

An Introduction to Quantum Mechanics:
Exercises and Solutions

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1 The Failure of Classical Physics

1.1 Atom stability

Exercise 1. Estimate the speed of the electron rotating around the nucleus for the hydrogen atom, assuming that it orbitates along a circular orbit of radius $r_0 = 10^{-8} \text{ cm}$. Compare it to the speed of light.

Solution.

$$\begin{aligned} v^2 &= \frac{e^2}{4\pi\epsilon_0} \frac{1}{m r_0} \approx (1.6)^2 \times 10^{-38} \cdot 9.0 \times 10^9 \frac{1}{9.1 \times 10^{-31}} \frac{1}{10^{10}} \frac{m^2}{\text{sec}^2} \approx \\ &\approx (1.6)^2 \cdot 0.99 \times 10^{12} \frac{m^2}{\text{sec}^2} \end{aligned} \quad (1.1)$$

Hence

$$\frac{v}{c} \approx \frac{1.6 \times 10^6}{3.0 \times 10^8} = 0.53 \times 10^{-2} \quad (1.2)$$

Exercise 2. Check that formula (1.7) of the lecture notes has the correct dimensions.

Solution.

Recall that $\frac{e^2}{4\pi\epsilon_0 r^2}$ has the dimension of a force. Therefore

$$\left[\frac{e^2}{4\pi\epsilon_0} \frac{a^2}{c^3} \right] = \left[\frac{M \times L^3}{T^2} \frac{L^2}{T^4} \frac{T^3}{L^3} \right] = \left[\frac{M \times L^2}{T^3} \right] = \left[\frac{E}{T} \right] \quad (1.3)$$

Exercise 3. Estimate the time that it takes an electron of the hydrogen atom to fall onto the nucleus, assuming it starts from a circular orbit of radius $r_0 = 10^{-8} \text{ cm}$.

Solution.

$$\begin{aligned} \tau &= \frac{(4\pi\epsilon_0)^2 c^3 m^2}{4e^4} r_0^3 = \left(\frac{4\pi\epsilon_0 m r_0 c^2}{e^2} \right)^2 \frac{r_0}{4c} = \frac{c^4}{v^4} \frac{r_0}{4c} \approx \\ &\approx \frac{1}{0.53^4 \times 10^{-8}} \times \frac{10^{-10}}{4 \times 3.0 \times 10^8} \text{ sec} \approx 1.1 \times 10^{-10} \text{ sec} \end{aligned} \quad (1.4)$$

1.2 Equipartition theorem

Exercise 3. Prove that a mass m which is constrained to move freely on a circle on a plane by a rigid rod of radius R is described by an Hamiltonian of the form

$$H(p, \theta) = \frac{p_\theta^2}{2I} \quad (1.5)$$

where p_θ is the momentum conjugate to angle θ which measures the position of the particle on the circle, and I is called the momentum of inertia. Express I in terms of m and R .

Solution.

The velocity of the particle is

$$v = R \frac{d\theta}{dt} \quad (1.6)$$

Therefore its energy is

$$H = \frac{1}{2} m v^2 = \frac{1}{2} m R^2 \dot{\theta}^2 \quad (1.7)$$

The momentum conjugate to θ is

$$p_\theta = m R^2 \dot{\theta} \quad (1.8)$$

Thus

$$H = \frac{1}{2} \frac{p_\theta^2}{m R^2} \quad (1.9)$$

Thus

$$I = m R^2 \quad (1.10)$$

Exercise 4. Prove that a diatomic molecule schematized as two identical masses $\frac{m}{2}$ held at a fixed distance R by a rigid rod of negligible mass is described by the Hamiltonian

$$H(p, q) = \frac{\vec{p}^2}{2m} + \frac{1}{2I} \left(p_\theta^2 + \frac{p_\phi^2}{\sin^2 \theta} \right) \quad (1.11)$$

Compute the momentum of inertia I in terms of m and R .

Problem 2. Generalize the derivation of the equipartition theorem to the Hamiltonian of the bi-atomic molecule (1.11).

1.3 The Photoelectric Effect

Problem 5. A lamp of 100 W emits light whose wave length is $5.890 \cdot 10^{-7} m$. How many photons are emitted in 1 second?

Solution The energy of photons of such frequency is

$$E_\nu = \frac{12400}{5890} eV = 2.10 eV = 3.37 \times 10^{-19} J \quad (1.12)$$

Therefore the number $\frac{dN}{dt}$ of photons emitted per unit of time is

$$\frac{dN}{dt} = \frac{100W}{3.37 \cdot 10^{-19} J} = 2.97 \times 10^{20} sec^{-1} \quad (1.13)$$

1.4 Bohr's quantum theory of atomic spectra.

Problem 6. Classical electromagnetism predicts that a charge rotating on a circular orbit with angular orbital frequency ω emits electromagnetic radiation with the same frequency. Show that the frequency of the photon emitted by an electron of the Bohr hydrogen atom which goes from the level E_{n+1}^H to the level E_n^H , is, for n large, approximately equal to the frequency of the classical circular motion corresponding to that energy.

