PHYS 660 - Quantum Mechanics I

Modern Quantum Mechanics by *J. J. Sakurai*

Student: **Ralph Razzouk**

Homework 3

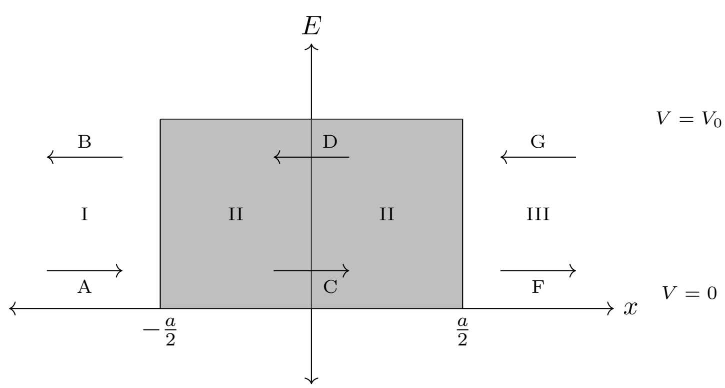
Problem 1

Consider an inverted square-well potential

$$V(x) = \begin{cases} V_0, & \text{if } |x| < \frac{a}{2}, \\ 0, & \text{if } |x| > \frac{a}{2}, \end{cases}$$

with $V_0 > 0$. Compute the scattering matrix S and the reflection and transmission coefficients. Consider both cases, $0 < E < V_0$ and $V_0 < E$. Check the unitarity and symmetries of S. Plot the transmission coefficient as a function of energy. Choose the parameters such that there are well-defined resonance peaks.

Proof. The system given looks like the following



The Hamiltonian of the system is given by

$$H = \frac{p^2}{2m} + V_0.$$

Notice that we have symmetry under parity inversion.

$\boxed{\text{For } 0 < E < V_0:}$

- **Region I**: The Schrodinger equation is given by

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi.$$

We are looking for a solution of the form

$$\psi_I(x) = c\mathrm{e}^{ikx},$$

where c is an arbitrary constant.

By separation of variables, we have that our constant k should be

$$k = \pm\frac{\sqrt{2mE}}{\hbar}.$$

Thus, the solution to the Schrodinger equation is given by

$$\psi_I(x) = A\mathrm{e}^{ikx} + B\mathrm{e}^{-ikx}.$$

- **Region II**: The Schrodinger equation is given by

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V_0\psi = E\psi.$$

We are looking for a solution of the form

$$\psi_{II}(x) = c\mathrm{e}^{ik'x},$$

where c is an arbitrary constant.

Similarly, by separation of variables, we have that our constant k should be

$$k' = \pm\frac{\sqrt{2m(E-V_0)}}{\hbar}, \quad (E - V_0 < 0).$$

This means that k' is an imaginary number. We could denote $k' = i\kappa$, where $\kappa = \frac{\sqrt{2m(V_0-E)}}{\hbar}$, but we will stick with the k' notation, keeping in mind that it is imaginary.

The solution to the Schrodinger equation is given by

$$\psi_{II}(x) = C\mathrm{e}^{ik'x} + D\mathrm{e}^{-ik'x}.$$

- **Region III**: Similar to Region I, the solution to the Schrodinger equation is given by

$$\psi_{III}(x) = F\mathrm{e}^{ikx} + G\mathrm{e}^{-ikx}.$$

For the second order partial differential equation to be defined, the wave function ψ and it's first derivative must be continuous. More formally, the wave function should be once-differentiable and belong to the first differentiability class, *i.e.* $\psi \in \mathcal{C}^1$. Thus, we must evaluate our wave function solutions and their derivatives at $x = \pm\frac{a}{2}$ and force continuity.
Applying boundary conditions at $x = -\frac{a}{2}$, we have

$$\begin{cases} \psi_I\left(-\frac{a}{2}\right) = \psi_{II}\left(-\frac{a}{2}\right) \\ \frac{\partial}{\partial x}\psi_I(x)\big|_{-\frac{a}{2}} = \frac{\partial}{\partial x}\psi_{II}(x)\big|_{-\frac{a}{2}} \end{cases} \implies \begin{cases} A\mathrm{e}^{-ik\frac{a}{2}} + B\mathrm{e}^{ik\frac{a}{2}} = C\mathrm{e}^{-ik'\frac{a}{2}} + D\mathrm{e}^{ik'\frac{a}{2}} \\ ikA\mathrm{e}^{-ik\frac{a}{2}} - ikB\mathrm{e}^{ik\frac{a}{2}} = ik'C\mathrm{e}^{-ik'\frac{a}{2}} - ik'D\mathrm{e}^{ik'\frac{a}{2}} \end{cases}$$

which gives us

$$\begin{pmatrix} \mathrm{e}^{-ik\frac{a}{2}} & \mathrm{e}^{ik\frac{a}{2}} \\ ik\mathrm{e}^{-ik\frac{a}{2}} & -ik\mathrm{e}^{ik\frac{a}{2}} \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} \mathrm{e}^{-ik'\frac{a}{2}} & \mathrm{e}^{ik'\frac{a}{2}} \\ ik'\mathrm{e}^{-ik'\frac{a}{2}} & -ik'\mathrm{e}^{ik'\frac{a}{2}} \end{pmatrix}\begin{pmatrix} C \\ D \end{pmatrix}$$

