_1 \right] - \frac{i \kappa \pi}{2} \right\}, \quad (342)$$

where κ is the number of times the quantity $\sin(\omega T)$ changes sign along the trajectory from $t = 0$ to $t = T$. It is hence the largest integer smaller than $\frac{\omega T}{\pi}$

$$\kappa = \left\lfloor \frac{\omega T}{\pi} \right\rfloor. \quad (343)$$

The semiclassical propagator in this case turns out to be exact as the potential is quadratic (see [35]). We even know the correct phase.

LIST OF FIGURES

1	A typical potential in one dimension with two turning points.....	10
2	Exact wave function and its semiclassical approximation for mode $n = 0$ of a one-dimensional Morse potential	14
3	Exact wave function and its semiclassical approximation for mode $n = 1$ of a one-dimensional Morse potential	14
4	Exact wave function and its semiclassical approximation for mode $n = 2$ of a one-dimensional Morse potential	15
5	Exact wave function and its semiclassical approximation for mode $n = 3$ of a one-dimensional Morse potential	15
6	Exact, TF, and semiclassical densities for two particles in a one-dimensional Morse potential	17
7	Exact, TF, and semiclassical densities for one particle in a one-dimensional Morse potential	19
8	Exact, TF, and semiclassical densities (dominant term) for two particles in a one-dimensional Morse potential	19
9	Exact, TF, and semiclassical densities (dominant term) for one particle in a three-dimensional harmonic oscillator potential	29
10	Exact, TF, and semiclassical densities (dominant term) for four particles in a three-dimensional harmonic oscillator potential	29
11	Exact, TF, and semiclassical densities (dominant term) for 10 particles in a three-dimensional harmonic oscillator potential	30
12	Exact, TF, and semiclassical densities (dominant term) for one particle in a three-dimensional Coulomb potential	32
13	Exact, TF, and semiclassical densities (dominant term) for two particles in a three-dimensional Coulomb potential	32
14	Exact, TF, and semiclassical densities (dominant term) for five particles in a three-dimensional Coulomb potential	33
15	Exact, TF, and semiclassical densities (dominant term) for six particles in a three-dimensional Coulomb potential	33

16	Exact wave function and its semiclassical approximation for mode $n_s = 0, l = 0$ of a two-dimensional harmonic oscillator potential	36
17	Exact wave function and its semiclassical approximation for mode $n_s = 1, l = 0$ of a two-dimensional harmonic oscillator potential	37
18	Exact wave function and its semiclassical approximation for mode $n_s = 2, l = 0$ of a two-dimensional harmonic oscillator potential	37
19	Exact and semiclassical radial densities (dominant term) for the first two orbitals with $l = 0$ of a two-dimensional harmonic oscillator potential	41
20	Exact, Thomas-Fermi and semiclassical densities for the first two orbitals with $l = 0$ of a two-dimensional harmonic oscillator potential	43
21	Exact, TF, and semiclassical densities for one particle in a two-dimensional harmonic oscillator potential	45
22	Exact, TF, and semiclassical densities for three particle in a two-dimensional harmonic oscillator potential	46
23	Exact, TF, and semiclassical densities for six particles in a two-dimensional harmonic oscillator potential	46
24	Exact wave function and its semiclassical approximation for mode $n_s = 2, l = 0$ of a two-dimensional Coulomb potential	48
25	Exact, TF, and semiclassical densities for one particle in a two-dimensional Coulomb potential	49
26	Exact, TF, and semiclassical densities for four particles in a two-dimensional Coulomb potential	49
27	Exact, TF, and semiclassical densities for nine particles in a two-dimensional Coulomb potential	50
28	Classical orbit in short-time approximation	57
29	Exact, TF, and semiclassical densities for three particles in a one-dimensional symmetric linear potential	63

LIST OF TABLES

I	Orbitals of the four smallest values of the principal quantum number for a three-dimensional harmonic oscillator	27
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II	Aufbau rule for filling electrons in orbitals	31
III	Orbitals corresponding to the first four values of the principal quantum number for the two-dimensional harmonic oscillator potential.	44
IV	Orbitals corresponding to the first three values of the principal quantum number for the two-dimensional Coulomb potential.	47
V	The first 20 energy eigenvalues for the symmetric linear potential	60

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