Solution: The difference of energy of the levels E_{n+1}^H and E_n^H for $n \gg 1$ is

$$\begin{aligned} E_{n+1}^H - E_n^H &= -\frac{e^4 m}{(4\pi\epsilon_0)^2 \hbar^2} \frac{1}{2(n+1)^2} + \frac{e^4 m}{(4\pi\epsilon_0)^2 \hbar^2} \frac{1}{2n^2} = \\ &\approx \frac{e^4 m}{(4\pi\epsilon_0)^2 \hbar^2} \frac{1}{n^3} \end{aligned} \quad (1.14)$$

The angular frequency of the corresponding emitted photon is

$$\omega_{n+1 \rightarrow n} = \frac{e^4 m}{(4\pi\epsilon_0)^2 \hbar^3} \frac{1}{n^3} \quad (1.15)$$

On the other hand, the angular frequency for a classical circular orbit of radius r is

$$\omega = \frac{v}{r} \quad (1.16)$$

Since

$$v^2 = \frac{e^2}{4\pi\epsilon_0 m} \frac{1}{r} \quad (1.17)$$

we have

$$\omega = \frac{4\pi\epsilon_0}{e^2} m v^3 \quad (1.18)$$

The velocity v_n of the electron in the circular orbit of energy E_n is given by

$$E_n = -\frac{1}{2} m v_n^2 = -\frac{e^4 m}{(4\pi\epsilon_0)^2 \hbar^2} \frac{1}{2n^2} \quad (1.19)$$

that is

$$v_n = \frac{1}{n} \frac{e^2}{(4\pi\epsilon_0) \hbar} \quad (1.20)$$

The angular frequency of the circular orbit with this energy is therefore

$$\omega = v_n^3 \frac{4 \pi \epsilon_0}{e^2} m = \frac{1}{n^3} \frac{e^4 m}{(4 \pi \epsilon_0)^2 \hbar^3} \quad (1.21)$$

which matches the frequency of the photon emitted in the transition $n+1 \rightarrow n$ as predicted by Bohr theory.

Problem 9. Apply the Bohr-Sommerfeld quantization condition to an unidimensional free particle moving in a potential well $V(x)$ defined by

$$V(x) = \begin{cases} -V_0 & \text{for } 0 < x < L \\ 0 & \text{for } x < 0 \text{ and } x > L \end{cases} \quad (1.22)$$

where $V_0 > 0$ is the depth of the well. Determine the discrete energy levels. How many they are? What is the minimum value of V_0 for which there exist discrete levels?

Solution: The bound classical trajectories are those with $E < 0$. The momentum for these orbits is quantized according to

$$p_n = \frac{n h}{2 L} \quad (1.23)$$

The energy is therefore

$$E_n = \frac{p_n^2}{2 m} - V_0 = \frac{n^2 h^2}{8 m L^2} - V_0 < 0 \quad (1.24)$$

Hence there are a finite number of closed trajectories, with $n = 1, 2, \dots, n_{max}$ where n_{max} is the highest positive integer such that

$$n_{max}^2 < \frac{8 m L^2 V_0}{h^2} \quad (1.25)$$

The minimal value of V_0 for which there are discrete levels is the minimal value for which this equation admits an integer positive solution

$$\frac{8 m L^2 V_0^{min}}{h^2} = 1 \Leftrightarrow V_0^{min} = \frac{h^2}{8 m L^2} \quad (1.26)$$

Problem 10. Apply Bohr-Sommerfeld quantization condition to a satellite of mass $m = 1 \text{ kg}$ rotating around the earth. Determine the allowed radiuses in terms of the mass of the earth M and the universal constant of gravitation

G. Suppose the satellite is on a circular orbit of radius near the radius of the earth $R = 6400 \text{ km}$, with a given Bohr integer number \bar{n} . How much does the radius change if the satellite shifts to an orbit with $n = \bar{n} + 1$? Express the answer in meters.

Solution: The classical equation of motion for a circular orbit of radius r is

$$\frac{GM}{r^2} = \frac{v^2}{r} \Leftrightarrow v^2 = \frac{GM}{r} \quad (1.27)$$

The momentum is therefore

$$p = mv = m \sqrt{\frac{GM}{r}} \quad (1.28)$$

and the Bohr-Sommerfeld quantization condition is

$$\oint p dr = 2\pi r p = 2\pi m \sqrt{GM r} = nh \quad (1.29)$$

that is

$$r_n = \frac{n^2 \hbar^2}{GM m^2} \quad (1.30)$$

If n changes from $n \rightarrow n + \Delta n = n + 1$ the radius changes

$$\Delta r_n = r_{n+1} - r_n \approx \frac{2n \Delta n \hbar^2}{GM m^2} = \frac{2 \Delta n r_n}{n} = \frac{2 r_n}{n} \quad (1.31)$$

We have

$$r_n = \frac{n^2 \hbar^2}{GM m^2} \approx R \Leftrightarrow n^2 \approx \frac{GM R m^2}{\hbar^2} = \frac{g m^2 R^3}{\hbar^2} \quad (1.32)$$

where $g = \frac{GM}{R^2} \approx 9.8 \frac{m}{sec^2}$ is the gravity acceleration. Thus

$$n^2 \approx \frac{9.8 \times 1^2 \times 6.4^3 \times 10^{18}}{1.05^2 \times 10^{-68}} \approx 24 \times 10^{88} \Rightarrow n \approx 5 \times 10^{44} \quad (1.33)$$

Then

$$\Delta r_n \approx \frac{2}{5 \times 10^{44}} \times 6.4 \times 10^6 m \approx 2.6 \times 10^{-38} m \quad (1.34)$$

Problem 12. Apply the Bohr-Sommerfeld quantization condition to compute the energy levels and the orbits of a particle of mass m moving in circular orbits of radius r in a potential $V(r) = \sigma r$.

