Problem 19

Summary of Approach

First, I calculate the equation that the exact energy eigenvalues must satisfy. Then I give a strategy for calculating the form of the exact eigenstates, and I show them graphically for a certain setup. Then, I calculate an approximate form for the energy eigenvalues for both large n and small L. I do this in two ways: by considering the asymptotic behavior of the exact wavefunction, and by using a WKB approximation. Lastly, I answer some of the further questions.

Many of the numerical calculations and plotting done in this solution can be found in the attached Mathematica notebook.

Exact Solution

The Hamiltonian in this problem is

$$H = \frac{P^2}{2m} + V(X),$$

where $V(X)$ in the X-basis is given by

$$V(x) = \begin{cases} \infty & x \geq L \\ Fx & 0 < x < L \\ \infty & x \leq 0. \end{cases}$$

First, we solve the time-independent Schrodinger equation for $0 < x < L$ and consider the boundary condition $\psi(0) = \psi(L) = 0$ afterwards.

$$\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + Fx\right)\psi(x) = E\psi(x)$$
$$\psi''(x) = \frac{2m(Fx - E)}{\hbar^2}\psi(x).$$

Let us now make the substitutions $u = x - E/F$ and $k = (2mF/\hbar^2)^{1/2}$. The differential equation becomes

$$\psi''(u) - k^2 u\psi(u) = 0. \tag{1}$$

We recognize (1) as the Airy equation. Its solutions are given by

$$\psi(u) = A\ \mathrm{Ai}(k^{2/3}u) + B\ \mathrm{Bi}(k^{2/3}u). \tag{2}$$

Taking into account the boundary conditions, we have the system of equations:

$$A\ \mathrm{Ai}\left[k^{2/3}\left(-\frac{E}{F}\right)\right] + B\ \mathrm{Bi}\left[k^{2/3}\left(-\frac{E}{F}\right)\right] = 0$$
$$A\ \mathrm{Ai}\left[k^{2/3}\left(L-\frac{E}{F}\right)\right] + B\ \mathrm{Bi}\left[k^{2/3}\left(L-\frac{E}{F}\right)\right] = 0.$$

Here, let us introduce the shorthand

$$\alpha = \frac{k^{2/3}E}{F} = \left(\frac{2m}{\hbar^2 F^2}\right)^{1/3} E$$
$$\beta = k^{2/3}L = \left(\frac{2mF}{\hbar^2}\right)^{1/3} L.$$

Note that α can be interpreted as a non-dimensional parameter for E, and β can be interpreted as a non-dimensional parameter for L. There exists a non-trivial solution to A and B in the previous system of equations only if

$$\det(\alpha,\beta) \equiv \mathrm{Ai}(-\alpha)\ \mathrm{Bi}(\beta-\alpha) - \mathrm{Ai}(\beta-\alpha)\ \mathrm{Bi}(-\alpha) = 0. \tag{3}$$

$\det(\alpha,\beta)$ is shown as a contour plot in Figure 1.

To illustrate some of the first few stationary energy eigenfunctions, we select $\beta = 10$. Then, we solve, numerically, for the first few values of α such that $\det(\alpha, 10) = 0$. We use these values of (α,β) to calculate the values of A and B, as defined in the system of equations found above:

$$A\ \mathrm{Ai}(-\alpha) + B\ \mathrm{Bi}(-\alpha) = 0.$$

Then, the un-normalized eigenstates are given by

$$\psi(y) = \mathrm{Ai}(y) + \frac{B}{A}\mathrm{Bi}(y),$$

on the domain $y \in [\alpha, \beta-\alpha]$. We plot the first 9 eigenstates in Figure 2.