Taking the inverse of the matrix on the right hand side, we get

$$\begin{aligned}
\begin{pmatrix} C \\ D \end{pmatrix} &= \frac{1}{-2ik'}\begin{pmatrix} -ik'\mathrm{e}^{ik'\frac{a}{2}} & -\mathrm{e}^{ik'\frac{a}{2}} \\ -ik'\mathrm{e}^{-ik'\frac{a}{2}} & \mathrm{e}^{-ik'\frac{a}{2}} \end{pmatrix}\begin{pmatrix} \mathrm{e}^{-ik\frac{a}{2}} & \mathrm{e}^{ik\frac{a}{2}} \\ ik\mathrm{e}^{-ik\frac{a}{2}} & -ik\mathrm{e}^{ik\frac{a}{2}} \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix} \\
&= \frac{1}{-2ik'}\begin{pmatrix} -ik'\mathrm{e}^{ik'\frac{a}{2}}\mathrm{e}^{-ik\frac{a}{2}} - ik\mathrm{e}^{ik'\frac{a}{2}}\mathrm{e}^{-ik\frac{a}{2}} & -ik'\mathrm{e}^{ik'\frac{a}{2}}\mathrm{e}^{ik\frac{a}{2}} + ik\mathrm{e}^{ik'\frac{a}{2}}\mathrm{e}^{ik\frac{a}{2}} \\ -ik'\mathrm{e}^{-ik'\frac{a}{2}}\mathrm{e}^{-ik\frac{a}{2}} + ik\mathrm{e}^{-ik'\frac{a}{2}}\mathrm{e}^{-ik\frac{a}{2}} & -ik'\mathrm{e}^{-ik'\frac{a}{2}}\mathrm{e}^{ik\frac{a}{2}} - ik\mathrm{e}^{-ik'\frac{a}{2}}\mathrm{e}^{ik\frac{a}{2}} \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix} \\
&= \frac{1}{2k'}\begin{pmatrix} (k+k')\mathrm{e}^{-i(k-k')\frac{a}{2}} & (-k+k')\mathrm{e}^{i(k+k')\frac{a}{2}} \\ (-k+k')\mathrm{e}^{-i(k+k')\frac{a}{2}} & (k+k')\mathrm{e}^{i(k-k')\frac{a}{2}} \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix}.
\end{aligned}$$

The large factor is the transfer matrix given from region I to region II.
Applying boundary conditions at $x = \frac{a}{2}$, we have

$$\begin{cases} \psi_{II}\left(\frac{a}{2}\right) = \psi_{III}\left(\frac{a}{2}\right) \\ \frac{\partial}{\partial x}\psi_{II}(x)\big|_{\frac{a}{2}} = \frac{\partial}{\partial x}\psi_{III}(x)\big|_{\frac{a}{2}} \end{cases} \implies \begin{cases} C\mathrm{e}^{ik'\frac{a}{2}} + D\mathrm{e}^{-ik'\frac{a}{2}} = F\mathrm{e}^{ik\frac{a}{2}} + G\mathrm{e}^{-ik\frac{a}{2}} \\ ik'C\mathrm{e}^{ik'\frac{a}{2}} - ik'D\mathrm{e}^{-ik'\frac{a}{2}} = ikF\mathrm{e}^{ik\frac{a}{2}} - ikG\mathrm{e}^{-ik\frac{a}{2}} \end{cases}$$

which gives us

$$\begin{pmatrix} e^{ik'\frac{a}{2}} & e^{-ik'\frac{a}{2}} \\ ik'e^{ik'\frac{a}{2}} & -ik'e^{-ik'\frac{a}{2}} \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} e^{ik\frac{a}{2}} & e^{-ik\frac{a}{2}} \\ ike^{ik\frac{a}{2}} & -ike^{-ik\frac{a}{2}} \end{pmatrix} \begin{pmatrix} F \\ G \end{pmatrix}$$

Taking the inverse of the matrix on the right hand side, we get

$$\begin{aligned}
\begin{pmatrix} F \\ G \end{pmatrix} &= \frac{1}{-2ik} \begin{pmatrix} -ike^{-ik\frac{a}{2}} & -e^{-ik\frac{a}{2}} \\ -ike^{ik\frac{a}{2}} & e^{ik\frac{a}{2}} \end{pmatrix} \begin{pmatrix} e^{ik'\frac{a}{2}} & e^{-ik'\frac{a}{2}} \\ ik'e^{ik'\frac{a}{2}} & -ik'e^{-ik'\frac{a}{2}} \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} \\
&= \frac{1}{-2ik} \begin{pmatrix} -ike^{-ik\frac{a}{2}}e^{ik'\frac{a}{2}} - ik'e^{-ik\frac{a}{2}}e^{ik'\frac{a}{2}} & -ike^{-ik\frac{a}{2}}e^{-ik'\frac{a}{2}} + ik'e^{-ik\frac{a}{2}}e^{-ik'\frac{a}{2}} \\ -ike^{ik\frac{a}{2}}e^{ik'\frac{a}{2}} + ik'e^{ik\frac{a}{2}}e^{ik'\frac{a}{2}} & -ike^{ik\frac{a}{2}}e^{-ik'\frac{a}{2}} - ik'e^{ik\frac{a}{2}}e^{-ik'\frac{a}{2}} \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} \\
&= \frac{1}{2k} \begin{pmatrix} (k+k')e^{-i(k-k')\frac{a}{2}} & (k-k')e^{-i(k+k')\frac{a}{2}} \\ (k-k')e^{i(k+k')\frac{a}{2}} & (k+k')e^{i(k-k')\frac{a}{2}} \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix}.
\end{aligned}$$

The large factor is the transfer matrix given from region II to region III.
Thus, we have

$$\begin{aligned}
\begin{pmatrix} F \\ G \end{pmatrix} &= \frac{1}{4kk'} \begin{pmatrix} (k+k')e^{-i(k-k')\frac{a}{2}} & (k-k')e^{-i(k+k')\frac{a}{2}} \\ (k-k')e^{i(k+k')\frac{a}{2}} & (k+k')e^{i(k-k')\frac{a}{2}} \end{pmatrix} \begin{pmatrix} (k+k')e^{-i(k-k')\frac{a}{2}} & (-k+k')e^{i(k+k')\frac{a}{2}} \\ (-k+k')e^{-i(k+k')\frac{a}{2}} & (k+k')e^{i(k-k')\frac{a}{2}} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} \\
&= \frac{1}{4kk'} \begin{pmatrix} (k+k')^2e^{-i(k-k')a} - (k-k')^2e^{-i(k+k')a} & -(k+k')(k-k')e^{ik'a} + (k+k')(k-k')e^{-ik'a} \\ (k+k')(k-k')e^{ik'a} - (k+k')(k-k')e^{-ik'a} & -(k-k')^2e^{i(k+k')a} + (k+k')^2e^{i(k-k')a} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} \\
&= \frac{1}{4kk'} \begin{pmatrix} (k+k')^2e^{-i(k-k')a} - (k-k')^2e^{-i(k+k')a} & -(k+k')(k-k')\left(e^{ik'a} - e^{-ik'a}\right) \\ (k+k')(k-k')\left(e^{ik'a} - e^{-ik'a}\right) & -(k-k')^2e^{i(k+k')a} + (k+k')^2e^{i(k-k')a} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} \\
&= \frac{1}{4kk'} \begin{pmatrix} (k+k')^2e^{-i(k-k')a} - (k-k')^2e^{-i(k+k')a} & -2i(k+k')(k-k')\sin(k'a) \\ 2i(k+k')(k-k')\sin(k'a) & -(k-k')^2e^{i(k+k')a} + (k+k')^2e^{i(k-k')a} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix}
\end{aligned}$$