Solution: The classical equation of motion is

$$\frac{m v^2}{r} = \sigma \quad (1.35)$$

The quantization condition on the angular momentum for a circular orbit of radius r is therefore

$$L = m r v = m r \sqrt{\frac{\sigma r}{m}} = \sqrt{m \sigma} r^{\frac{3}{2}} = n \hbar \quad (1.36)$$

The orbits have therefore radiuses

$$r_n = \frac{(n \hbar)^{\frac{2}{3}}}{(m \sigma)^{\frac{1}{3}}} \quad (1.37)$$

and the corresponding energies are

$$E_n = \frac{3}{2} \sigma r_n = \frac{3}{2} \frac{(n \hbar \sigma)^{\frac{2}{3}}}{m^{\frac{1}{3}}} \quad (1.38)$$

Problem 13. Apply the Bohr-Sommerfeld quantization condition to derive energy levels and allowed orbit radiuses for a particle of mass m moving in circular orbits of radius r attracted toward the center of the orbit by an elastic force $F = -k r$.

Solution: The classical equations of motion for circular orbits are

$$m \frac{v^2}{r} = k r \quad (1.39)$$

Therefore

$$v^2 = \frac{k}{m} r^2 \Rightarrow v = \sqrt{\frac{k}{m}} r \equiv \omega r \quad (1.40)$$

where $\omega = \sqrt{\frac{k}{m}}$ is the angular frequency of the harmonic oscillations. The angular momentum of the circular orbit is therefore

$$L = m v r = m \omega r^2 \quad (1.41)$$

and the Bohr quantization condition $L_n = n \hbar$ gives for the radii of the circular orbits

$$r_n^2 = \frac{n \hbar}{m \omega} \quad (1.42)$$

The corresponding energy levels are therefore

$$\begin{aligned} E_n &= \frac{1}{2} m v_n^2 + \frac{1}{2} m \omega^2 r_n^2 = \frac{1}{2} m \omega^2 r_n^2 + \frac{1}{2} m \omega^2 r_n^2 = \\ &= m \omega^2 r_n^2 = n \hbar \omega \end{aligned} \quad (1.43)$$

Problem 14. Derive the numerical values for the Rydberg constants predicted by Bohr atomic model for the following hydrogenoids: hydrogen H , deuteron D (whose nucleus has one proton and one neutron), He^+ , Li^{++} and, for the same elements, the wave lengths of the spectral lines corresponding to the transition between the first excited level and the fundamental level.

Solution:

Let us denote by R_∞ the Rydberg constant for an infinitely massive nucleus

$$R_\infty = \left(\frac{e^2}{4 \pi \epsilon_0} \right)^2 \frac{1}{4 \pi \hbar^3 c} \frac{m_e}{c} \approx 109737 \text{ cm}^{-1} \quad (1.44)$$

The Rydberg constant $R(M)$ for a nucleus of mass M and charge Z is related to the energy levels by the formula

$$E_n = -Z^2 \frac{R(M) h c}{n^2} \quad (1.45)$$

a

$$R(M) = R_\infty \frac{1}{1 + \frac{m_e}{M}} \approx R_\infty \left(1 - \frac{m_e}{M} \right) \quad (1.46)$$

Recall that

$$\frac{m_p}{m_e} = 1836.15 \quad (1.47)$$

Therefore

$$\begin{aligned}
 R_H &= R(m_p) \approx R_\infty \left(1 - \frac{m_e}{m_p}\right) = 109677 \text{ cm}^{-1} \\
 R_D &= R(2 * m_p) \approx R_\infty \left(1 - \frac{m_e}{2 m_p}\right) = 109707 \text{ cm}^{-1} \\
 R_{He^+} &= R(4 * m_p) \approx R_\infty \left(1 - \frac{m_e}{4 m_p}\right) = 109722 \text{ cm}^{-1} \\
 R_{Li^{++}} &= R(7 * m_p) \approx R_\infty \left(1 - \frac{m_e}{7 m_p}\right) = 109728 \text{ cm}^{-1} \quad (1.48)
 \end{aligned}$$

The wave lengths of the first spectral line corresponding to the transition from $n = 1$ to $n = 2$ are

$$\begin{aligned}
 \lambda_H &= \frac{4}{3} \frac{1}{R_H} = 1215.69 \text{ \AA} \\
 \lambda_D &= \frac{4}{3} \frac{1}{R_D} = 1215.36 \text{ \AA} \\
 \lambda_{He^+} &= \frac{4}{3} \frac{1}{4 R_{He^+}} = 303.798 \text{ \AA} \\
 \lambda_{Li^{++}} &= \frac{4}{3} \frac{1}{9 R_{Li^{++}}} = 135.013 \text{ \AA} \quad (1.49)
 \end{aligned}$$

1.5 Quantum theory of gas specific heat capacities

1.5.1 Einstein and Debye theories of specific heat capacities of solids

Problem 16. Suppose that the density of states of phonons grows quadratically with the frequency

$$\frac{dn(\omega)}{d\omega} = A\omega^2 + O(\omega^3) \quad \text{for } \omega \ll \omega_{max} \quad (1.50)$$

only for small frequencies ω . $n(\omega)$ is an otherwise generic function of ω for bigger ω up to a certain given ω_{max} , which defines a Debye temperature T_D . Derive the predictions of the Debye model for the internal energy in the low and high temperature limit.