Larger Energy Eigenvalues

To find a simpler formula for larger energy eigenvalues, we examine our method in the limit $\alpha \to \infty$. The limiting behavior of the Airy functions in this limit is:

$$\mathrm{Ai}(y) \approx \left(\frac{1}{\pi^2|y|}\right)^{1/4} \sin\left(\frac{2}{3}|y|^{3/2} + \frac{\pi}{4}\right)$$
$$\mathrm{Bi}(y) \approx \left(\frac{1}{\pi^2|y|}\right)^{1/4} \cos\left(\frac{2}{3}|y|^{3/2} + \frac{\pi}{4}\right)$$

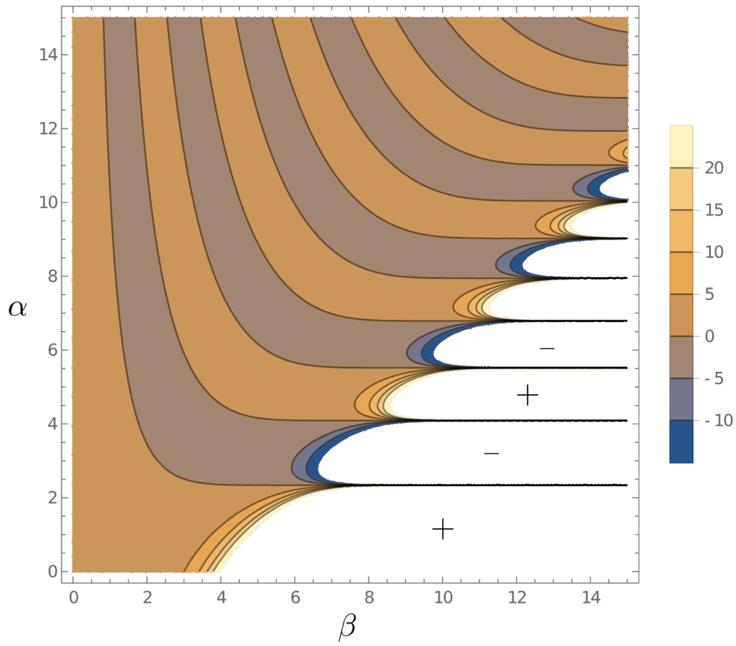

Figure 1: A contour plot of $\det(\alpha, \beta)$. α is proportional to the energy eigenvalue and β is proportional to the length of the box, so the curves $\det(\alpha, \beta) = 0$ are the plots of the lower energy eigenvalues as a function of box length.

Thus, our condition $\det(\alpha, \beta) = 0$ reduces to

$$\sin\left(\frac{2}{3}\alpha^{3/2} + \frac{\pi}{4}\right)\cos\left[\frac{2}{3}(\alpha-\beta)^{3/2} + \frac{\pi}{4}\right] = \sin\left[\frac{2}{3}(\alpha-\beta)^{3/2} + \frac{\pi}{4}\right]\cos\left(\frac{2}{3}\alpha^{3/2} + \frac{\pi}{4}\right)$$

$$\implies \qquad \tan\left(\frac{2}{3}\alpha^{3/2} + \frac{\pi}{4}\right) = \tan\left[\frac{2}{3}(\alpha-\beta)^{3/2} + \frac{\pi}{4}\right].$$

This means that the bracketed quantities must be separated by integral values of π. This gives