Define $k_\pm = k \pm k'$, which reduces our total transfer matrix to

$$\begin{pmatrix} F \\ G \end{pmatrix} = \begin{pmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \frac{1}{4kk'} \begin{pmatrix} k_+^2e^{-ik_-a} - k_-^2e^{-ik_+a} & -2ik_+k_-\sin(k'a) \\ 2ik_+k_-\sin(k'a) & -k_-^2e^{ik_+a} + k_+^2e^{ik_-a} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix}$$

The scattering matrix is given by

$$S = \begin{pmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{pmatrix}$$

such that

$$\begin{pmatrix} G \\ A \end{pmatrix} = S \begin{pmatrix} B \\ F \end{pmatrix}.$$

This means that

$$\begin{cases} F = t_{11}A + t_{12}B, \\ G = t_{21}A + t_{22}B, \end{cases} \implies \begin{cases} A = \frac{1}{t_{11}}F - \frac{t_{12}}{t_{11}}B, \\ G = \frac{t_{21}}{t_{11}}F + \frac{1}{t_{11}}\left(t_{11}t_{22} - t_{12}t_{21}\right)B, \end{cases}$$

where $t_{11}t_{22} - t_{12}t_{21}$ is the determinant of the transfer matrix, which is equal to 1. Thus,

$$\begin{cases} A = -\frac{t_{12}}{t_{11}}B + \frac{1}{t_{11}}F, \\ G = \frac{1}{t_{11}}B + \frac{t_{21}}{t_{11}}F. \end{cases}$$

Rewriting this, we have

$$\begin{pmatrix} G \\ A \end{pmatrix} = \frac{1}{t_{11}} \begin{pmatrix} 1 & t_{21} \\ -t_{12} & 1 \end{pmatrix} \begin{pmatrix} B \\ F \end{pmatrix}.$$

Therefore, the scattering matrix S is given by

$$\begin{aligned}
S = \begin{pmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{pmatrix} &= \frac{4kk'}{k_+^2 \mathrm{e}^{-ik_- a} - k_-^2 \mathrm{e}^{-ik_+ a}} \begin{pmatrix} 1 & \frac{2ik_+k_-}{4kk'} \sin(k'a) \\ \frac{2ik_+k_-}{4kk'} \sin(k'a) & 1 \end{pmatrix} \\
&= \frac{2}{k_+^2 \mathrm{e}^{-ik_- a} - k_-^2 \mathrm{e}^{-ik_+ a}} \begin{pmatrix} 2kk' & ik_+k_- \sin(k'a) \\ ik_+k_- \sin(k'a) & 2kk' \end{pmatrix} \\
&= \frac{2}{(k+k')^2 \mathrm{e}^{-i(k-k')a} - (k-k')^2 \mathrm{e}^{-i(k+k')a}} \begin{pmatrix} 2kk' & i(k+k')(k-k')\sin(k'a) \\ i(k+k')(k-k')\sin(k'a) & 2kk' \end{pmatrix} \\
&= \frac{2\mathrm{e}^{ika}}{(k^2+2kk'+k'^2)\mathrm{e}^{ik'a} - (k^2-2kk'+k'^2)\mathrm{e}^{-ik'a}} \begin{pmatrix} 2kk' & i(k^2-k'^2)\sin(k'a) \\ i(k^2-k'^2)\sin(k'a) & 2kk' \end{pmatrix} \\
&= \frac{2\mathrm{e}^{ika}}{(k^2+k'^2)\left(\mathrm{e}^{ik'a} - \mathrm{e}^{-ik'a}\right) + 2kk'\left(\mathrm{e}^{ik'a} + \mathrm{e}^{-ik'a}\right)} \begin{pmatrix} 2kk' & i(k^2-k'^2)\sin(k'a) \\ i(k^2-k'^2)\sin(k'a) & 2kk' \end{pmatrix} \\
&= \frac{\mathrm{e}^{ika}}{(k^2+k'^2)i\sin(k'a) + 2kk'\cos(k'a)} \begin{pmatrix} 2kk' & i(k^2-k'^2)\sin(k'a) \\ i(k^2-k'^2)\sin(k'a) & 2kk' \end{pmatrix} \\
&= \frac{\mathrm{e}^{ika}}{(k^2+k'^2)\sin(k'a) + 2ikk'\cos(k'a)} \begin{pmatrix} 2ikk' & -(k^2-k'^2)\sin(k'a) \\ -(k^2-k'^2)\sin(k'a) & 2ikk' \end{pmatrix}.
\end{aligned}$$

The transmission coefficient is given by

$$\begin{aligned}
T &= |s_{11}|^2 \\
&= \left| \frac{2ikk'\mathrm{e}^{ika}}{(k^2+k'^2)\sin(k'a) + 2ikk'\cos(k'a)} \right|^2 \\
&= \frac{4k^2k'^2}{(k^2+k'^2)^2\sin^2(k'a) + 4k^2k'^2\cos^2(k'a)} \\
&= \frac{4k^2k'^2}{(k^2-k'^2)^2\sin^2(k'a) + 4k^2k'^2} \\
&= \frac{1}{\frac{(k^2-k'^2)^2\sin^2(k'a)}{4k^2k'^2} + 1}.
\end{aligned}$$