Solution:

Let us start from

$$U = \int_0^{\omega_{max}} d\omega n'(\omega) \frac{\hbar\omega e^{-\beta\hbar\omega}}{1 - e^{-\beta\hbar\omega}} \quad (1.51)$$

For $T \gg T_D \equiv \frac{\hbar \omega_{max}}{k}$,

$$\hbar \beta \omega \leq \hbar \beta \omega_{max} \ll 1 \quad (1.52)$$

Therefore the high temperature limit of the internal energy coincides with the classical result, as expected on general grounds

$$U \approx \int_0^{\omega_{max}} d\omega n'(\omega) \frac{\hbar \omega}{\beta \hbar \omega} = \frac{1}{\beta} \int_0^{\omega_{max}} d\omega n'(\omega) = \frac{3N_A}{\beta} \quad T \gg T_D \quad (1.53)$$

On the other hand for low temperatures, when $T \ll T_D$,

$$\frac{1}{\hbar \beta} \ll \omega_{max} \quad (1.54)$$

the integrand in (1.51) is significantly different than zero only if

$$\omega \lesssim \frac{1}{\hbar \beta} \ll \omega_{max} \quad (1.55)$$

Therefore, in the region of frequencies when the integrand is significantly different than zero we can approximate the density of state with (1.50) and

$$\begin{aligned} U &\approx A \int_0^{\omega_{max}} d\omega \frac{\hbar \omega^3 e^{-\beta \hbar \omega}}{1 - e^{-\beta \hbar \omega}} \approx \frac{A \hbar}{(\hbar \beta)^4} \int_0^{\infty} dx \frac{x^3 e^{-x}}{1 - e^{-x}} = \\ &= \frac{A}{\hbar^3} \frac{\pi^4}{15} \frac{1}{\beta^4} \end{aligned} \quad (1.56)$$

In the lecture notes we derived the expression of A in terms of the sound speed in the solid and the volume

$$A = \frac{3L^3}{2\pi^2 v^3} \quad (1.57)$$

Therefore

$$U \approx \frac{L^3}{v^3 \hbar^3} \frac{\pi^2}{10} k^4 T^4 \quad T \ll T_D \quad (1.58)$$

Problem 17. Discuss the effect of quantization on the specific heat capacities of bi-atomic gases, knowing that: a) the rotational degrees of freedom around an axis orthogonal to the axis connecting the two atoms give rise to discrete energy levels with separation $\Delta E \sim 10^{-4} - 10^{-2} eV$; b) vibrational degrees of freedom have $\Delta E \sim 10^{-1} eV$; c) rotational degrees of freedom around the axis connecting the two atoms have $\Delta E \sim 10 eV$.

Solution. TO BE GIVEN

2 The Principles of Quantum Mechanics

Problem 10. A system is described by a 2-dimensional space of states. Let $|1\rangle$ and $|2\rangle$ be the normalized eigenstates of an observable \mathcal{O} with eigenvalues $\lambda = 1$ and $\lambda = 2$ respectively. Let $v = |1\rangle + i\sqrt{3}|2\rangle$ be a state of the system.

a) What is the probability that the measure of \mathcal{O} on v gives the result $\lambda = 2$?

b) Write the 2×2 matrix which represents \mathcal{O} in the basis $\{|1\rangle, |2\rangle\}$.

c) Let \mathcal{O}' be another observable, such that $\mathcal{O}'|1\rangle = |2\rangle$ and $\mathcal{O}'|2\rangle = |1\rangle$. Write the 2×2 matrix which represents \mathcal{O}' in the basis $\{|1\rangle, |2\rangle\}$.

d) What are the eigenvalues of \mathcal{O}' ?

e) What is the average of \mathcal{O}' on the state v ?

Solution:

- a) Let us compute the norm of v

$$|v|^2 = 1 + |i\sqrt{3}|^2 = 1 + 3 = 4 \quad (2.1)$$

Thus the normalized vector

$$v' = \frac{1}{2} (|1\rangle + i\sqrt{3}|2\rangle) \quad (2.2)$$

describes the same physical state as v . From (2.2) we read the probabilities

$$P_{\lambda=1}(v) = \left|\frac{1}{2}\right|^2 = \frac{1}{4} \quad P_{\lambda=2}(v) = \left|\frac{i\sqrt{3}}{2}\right|^2 = \frac{3}{4} \quad (2.3)$$

- b) Since $\{|1\rangle, |2\rangle\}$ are the eigenstates of \mathcal{O} , in this basis \mathcal{O} is represented by a diagonal matrix

$$\mathcal{O} = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix} \quad (2.4)$$