$$\alpha^{3/2} - (\alpha-\beta)^{3/2} = \frac{3\pi n}{2}.$$

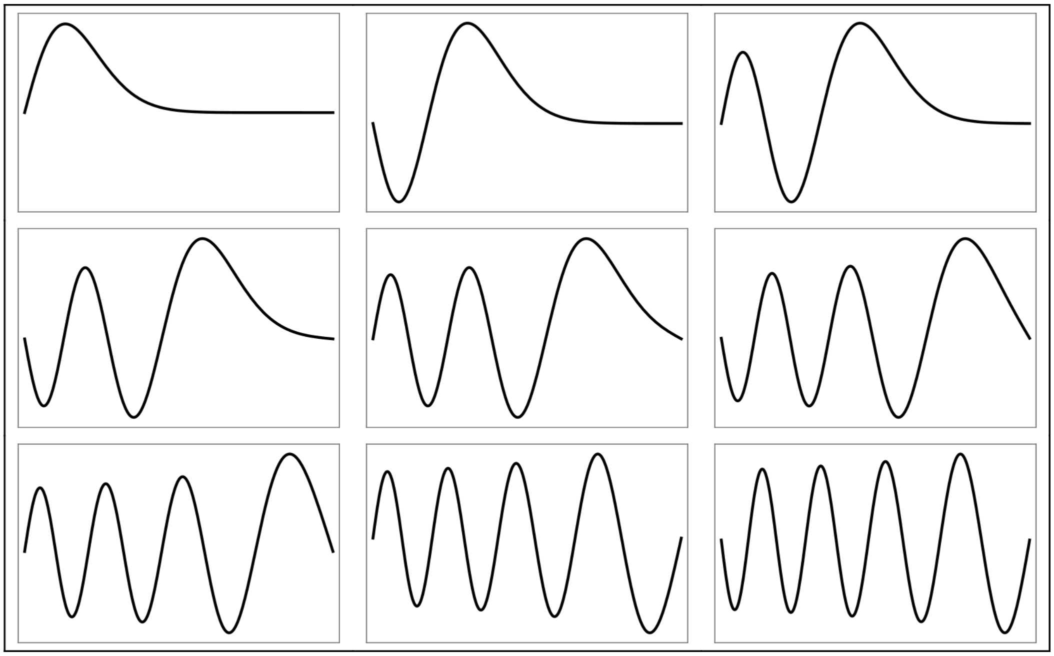

Figure 2: The first 9 un-normalized energy eigenstates with $\beta = 10$.

Since we work under the assumption that we are examining large eigenvalues, we can assume that $\alpha \gg \beta$. Under this approximation,

$$\begin{aligned} \alpha^{3/2}\left[1-\left(1-\frac{\beta}{\alpha}\right)^{3/2}\right] &= \frac{3}{2}\beta\alpha^{1/2} \\ \implies \qquad \alpha &= \frac{\pi^2 n^2}{\beta^2} \\ \implies \qquad E &= \frac{\hbar^2\pi^2 n^2}{2mL^2}. \end{aligned}$$

Of course, this is the well known quantization formula for the particle in a normal box.

Semi-classical (WKB) approximation

The turning points are $x = 0$ and L. The quantization condition is given by

$$\int_0^L \left[2m(E_n - Fx)\right]^{1/2}\ \mathrm{d}x = n\pi\hbar.$$

Integrating this, we have

$$
\begin{aligned}
n\pi\hbar &= -(2mF)^{1/2}\left(\frac{2}{3}\right)\left[-x+\frac{E_n}{F}\right]^{3/2}\Bigg|_0^L \\
&= \left(\frac{2}{3}\right)(2mF)^{1/2}\left[-\left(-L+\frac{E_n}{F}\right)^{3/2}+\left(\frac{E_n}{F}\right)^{3/2}\right] \\
n\pi &= \left(\frac{2}{3}\right)\left\{-\left[-\left(\frac{2mF}{\hbar^2}\right)^{1/3}L+\left(\frac{2m}{\hbar^2F^2}\right)^{1/3}E_n\right]^{3/2}+\left[\left(\frac{2m}{\hbar^2F^2}\right)^{1/3}E_n\right]^{3/2}\right\} \\
\frac{3\pi n}{2} &= \alpha^{3/2}-(\alpha-\beta)^{3/2},
\end{aligned}
$$

which is the same quantization condition as our previous approximation. Let us compare this formula to some of the known levels of α as calculated by the exact formula (3). Figure 3 shows a plot of $\det(\alpha,\beta)$ as well as the lowest energy eigenvalues α as calculated by the semi-classical approximation. There is an excellent match for $\beta=1$, a relatively low value of β.