The reflection coefficient is given by

$$\begin{aligned}
R &= |s_{21}|^2 \\
&= \left| \frac{-(k^2-k'^2)\sin(k'a)\mathrm{e}^{ika}}{(k^2+k'^2)\sin(k'a) + 2ikk'\cos(k'a)} \right|^2 \\
&= \frac{(k^2-k'^2)^2\sin^2(k'a)}{(k^2+k'^2)^2\sin^2(k'a) + 4k^2k'^2\cos^2(k'a)} \\
&= \frac{(k^2-k'^2)^2\sin^2(k'a)}{(k^2-k'^2)^2\sin^2(k'a) + 4k^2k'^2} \\
&= \frac{1}{1 + \frac{4k^2k'^2}{(k^2-k'^2)^2\sin^2(k'a)}}.
\end{aligned}$$

Checking the unitarity of S, we have

$$\begin{aligned}
SS^\dagger &= \frac{\mathrm{e}^{ika}\mathrm{e}^{-ika}}{(k^2+k'^2)^2\sin^2(k'a) + 4k^2k'^2\cos^2(k'a)} \begin{pmatrix} 4k^2k'^2 + (k^2-k'^2)^2\sin^2(k'a) & 0 \\ 0 & 4k^2k'^2 + (k^2-k'^2)^2\sin^2(k'a) \end{pmatrix} \\
&= \frac{1}{(k^2-k'^2)^2\sin^2(k'a) + 4k^2k'^2} \begin{pmatrix} 4k^2k'^2 + (k^2-k'^2)^2\sin^2(k'a) & 0 \\ 0 & 4k^2k'^2 + (k^2-k'^2)^2\sin^2(k'a) \end{pmatrix} \\
&= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\
&= \mathbb{I},
\end{aligned}$$

which means S is unitary. It is also clear that S is a symmetric matrix.
The symmetries of the scattering matrix are the following

- **Symmetry under parity inversion:** If we make the transformation

  $$\psi(x) \mapsto \psi(-x),$$

  which is equivalent to switching regions I and III, then S also describes a solution to the new system. In fact,

  $$\begin{cases} \tilde{\psi}_I(x) = G\mathrm{e}^{ikx} + F\mathrm{e}^{-ikx} \\ \tilde{\psi}_{III}(x) = B\mathrm{e}^{ikx} + A\mathrm{e}^{-ikx} \end{cases}$$

  which gives us

  $$\begin{pmatrix} A \\ G \end{pmatrix} = \begin{pmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{pmatrix} \begin{pmatrix} F \\ B \end{pmatrix} \implies \begin{pmatrix} G \\ A \end{pmatrix} = \begin{pmatrix} s_{22} & s_{21} \\ s_{12} & s_{11} \end{pmatrix} \begin{pmatrix} B \\ F \end{pmatrix}$$

  This is satisfied when $s_{11} = s_{22}$ and $s_{12} = s_{21}$, which is true since S is symmetric. Thus, the scattering matrix S is symmetric under parity inversion.

- **Symmetry under time reversal:** If we make the transformation

  $$t \mapsto -t,$$

  which is equivalent to flipping the directions of the waves in regions I and III, then S also describes a solution to the new system. In fact,

  $$\begin{cases} \psi_I^*(x) = B^*\mathrm{e}^{ikx} + A^*\mathrm{e}^{-ikx} \\ \psi_{III}^*(x) = G^*\mathrm{e}^{ikx} + F^*\mathrm{e}^{-ikx} \end{cases}$$

  which gives us

  $$\begin{pmatrix} A^* \\ G^* \end{pmatrix} = \begin{pmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{pmatrix} \begin{pmatrix} F^* \\ B^* \end{pmatrix}$$

  Additionally, if the potential $V(x)$ is real, then the system possesses time-reversal symmetry. Thus, the scattering matrix S is symmetric under parity inversion.

$\boxed{\text{For } V_0 < E\text{:}}$

In this case, practically everything works out the same, except that, in Region II, k' is real, and, in the scattering matrix, $k^2 \pm k'^2 \to k^2 \mp k'^2$.
Going back to the transmission coefficient T, we will use the small-angle approximation for sin to get $\sin(x) \approx x$, and thus

$$\begin{aligned} T &= \frac{1}{\frac{(k^2-k'^2)^2 \sin^2(k'a)}{4k^2k'^2} + 1} \\ &= \frac{1}{\frac{(k^2-k'^2)^2 a^2}{4k^2} + 1}. \end{aligned}$$

Replacing the values of k and k', we get

$$T = \frac{1}{\frac{mV_0^2}{2\hbar^2 E} a^2 + 1}.$$

The interesting points are when $\sin(k'a) = 0 \implies k'a = n\pi$ for integer values of n. Replacing k', we get

$$\frac{\sqrt{2m(E - V_0)}}{\hbar} a = n\pi \implies E = V_0 + \frac{(n\pi\hbar)^2}{2ma^2}.$$

Setting $\hbar = m = 1$ and some arbitrary values for V_0 and a, we plot the transmission coefficient T as a function of energy E, getting

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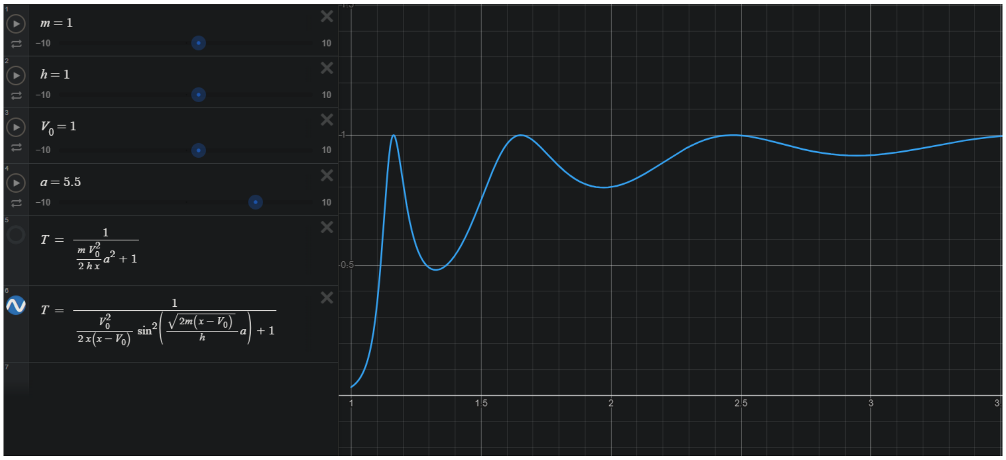


Figure 1: Transmission Coefficient T as a Function of Energy E.