- c) The matrix representing \mathcal{O}' in the basis $\{|1\rangle, |2\rangle\}$ is

$$\mathcal{O}' = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (2.5)$$

- d) The eigenvalues of \mathcal{O}' are obtained from the secular equation

$$\det \begin{pmatrix} -\lambda' & 1 \\ 1 & -\lambda' \end{pmatrix} = (\lambda')^2 - 1 = 0 \Leftrightarrow \lambda' = 1, -1 \quad (2.6)$$

- e) The average of \mathcal{O}' on v is

$$\begin{aligned} \langle v', \mathcal{O}' v' \rangle &= \langle v', \mathcal{O}' \frac{1}{2} (|1\rangle + i\sqrt{3}|2\rangle) \rangle = \\ &= \langle v', \frac{1}{2} (|2\rangle + i\sqrt{3}|1\rangle) \rangle = \\ &= \langle \frac{1}{2} (|1\rangle + i\sqrt{3}|2\rangle), \frac{1}{2} (|2\rangle + i\sqrt{3}|1\rangle) \rangle = \\ &= \frac{1}{4} (i\sqrt{3} - i\sqrt{3}) = 0 \end{aligned} \quad (2.7)$$

Problem 11. On a spin 1/2 system the following 3 observables are defined

$$S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad (2.8)$$

- Find the eigenvalues and the normalized eigenvectors of the 3 observables $\{S_x, S_y, S_z\}$.
- Suppose the system is in the state described by the vector

$$v = \begin{pmatrix} 1 \\ 3i \end{pmatrix} \quad (2.9)$$

Find the probabilities to obtain the various possible values of $\{S_x, S_y, S_z\}$ on v . (You should in other words compute 6 probabilities, 2 for each of the 3 observables.)

- Compute the 2x2 unitary matrix which connects the basis of eigenvectors of S_z with the basis of eigenvectors of S_y .
- Find the eigenvalues and the normalized eigenvectors of the observable

$$S_{\vec{n}} \equiv n_x S_x + n_y S_y + n_z S_z \quad (2.10)$$

where

$$\vec{n} = (n_x, n_y, n_z) = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta) \quad (2.11)$$

θ and ϕ are polar coordinates: $0 \leq \phi \leq 2\pi$ and $0 \leq \theta \leq \pi$.

e) Compute the 2x2 unitary matrix which connects the basis of eigenvectors of S_z with the basis of eigenvectors of $S_{\vec{n}}$.

Solution:

a) The eigenvalues of any of $\{S_x, S_y, S_z\}$ are

$$\lambda_{\pm} = \pm \frac{\hbar}{2} \quad (2.12)$$

The eigenvectors of S_x are obtained from

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x_{\pm} \\ y_{\pm} \end{pmatrix} = \pm \begin{pmatrix} x_{\pm} \\ y_{\pm} \end{pmatrix} \quad (2.13)$$

that is

$$|S_x = \pm \frac{\hbar}{2}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} \quad (2.14)$$

The eigenvectors of S_y are obtained from

$$\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} x_{\pm} \\ y_{\pm} \end{pmatrix} = \pm \begin{pmatrix} x_{\pm} \\ y_{\pm} \end{pmatrix} \quad (2.15)$$

that is

$$|S_y = \pm \frac{\hbar}{2}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm i \end{pmatrix} \quad (2.16)$$

Finally, the eigenvectors of S_z are obtained from

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} x_{\pm} \\ y_{\pm} \end{pmatrix} = \pm \begin{pmatrix} x_{\pm} \\ y_{\pm} \end{pmatrix} \quad (2.17)$$

that is

$$|S_z = \frac{\hbar}{2}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |S_z = -\frac{\hbar}{2}\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (2.18)$$

b) Let us consider the normalized vector

$$|v\rangle = \frac{1}{\sqrt{10}} \begin{pmatrix} 1 \\ 3i \end{pmatrix} \quad (2.19)$$

The transition amplitudes are given by the scalar products

$$\begin{aligned}
 \langle S_x = \frac{\hbar}{2} | v \rangle &= \frac{1}{\sqrt{20}} (1 + 3i) \\
 \langle S_y = \frac{\hbar}{2} | v \rangle &= \frac{1}{\sqrt{20}} (1 + 3) = \frac{1}{\sqrt{20}} 4 \\
 \langle S_z = \frac{\hbar}{2} | v \rangle &= \frac{1}{\sqrt{10}}
 \end{aligned} \tag{2.20}$$

The corresponding probabilities are therefore

$$\begin{aligned}
 |\langle S_x = \frac{\hbar}{2} | v \rangle|^2 &= \frac{1}{20} |1 + 3i|^2 = \frac{1}{2} \\
 |\langle S_y = \frac{\hbar}{2} | v \rangle|^2 &= \frac{16}{20} = \frac{4}{5} \\
 |\langle S_z = \frac{\hbar}{2} | v \rangle|^2 &= \frac{1}{10}
 \end{aligned} \tag{2.21}$$