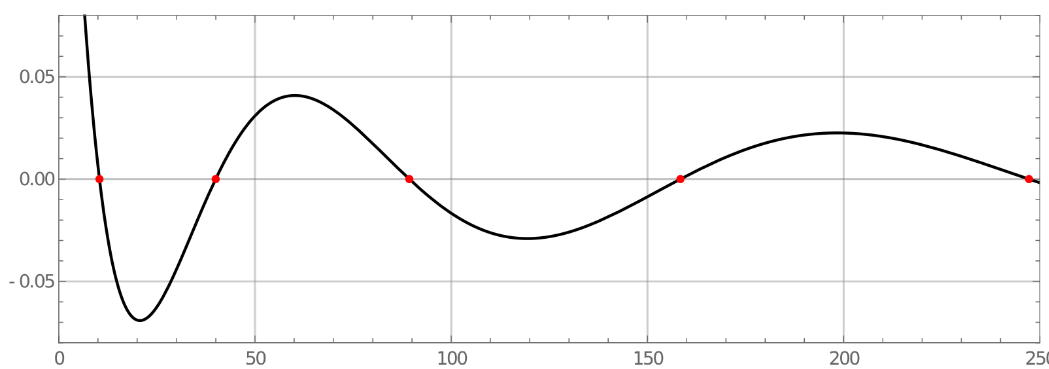

Figure 3: A comparison of the exact eigenvalues α (the roots of the black curve $\det(\alpha,\beta=1)$), and the approximated eigenvalues (the red points).

The approximation breaks down for larger values of β. This occurs because the lowest energy eigenvalues obey $\alpha<\beta$. However, our formula for the asymptotic behavior of the Airy functions required that $\beta-\alpha<0$. Hence, the lowest energy eigenvalues are incalculable with the approximation. However, the higher energy eigenvalues calculated by the approximation still match very well. Figure 4 is the same as Figure 3, but shows the situation for $\beta=10$.

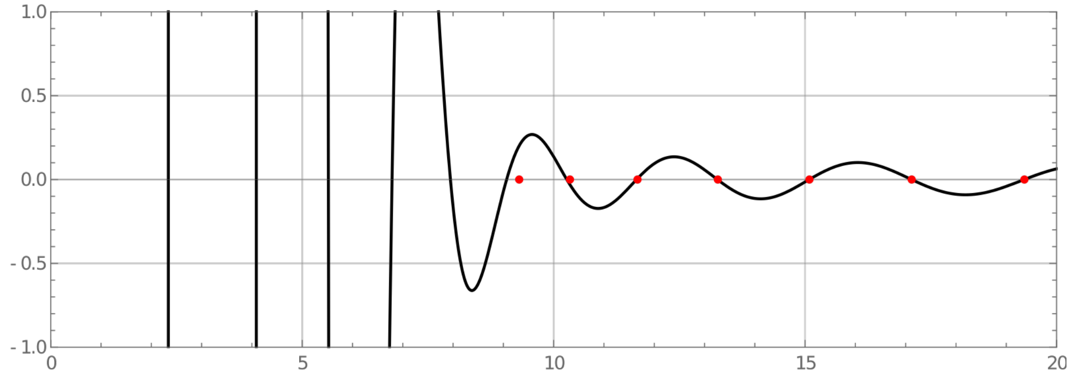

Figure 4: A comparison of the exact eigenvalues α (the roots of the black curve $\det(\alpha, \beta)$ and the approximated eigenvalues (the red points), for $\beta = 10$. The first five eigenvalues cannot be calculated with the approximation, but the larger eigenvalues match the exact ones well.

Further Questions

(a) For small L, the approximation being made is identical to that of large energy. In both cases, $\alpha \gg \beta$.

(b) For what parameters will the ground state energy equal FL? Note that at $E = FL$, $\alpha = \beta$. By examining the plot in Figure 1, we see that there are many (α, β) that satisfy both $\alpha = \beta$ and $\det(\alpha, \beta) = 0$. However, only one such point is a ground state. By inspection that point is near $(3, 3)$. The exact location, which can be found numerically, is $(2.666, 2.666)$. For α and β to take on these values, the parameters of the problem will satisfy

$$\frac{mFL^3}{\hbar^2} = 9.47.$$

(c) It is clear just from examining Figure 1 that for all $\beta < 2.666$, the first ground state will be larger than $E = FL$, or $\alpha = 2.666$.

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