Problem 2

Consider the spin $\frac{1}{2}$ Heisenberg chain and the operator $\hat{n} = \frac{1}{2}(1 + \sigma_z)$ that has expectation value 0 for a spin down and 1 for a spin up. It can be thought as the particle number in the interpretation where the vacuum are all spins down and a few spins are up.

(a) Compute the mean value of $\left\langle k \middle| n^{(i)} \middle| k \right\rangle$ for a given site i in the one particle state, assuming the spin chain has a finite length $N \gg 1$ for normalization purposes (but ignoring boundary effects).

(b) Compute the correlation

$$C_{ij} = \left\langle \psi \middle| n^{(i)} n^{(j)} \middle| \psi \right\rangle, \quad i < j$$

as a function of $|i - j|$ for the two particle state, *i.e.* $|\psi\rangle = |k_1, k_2\rangle$ in the infinite chain. Pay particular attention to the bound states and argue that the two particles are combined.

Proof. The Hamiltonian of a spin $\frac{1}{2}$ Heisenberg chain is given by

$$H = 2\lambda \sum_j \left(\mathbb{I}_{j,j+1} - \mathbb{P}_{j,j+1} \right),$$

where

$$\mathbb{P}_{j,j+1} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

is the permutation matrix.

(a) We have

$$\begin{aligned} H |j\rangle &= 2\lambda(|j\rangle - |j-1\rangle + |j\rangle - |j+1\rangle) \\ &= 2\lambda(2|j\rangle - |j-1\rangle - |j+1\rangle) \end{aligned}$$

and

$$\begin{aligned} H |\psi\rangle &= \sum_j H |j\rangle \\ &= 2\lambda \sum_j (2|j\rangle - |j-1\rangle - |j+1\rangle) \\ &= \epsilon |\psi\rangle \end{aligned}$$

$$\implies \epsilon c_j = 2\lambda(2c_j - c_{j-1} - c_{j+1}).$$

Since the coefficients are constant, we try a solution of $c_j = \mathrm{e}^{jm}$, which gives us

$$\epsilon \mathrm{e}^{jm} = 2\lambda \mathrm{e}^{jm}\left(2 - \mathrm{e}^{-m} - \mathrm{e}^{m}\right)$$
$$\epsilon = 4\lambda - 2\lambda\left(\mathrm{e}^{m} + \mathrm{e}^{-m}\right).$$

The only way to stay finite is if we analytically continue $m \to ik$, which gives us

$$\begin{aligned}\epsilon &= 4\lambda - 2\lambda\left(\mathrm{e}^{ik} + \mathrm{e}^{-ik}\right)\\ &= 4\lambda - 4\lambda\cos(k)\\ &= 8\lambda\sin^2\left(\frac{k}{2}\right).\end{aligned}$$

We have that $|\epsilon\rangle = \sum_j e^{ikj}|j\rangle$, which gives us

$$\begin{aligned}\langle\epsilon|\epsilon\rangle &= \left(\sum_{j'} e^{-ikj'}\langle j'|\right)\left(\sum_j e^{ikj}|j\rangle\right)\\ &= \sum_{j,j'} e^{ik(j-j')}\langle j'|j\rangle\\ &= N.\end{aligned}$$

Normalizing, we get

$$|k\rangle = \frac{1}{\sqrt{N}}\sum_j e^{ikj}|j\rangle.$$

Computing the mean value, we have

$$\begin{aligned}\left\langle k\middle|n^{(i)}\middle|k\right\rangle &= \left(\frac{1}{\sqrt{N}}\sum_{j'} e^{-ikj'}\langle j'|\right)\frac{1}{2}(\mathbb{I}^{(i)} + \sigma_z^{(i)})\left(\frac{1}{\sqrt{N}}\sum_j e^{ikj}|j\rangle\right)\\ &= \frac{1}{2N}\sum_{j,j'} e^{ik(j-j')}\left\langle j'\middle|\mathbb{I}^{(i)} + \sigma_z^{(i)}\middle|j\right\rangle\\ &= \frac{1}{2N}\sum_{j,j'} e^{ik(j-j')}\left\langle j'\middle|\mathbb{I}^{(i)} + \sigma_z^{(i)}\middle|j\right\rangle\\ &= \frac{1}{N}\sum_{j,j'} e^{ik(j-j')}\langle j'|\delta_{ij}|j\rangle\\ &= \frac{1}{N}\sum_{j,j'} e^{ik(j-j')}\delta_{ij}\delta_{jj'}\\ &= \frac{1}{N}.\end{aligned}$$

(b) For the two-particle spin $\frac{1}{2}$ Heisenberg chain, we will denote the first particle by j_1 and the second by j_2 (to prevent confusion with the particle i and the imaginary unit i). We have

$$|\epsilon\rangle = \sum_{j_1,j_2} A_{j_1,j_2}|j_1,j_2\rangle,$$

where

$$A_{j_1,j_2} = \mathrm{e}^{i\frac{\theta}{2}}\mathrm{e}^{ik_1j_1}\mathrm{e}^{ik_2j_2} + \mathrm{e}^{-i\frac{\theta}{2}}\mathrm{e}^{ik_2j_1}\mathrm{e}^{ik_1j_2}$$