Hence the other probabilities are therefore

$$\begin{aligned}
 |\langle S_x = -\frac{\hbar}{2} | v \rangle|^2 &= 1 - \frac{1}{2} = \frac{1}{2} \\
 |\langle S_y = -\frac{\hbar}{2} | v \rangle|^2 &= 1 - \frac{4}{5} = \frac{1}{5} \\
 |\langle S_z = -\frac{\hbar}{2} | v \rangle|^2 &= 1 - \frac{1}{10} = \frac{9}{10}
 \end{aligned} \tag{2.22}$$

c)

$$\begin{aligned}
 |S_y = \frac{\hbar}{2}\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix} = \frac{1}{\sqrt{2}} |S_z = \frac{\hbar}{2}\rangle + \frac{i}{\sqrt{2}} |S_z = -\frac{\hbar}{2}\rangle \\
 |S_y = -\frac{\hbar}{2}\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} = \frac{1}{\sqrt{2}} |S_z = \frac{\hbar}{2}\rangle - \frac{i}{\sqrt{2}} |S_z = -\frac{\hbar}{2}\rangle
 \end{aligned} \tag{2.23}$$

The unitary matrix is therefore

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} \tag{2.24}$$

d) The matrix

$$S_{\vec{n}} = S_x = \frac{\hbar}{2} \begin{pmatrix} n_z & n_x - in_y \\ n_z + in_y & n_z \end{pmatrix} \tag{2.25}$$

has eigenvalues

$$\lambda_{\pm} = \pm \frac{\hbar}{2} \quad (2.26)$$

The eigenvectors are obtained from

$$\begin{pmatrix} n_z & n_x - i n_y \\ n_x + i n_y & -n_z \end{pmatrix} \begin{pmatrix} x_{\pm} \\ y_{\pm} \end{pmatrix} = \pm \begin{pmatrix} x_{\pm} \\ y_{\pm} \end{pmatrix} \quad (2.27)$$

that is

$$n_z x_{\pm} + (n_x - i n_y) y_{\pm} = \pm x_{\pm} \quad (2.28)$$

Hence

$$|S_{\vec{n}} = \pm \frac{\hbar}{2}\rangle = \frac{1}{\sqrt{2(1 \mp n_z)}} \begin{pmatrix} n_x - i n_y \\ \pm 1 - n_z \end{pmatrix} = \frac{1}{\sqrt{2(1 \mp \cos \theta)}} \begin{pmatrix} \sin \theta e^{-i\phi} \\ \pm 1 - \cos \theta \end{pmatrix}$$

Therefore

$$|S_{\vec{n}} = \frac{\hbar}{2}\rangle = \begin{pmatrix} \cos \frac{\theta}{2} e^{-i\phi} \\ \sin \frac{\theta}{2} \end{pmatrix} \quad |S_{\vec{n}} = -\frac{\hbar}{2}\rangle = \begin{pmatrix} \sin \frac{\theta}{2} e^{-i\phi} \\ -\cos \frac{\theta}{2} \end{pmatrix} \quad (2.29)$$

e)

$$U = \begin{pmatrix} \cos \frac{\theta}{2} e^{-i\phi} & \sin \frac{\theta}{2} e^{-i\phi} \\ \sin \frac{\theta}{2} & -\cos \frac{\theta}{2} \end{pmatrix} \quad (2.30)$$

Problem 13. Show that

$$v_{\vec{p}_0, \Delta}(\vec{x}) = \int d^3 \vec{p} v_{\vec{p}}(\vec{x}) \phi_{\vec{p}_0, \Delta}(\vec{p}) \quad (2.31)$$

with

$$v_{\vec{p}}(\vec{x}) = \frac{e^{\frac{i}{\hbar} \vec{x} \cdot \vec{p}}}{(2\pi \hbar)^{\frac{3}{2}}} \quad \phi_{\vec{p}_0, \Delta}(\vec{p}) = \frac{1}{(\pi)^{\frac{3}{4}} \Delta^{\frac{3}{2}}} e^{-\frac{(\vec{p} - \vec{p}_0)^2}{2\Delta^2}} \quad (2.32)$$

is a normalizable wave function of unit norm. Compute the average of \vec{x} , \vec{p} , Δp^2 and Δx^2 on the state described by the packet (2.31). Make use of the formula for gaussian integrals

$$\int_{-\infty}^{\infty} dx e^{-\alpha x^2 + \beta x} = \sqrt{\frac{\pi}{\alpha}} e^{\frac{\beta^2}{4\alpha}} \quad (2.33)$$

where $\alpha > 0$ and β is a generic *complex* number.

Solution: Let us compute the norm of this vector in the momentum representation

$$\begin{aligned}\langle v, v \rangle &= \int d^3 \vec{p} |\phi_{\vec{p}_0, \Delta}(\vec{p})|^2 = \int \frac{d^3 \vec{p}}{(\pi)^{\frac{3}{2}} \Delta^3} e^{-\frac{(\vec{p}-\vec{p}_0)^2}{\Delta^2}} = \\ &= \int \frac{d^3 \vec{p}}{(\pi)^{\frac{3}{2}} \Delta^3} e^{-\frac{\vec{p}^2}{\Delta^2}} = \frac{1}{(\pi)^{\frac{3}{2}} \Delta^3} \pi^{\frac{3}{2}} (\Delta^2)^{\frac{3}{2}} = 1\end{aligned}\quad (2.34)$$

Let us compute the average of \vec{x} in the momentum representation

$$\begin{aligned}\langle v, \vec{x} v \rangle &= \int \frac{d^3 \vec{p}}{(\pi)^{\frac{3}{2}} \Delta^3} e^{-\frac{(\vec{p}-\vec{p}_0)^2}{2\Delta^2}} i \hbar \vec{\nabla}_{\vec{p}} e^{-\frac{(\vec{p}-\vec{p}_0)^2}{2\Delta^2}} = \\ &= -i \hbar \int \frac{d^3 \vec{p}}{(\pi)^{\frac{3}{2}} \Delta^3} e^{-\frac{(\vec{p}-\vec{p}_0)^2}{\Delta^2}} \times \frac{(\vec{p} - \vec{p}_0)}{\Delta^2} = \\ &= -i \hbar \int \frac{d^3 \vec{p}}{(\pi)^{\frac{3}{2}} \Delta^3} e^{-\frac{\vec{p}^2}{\Delta^2}} \times \frac{\vec{p}}{\Delta^2} = 0\end{aligned}\quad (2.35)$$

Let us compute the average of \vec{p} in the momentum representation

$$\begin{aligned}\langle v, \vec{p} v \rangle &= \int \frac{d^3 \vec{p}}{(\pi)^{\frac{3}{2}} \Delta^3} e^{-\frac{(\vec{p}-\vec{p}_0)^2}{2\Delta^2}} \vec{p} e^{-\frac{(\vec{p}-\vec{p}_0)^2}{2\Delta^2}} = \\ &= \int \frac{d^3 \vec{p}}{(\pi)^{\frac{3}{2}} \Delta^3} e^{-\frac{\vec{p}^2}{\Delta^2}} (\vec{p} + \vec{p}_0) = \vec{p}_0\end{aligned}\quad (2.36)$$

Let us compute the average of \vec{x}^2 in the momentum representation

$$\begin{aligned}\langle v, \vec{x}^2 v \rangle &= - \int \frac{d^3 \vec{p}}{(\pi)^{\frac{3}{2}} \Delta^3} e^{-\frac{(\vec{p}-\vec{p}_0)^2}{2\Delta^2}} \hbar^2 \vec{\nabla}_{\vec{p}}^2 e^{-\frac{(\vec{p}-\vec{p}_0)^2}{2\Delta^2}} = \\ &= + \hbar^2 \int \frac{d^3 \vec{p}}{(\pi)^{\frac{3}{2}} \Delta^3} e^{-\frac{(\vec{p}-\vec{p}_0)^2}{2\Delta^2}} \times \vec{\nabla}_{\vec{p}} \left[\frac{(\vec{p} - \vec{p}_0)}{\Delta^2} e^{-\frac{(\vec{p}-\vec{p}_0)^2}{2\Delta^2}} \right] = \\ &= + \hbar^2 \int \frac{d^3 \vec{p}}{(\pi)^{\frac{3}{2}} \Delta^3} e^{-\frac{(\vec{p}-\vec{p}_0)^2}{\Delta^2}} \times \left[-\frac{(\vec{p} - \vec{p}_0)^2}{\Delta^4} + \frac{3}{\Delta^2} \right] = \\ &= + \frac{3 \hbar^2}{\Delta^2} - \hbar^2 \int \frac{d^3 \vec{p}}{(\pi)^{\frac{3}{2}} \Delta^3} e^{-\frac{\vec{p}^2}{\Delta^2}} \frac{\vec{p}^2}{\Delta^4}\end{aligned}\quad (2.37)$$

Integrals like those which appear in the r.h.s. can be computed in the following way

$$\int d^3 \vec{x} e^{-\alpha \vec{x}^2} \vec{x}^2 = -\partial_\alpha \int d^3 \vec{x} e^{-\alpha \vec{x}^2} = -\partial_\alpha \frac{\pi^{\frac{3}{2}}}{\alpha^{\frac{3}{2}}} = \frac{3}{2} \frac{\pi^{\frac{3}{2}}}{\alpha^{\frac{5}{2}}} \quad (2.38)$$

Hence

$$\langle v, \vec{x}^2 v \rangle = +\frac{3 \hbar^2}{\Delta^2} - \frac{3}{2} \frac{\hbar^2}{\Delta^2} = \frac{3 \hbar^2}{2 \Delta^2} \quad (2.39)$$

Therefore the uncertainty on \vec{x}^2 is

$$\Delta \vec{x}^2 = \langle v, \vec{x}^2 v \rangle - \langle v, \vec{x} v \rangle^2 = \frac{3 \hbar^2}{2 \Delta^2} \quad (2.40)$$

Let us compute the average of \vec{p}^2

$$\begin{aligned} \langle v, \vec{p}^2 v \rangle &= \int \frac{d^3 \vec{p}}{(\pi)^{\frac{3}{2}} \Delta^3} e^{-\frac{(\vec{p}-\vec{p}_0)^2}{2 \Delta^2}} \vec{p}^2 e^{-\frac{(\vec{p}-\vec{p}_0)^2}{2 \Delta^2}} = \\ &= \int \frac{d^3 \vec{p}}{(\pi)^{\frac{3}{2}} \Delta^3} e^{-\frac{\vec{p}^2}{\Delta^2}} (\vec{p} + \vec{p}_0)^2 = \\ &= \vec{p}_0^2 + \frac{3}{2} \Delta^2 \end{aligned} \quad (2.41)$$