Calculating, we have

$$\begin{aligned}
\langle \epsilon|\epsilon\rangle &= \left(\sum_{j_1',j_2'} A^*_{j_1',j_2'}\left\langle j_1',j_2'\right|\right)\left(\sum_{j_1,j_2} A_{j_1,j_2}\left|j_1,j_2\right\rangle\right)\\
&= \sum_{j_1,j_2,j_1',j_2'} A^*_{j_1',j_2'}A_{j_1,j_2}\left\langle j_1',j_2'|j_1,j_2\right\rangle\\
&= \sum_{j_1,j_2,j_1',j_2'}\left(\mathrm{e}^{-i\frac{\theta}{2}}\mathrm{e}^{-ik_1j_1'}\mathrm{e}^{-ik_2j_2'}+\mathrm{e}^{i\frac{\theta}{2}}\mathrm{e}^{-ik_2j_1'}\mathrm{e}^{-ik_1j_2'}\right)\left(\mathrm{e}^{i\frac{\theta}{2}}\mathrm{e}^{ik_1j_1}\mathrm{e}^{ik_2j_2}+\mathrm{e}^{-i\frac{\theta}{2}}\mathrm{e}^{ik_2j_1}\mathrm{e}^{ik_1j_2}\right)\left\langle j_1',j_2'|j_1,j_2\right\rangle\\
&= \sum_{j_1,j_2,j_1',j_2'}\left(\mathrm{e}^{ik_1(j_1-j_1')}\mathrm{e}^{ik_2(j_2-j_2')}+\mathrm{e}^{-i\theta}\mathrm{e}^{ik_1(j_2-j_1')}\mathrm{e}^{ik_2(j_1-j_2')}\right.\\
&\qquad\left.+\mathrm{e}^{i\theta}\mathrm{e}^{ik_2(j_2-j_1')}\mathrm{e}^{ik_1(j_1-j_2')}+\mathrm{e}^{ik_2(j_1-j_1')}\mathrm{e}^{ik_1(j_2-j_2')}\right)\left\langle j_1',j_2'|j_1,j_2\right\rangle.
\end{aligned}$$

We have that $j_1<j_2$ and $j_1'<j_2'$, in addition to $\langle j_1',j_2'|j_1,j_2\rangle=\delta_{j_1,j_1'}\delta_{j_2,j_2'}$, which gives us

$$\begin{aligned}
\langle \epsilon|\epsilon\rangle &= \sum_{j_1<j_2}\left(2+\mathrm{e}^{-i\theta}\mathrm{e}^{ik_1(j_2-j_1)}\mathrm{e}^{ik_2(j_1-j_2)}+\mathrm{e}^{i\theta}\mathrm{e}^{ik_2(j_2-j_1)}\mathrm{e}^{ik_1(j_1-j_2)}\right)\\
&= \sum_{j_1<j_2}\left(2+\mathrm{e}^{i\theta}\mathrm{e}^{ik_1(j_1-j_2)}\mathrm{e}^{ik_2(j_2-j_1)}+\mathrm{e}^{-i\theta}\mathrm{e}^{-ik_1(j_1-j_2)}\mathrm{e}^{-ik_2(j_2-j_1)}\right)\\
&= \sum_{j_1<j_2}\left[2+2\cos(\theta+k_1(j_1-j_2)+k_2(j_2-j_1))\right]\\
&= \sum_{j_1<j_2}\left[2+2\cos(\theta+(k_1-k_2)(j_1-j_2))\right].
\end{aligned}$$

Then, $|\psi\rangle=|k_1,k_2\rangle=\frac{1}{\sqrt{\langle\epsilon|\epsilon\rangle}}|\epsilon\rangle$.

Calculating the correlation C_{j_1,j_2}, we have

$$\begin{aligned}
C_{j_1,j_2} &= \left\langle\psi\middle|n^{(i)}n^{(j)}\middle|\psi\right\rangle\\
&= \frac{1}{\sqrt{\langle\epsilon|\epsilon\rangle}}\left\langle\epsilon\middle|n^{(i)}n^{(j)}\middle|\epsilon\right\rangle\\
&= \frac{1}{\sqrt{\langle\epsilon|\epsilon\rangle}}\sum_{j_1<j_2,j_1'<j_2'}\left(\mathrm{e}^{ik_1(j_1-j_1')}\mathrm{e}^{ik_2(j_2-j_2')}+\mathrm{e}^{-i\theta}\mathrm{e}^{ik_1(j_2-j_1')}\mathrm{e}^{ik_2(j_1-j_2')}\right.\\
&\qquad\left.+\mathrm{e}^{i\theta}\mathrm{e}^{ik_2(j_2-j_1')}\mathrm{e}^{ik_1(j_1-j_2')}+\mathrm{e}^{ik_2(j_1-j_1')}\mathrm{e}^{ik_1(j_2-j_2')}\right)\left\langle j_1',j_2'\middle|n^{(i)}n^{(j)}\middle|j_1,j_2\right\rangle\\
&= \frac{1}{\sqrt{\langle\epsilon|\epsilon\rangle}}\sum_{j_1<j_2,j_1'<j_2'}\left(\mathrm{e}^{ik_1(j_1-j_1')}\mathrm{e}^{ik_2(j_2-j_2')}+\mathrm{e}^{-i\theta}\mathrm{e}^{ik_1(j_2-j_1')}\mathrm{e}^{ik_2(j_1-j_2')}\right.\\
&\qquad\left.+\mathrm{e}^{i\theta}\mathrm{e}^{ik_2(j_2-j_1')}\mathrm{e}^{ik_1(j_1-j_2')}+\mathrm{e}^{ik_2(j_1-j_1')}\mathrm{e}^{ik_1(j_2-j_2')}\right)\delta_{j_1j_1'}\delta_{j_2j_2'}\delta_{j_1'i}\delta_{j_2'j}\\
&= \frac{1}{\sqrt{\langle\epsilon|\epsilon\rangle}}\left[2+2\cos(\theta+(k_1-k_2)(j_1-j_2))\right].
\end{aligned}$$

Returning to the needed notation as per the problem, we have

$$C_{ij}=\frac{1+\cos(\theta+(k_1-k_2)(i-j))}{\sum_{j_1<j_2}\left[1+\cos(\theta+(k_1-k_2)(j_1-j_2))\right]}.$$

We define

$$\begin{cases}\kappa=k_1+k_2\\ q=\frac{k_2-k_1}{2}\end{cases}$$

and, thus, get

$$C_{ij} = \frac{1+\cos(\theta - 2q(i-j))}{\sum_{j_1<j_2}\left[1+\cos(\theta-2q(j_1-j_2))\right]}.$$

This creates a bound state when the wave function of j_2 is far away from j_1. For bound states, we have $\theta = i\alpha$, $\alpha \to -\infty$ and $q = i\eta$, $\eta = -2\ln(\cos(\kappa)) > 0$, which gives us

$$\begin{aligned}
C_{ij} &= \frac{1+\cosh(\alpha - 2\eta(i-j))}{\sum_{j_1<j_2}\left[1+\cosh(\alpha-2\eta(j_1-j_2))\right]} \\
&= \frac{2+\mathrm{e}^{\alpha+2\eta(j-i)}+\mathrm{e}^{-\alpha-2\eta(j-i)}}{\sum_{j_1<j_2}\left[2+\mathrm{e}^{\alpha+2\eta(j_2-j_1)}+\mathrm{e}^{-\alpha-2\eta(j_2-j_1)}\right]} \\
&= \frac{2\mathrm{e}^{\alpha}+\mathrm{e}^{2\alpha+2\eta(j-i)}+\mathrm{e}^{-2\eta(j-i)}}{\sum_{j_1<j_2}\left[2\mathrm{e}^{\alpha}+\mathrm{e}^{2\alpha+2\eta(j_2-j_1)}+\mathrm{e}^{-2\eta(j_2-j_1)}\right]} \\
&\to \frac{\mathrm{e}^{-2\eta(j-i)}}{\sum_{j_1<j_2}\mathrm{e}^{-2\eta(j_2-j_1)}} \quad \text{as } \alpha \to -\infty
\end{aligned}$$

Since we are assuming that the chain is infinitely long, then there is no need to normalize to the states. Thus, we can just write

$$C_{ij} = 1+\cos(\theta + 2q(i-j)).$$

For bound states

$$C_{ij} = \mathrm{e}^{-2\eta(j-1)}.$$

■

Problem 3
Consider a particle in the one dimensional potential $V(x) = \lambda x^4$ such that the Hamiltonian is

$$H = \frac{p^2}{2m} + \lambda x^4.$$

(a) Write the corresponding Schrodinger equation for the (possible) wave function of energy E. Rescale the variable x by a constant a, namely define $z = ax$ and find a to eliminate λ from the equation (after appropriately rescaling E).

(b) Solve the resulting equation numerically for different values of E. [Use the boundary condition $\psi(0) = 1$, $\psi'(0) = 0$]. By considering the behavior of ψ at infinity, determine the lowest eigenvalue of the energy. After that, compute two other eigenvalues.

(c) Consider the wave function

$$\psi = A\mathrm{e}^{-\alpha x^2}.$$

Choose A such that the wave function $\psi(x)$ is normalized and then compute $E(\alpha) = \langle\psi|H|\psi\rangle$. Minimize $E(\alpha)$ with respect to α and compare the minimum value of $E(\alpha)$ with the result of the previous point to see how good the approximation is.

Note: This problem requires the use of a compute algebra program such as Mathematica, Maple, Matlab etc. (or the coding the integration in some computer language such as C, Fortran etc.). It is more difficult and requires some extra research but playing with the numerics is always useful to understand what one is doing analytically.

Proof. (a) Writing the corresponding Schrodinger equation, we have

$$\left\langle x\middle|\hat{H}\middle|\psi\right\rangle = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + \lambda x^4\psi(x) = E\psi(x).$$

Letting $z = ax \implies x = \frac{z}{a}$, and denoting $\phi(z) = \psi\left(\frac{z}{a}\right)$ and we get

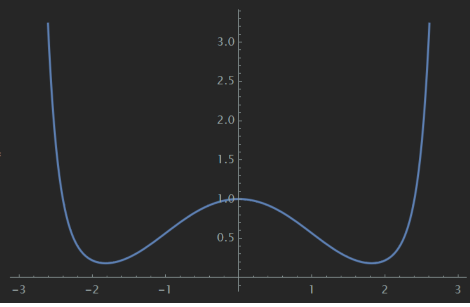
$$\begin{aligned}
-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\left(\frac{z}{a}\right)^2}\psi\left(\frac{z}{a}\right) + \lambda\left(\frac{z}{a}\right)^4\psi\left(\frac{z}{a}\right) &= E\psi\left(\frac{z}{a}\right)\\
-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}\phi(z) + \lambda\frac{z^4}{a^6}\phi(z) &= \frac{E}{a^2}\phi(z)\\
-\frac{\partial^2\phi(z)}{\partial z^2} + \frac{2m\lambda}{a^6\hbar^2}z^4\phi(z) &= \frac{2mE}{a^2\hbar^2}\phi(z).
\end{aligned}$$

Now, to eliminate λ, we set $\lambda = \frac{a^6\hbar^2}{2m} \implies a^2 = \left(\frac{2m\lambda}{\hbar^2}\right)^{\frac{1}{3}} \implies \epsilon = \left(\frac{2m}{\hbar^2}\right)^{\frac{2}{3}}\frac{E}{\lambda^{\frac{1}{3}}}$, and we get

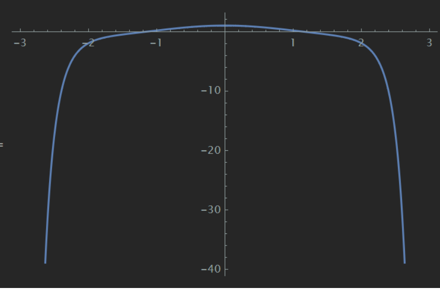
$$-\frac{\partial^2\phi(z)}{\partial z^2} + z^4\phi(z) = \epsilon\phi(z).$$

(b) We are given the boundary conditions $\psi(0) = 1$ and $\psi'(0) = 0$, which, after our transformation to z, we have $\phi(0) = 1$ and $\phi'(0) = 0$. Plugging our second-order IVP differential equation into Mathematica, we first change ϵ in a way that helps us see the change of our solution to the ODE. We then pick arbitrary starting and ending energies and search for the energy eigenvalue in between these two bounds. This effectively is solving for when the solution to the ODE coincides with the x-axes, up to a certain degree of precision.

```
In[1]:= epsilon = 1
        s = NDSolve[{-phi''[z] + z^4*phi[z] == epsilon * phi[z], phi[0] == 1, phi'[0] == 0}, phi, {z, -3, 3}]
        Plot[Evaluate[phi[z] /. %], {z, -3, 3}]

Out[1]= 1

Out[2]= {{phi → InterpolatingFunction[ Domain: {{-3., 3.}} Output: scalar ]}}

Out[3]=
```




```
In[4]:= epsilon = 2;
        NDSolve[{-D[D[phi[z], z], z] + z^4 * phi[z] == epsilon*phi[z], phi[0] == 1, phi'[0] == 0}, phi[z], {z, -3, 3}]
        Plot[Evaluate[phi[z] /. %], {z, -3, 3}]

Out[5]= {{phi[z] → InterpolatingFunction[ Domain: {{-3., 3.}} Output: scalar ][z]}}

Out[6]=
```




```
In[7]:= e1 = 1.0;
        e2 = 2.0;
        precision = 0.000001;
        While[e2 - e1 > precision,
         avg = (e1 + e2) / 2;
         sol = NDSolve[{-phi''[z] + z^4*phi[z] == avg*phi[z], phi[0] == 1, phi'[0] == 0}, phi, {z, -4, 4}];
         If[Part[phi[4] /. sol, 1] > 0, e1 = avg];
         If[Part[phi[4] /. sol, 1] < 0, e2 = avg];
        ]
        NumberForm[e1, 7]
        NumberForm[e2, 7]

Out[11]//NumberForm=
        1.060362

Out[12]//NumberForm=
        1.060363
```

Thus, the numerical result for our lowest energy eigenvalue is $\epsilon = 1.060362$. By the same method, and by searching using trial-and-error, we get the next two energy eigenvalues, which are $\epsilon_1 = 16.26183$ and $\epsilon_2 = 37.923$.

(c) Given $\psi(x) = A\mathrm{e}^{-\alpha x^2}$, we find A such that ψ is normalized

$$\begin{aligned}
\langle\psi|\psi\rangle &= \int_{-\infty}^{\infty} \psi^*\psi \,\mathrm{d}x \\
&= |A|^2 \int_{-\infty}^{\infty} \mathrm{e}^{-2\alpha x^2}\,\mathrm{d}x \\
&= \sqrt{\frac{\pi}{2\alpha}}|A|^2 \\
&= 1 \\
\implies A &= \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}}.
\end{aligned}$$

Thus, we can write

$$\psi(x) = \left(\frac{2\alpha}{\pi}\right)^{\frac{1}{4}} \mathrm{e}^{-\alpha x^2}.$$

Computing $\left\langle\psi\middle|\hat{H}\middle|\psi\right\rangle$, we have

$$\begin{aligned}
E(\alpha) = \left\langle\psi\middle|\hat{H}\middle|\psi\right\rangle &= \sqrt{\frac{2\alpha}{\pi}}\int_{-\infty}^{\infty}\psi^*\left(\frac{\hat{p}^2}{2m} + \lambda\hat{x}^4\right)\psi\,\mathrm{d}x \\
&= \sqrt{\frac{2\alpha}{\pi}}\int_{-\infty}^{\infty}\mathrm{e}^{-\alpha x^2}\left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \lambda x^4\right)\mathrm{e}^{-\alpha x^2}\,\mathrm{d}x \\
&= \sqrt{\frac{2\alpha}{\pi}}\int_{-\infty}^{\infty}\mathrm{e}^{-\alpha x^2}\left(\frac{-\hbar^2}{2m}\left(-2\alpha + 4\alpha^2x^2\right) + \lambda x^4\right)\mathrm{e}^{-\alpha x^2}\,\mathrm{d}x \\
&= \sqrt{\frac{2\alpha}{\pi}}\int_{-\infty}^{\infty}\left(\frac{-\hbar^2}{2m}\left(-2\alpha + 4\alpha^2x^2\right) + \lambda x^4\right)\mathrm{e}^{-2\alpha x^2}\,\mathrm{d}x \\
&= \sqrt{\frac{2\alpha}{\pi}}\left[\frac{\hbar^2}{m}\int_{-\infty}^{\infty}\alpha\mathrm{e}^{-2\alpha x^2}\,\mathrm{d}x - \frac{2\hbar^2}{m}\int_{-\infty}^{\infty}\alpha^2x^2\mathrm{e}^{-2\alpha x^2}\,\mathrm{d}x + \int_{-\infty}^{\infty}\lambda x^4\mathrm{e}^{-2\alpha x^2}\,\mathrm{d}x\right] \\
&= \sqrt{\frac{2\alpha}{\pi}}\left[\frac{\hbar^2}{m}\left(\sqrt{\frac{\pi\alpha}{2}}\right) - \frac{2\hbar^2}{m}\left(\frac{\sqrt{\pi\alpha}}{4\sqrt{2}}\right) + \left(\frac{3\lambda\sqrt{\pi}}{16\alpha^2\sqrt{2\alpha}}\right)\right] \\
&= \frac{\alpha\hbar^2}{2m} + \frac{3\lambda}{16\alpha^2}.
\end{aligned}$$

To minimize $E(\alpha)$, we take the derivative of E with respect to α and set it to zero, and we get

$$\frac{\mathrm{d}E}{\mathrm{d}\alpha} = \frac{\hbar^2}{2m} - \frac{3\lambda}{8\alpha^3} = 0$$

$$\implies \alpha = \left(\frac{3m\lambda}{4\hbar^2}\right)^{\frac{1}{3}}.$$

Thus, the energy E is minimum when

$$\begin{aligned}
E_{\min} &= \left(\frac{3m\lambda}{4\hbar^2}\right)^{\frac{1}{3}}\frac{\hbar^2}{2m} + \frac{3\lambda}{16}\left(\frac{4\hbar^2}{3m\lambda}\right)^{\frac{2}{3}} \\
&= \frac{9\lambda}{16}\left(\frac{4\hbar^2}{3m\lambda}\right)^{\frac{2}{3}}.
\end{aligned}$$

Now, if we replace E_{min} into ϵ, we get

$$\begin{aligned}
\epsilon &= \left(\frac{2m}{\hbar^2}\right)^{\frac{2}{3}} \frac{E}{\lambda^{\frac{1}{3}}} \\
&= \left(\frac{2m}{\hbar^2}\right)^{\frac{2}{3}} \frac{1}{\lambda^{\frac{1}{3}}} \frac{9\lambda}{16} \left(\frac{4\hbar^2}{3m\lambda}\right)^{\frac{2}{3}} \\
&= \frac{9}{4}\left(\frac{1}{3}\right)^{\frac{2}{3}} \\
&\approx 1.08168,
\end{aligned}$$

which matches the value we got numerically in part (b).

■