Therefore the uncertainty on the \vec{p}^2 is

$$\Delta \vec{p}^2 = \langle v, \vec{p}^2 v \rangle - \langle v, \vec{p} v \rangle^2 = \frac{3}{2} \Delta^2 \quad (2.42)$$

Note that

$$\sqrt{\Delta \vec{x}^2} \sqrt{\Delta \vec{p}^2} = \frac{3}{2} \hbar \quad (2.43)$$

Since the state is rotation invariant

$$\begin{aligned} \Delta \vec{x}^2 &= \Delta(x^2 + y^2 + z^2) = 3 \Delta x^2 \\ \Delta \vec{p}^2 &= \Delta(p_x^2 + p_y^2 + p_z^2) = 3 \Delta p_x^2 \end{aligned} \quad (2.44)$$

Therefore

$$\Delta x \times \Delta p_x = \Delta y \times \Delta p_y = \Delta z \times \Delta p_z = \frac{\hbar}{2} \quad (2.45)$$

The state considered is therefore a state of *minimal* uncertainty.

The same computation could be done in the Schrödinger representation. Let us first compute the wave function in the Schrödinger representation

$$\begin{aligned}
v_{\vec{p}_0, \Delta}(\vec{x}) &= \frac{1}{(2\hbar\pi)^{\frac{3}{2}}} \int d^3\vec{p} e^{\frac{i}{\hbar}\vec{p}\cdot\vec{x}} \frac{1}{(\pi)^{\frac{3}{4}} \Delta^{\frac{3}{2}}} e^{-\frac{(\vec{p}-\vec{p}_0)^2}{2\Delta^2}} = \\
&= \frac{e^{\frac{i}{\hbar}\vec{p}_0\cdot\vec{x}}}{(2\hbar\pi)^{\frac{3}{2}}} \int d^3\vec{p} \frac{1}{(\pi)^{\frac{3}{4}} \Delta^{\frac{3}{2}}} e^{\frac{i}{\hbar}\vec{p}\cdot\vec{x} - \frac{\vec{p}^2}{2\Delta^2}} = \\
&= \frac{e^{\frac{i}{\hbar}\vec{p}_0\cdot\vec{x}}}{(2\hbar\pi)^{\frac{3}{2}}} \int d^3\vec{p} \frac{1}{(\pi)^{\frac{3}{4}} \Delta^{\frac{3}{2}}} e^{-\frac{(\vec{p}-\frac{i}{\hbar}\Delta^2\vec{x})^2}{2\Delta^2}} \times e^{-\frac{\Delta^2\vec{x}^2}{2\hbar^2}} = \\
&= \left(\frac{\Delta}{\hbar}\right)^{\frac{3}{2}} \frac{e^{\frac{i}{\hbar}\vec{p}_0\cdot\vec{x}}}{(\pi)^{\frac{3}{4}}} e^{-\frac{\Delta^2\vec{x}^2}{2\hbar^2}} \tag{2.46}
\end{aligned}$$

The averages of \vec{x} and \vec{p} are

$$\begin{aligned}
\langle v, \vec{x} v \rangle &= \left(\frac{\Delta}{\hbar}\right)^3 \frac{1}{\pi^{\frac{3}{2}}} \int d^3\vec{x} e^{-\frac{\Delta^2\vec{x}^2}{\hbar^2}} \vec{x} = 0 \\
\langle v, \vec{p} v \rangle &= \left(\frac{\Delta}{\hbar}\right)^3 \frac{1}{\pi^{\frac{3}{2}}} \int d^3\vec{x} e^{-\frac{\Delta^2\vec{x}^2}{\hbar^2}} \left[i \frac{\Delta^2\vec{x}}{\hbar} + \vec{p}_0 \right] = \vec{p}_0 \tag{2.47}
\end{aligned}$$

The averages of \vec{x}^2 and \vec{p}^2 write

$$\begin{aligned}
\langle v, \vec{x}^2 v \rangle &= \left(\frac{\Delta}{\hbar}\right)^3 \frac{1}{\pi^{\frac{3}{2}}} \int d^3\vec{x} e^{-\frac{\Delta^2\vec{x}^2}{\hbar^2}} \vec{x}^2 = \frac{3\hbar^2}{2\Delta^2} \\
\langle v, \vec{p}^2 v \rangle &= \left(\frac{\Delta}{\hbar}\right)^3 \frac{1}{\pi^{\frac{3}{2}}} \int d^3\vec{x} e^{-\frac{\Delta^2\vec{x}^2}{\hbar^2}} \left[3\Delta^2 + \vec{p}_0^2 - \frac{\Delta^4\vec{x}^2}{\hbar^2} \right] = \\
&= \vec{p}_0^2 + 3\Delta^2 - \frac{3}{2}\Delta^2 = \vec{p}_0^2 + \frac{3}{2}\Delta^2 \tag{2.48}
\end{aligned}$$

in agreement with the results obtained above in the momentum representation.

3 Simple systems

Problem 3. Show that the exponential factor which controls the probability of tunneling through the barrier

$$V(x) = \begin{cases} +\infty & \text{if } x < 0, \\ -V_0 & \text{if } 0 < x < L \\ \frac{Z e^2}{4\pi\epsilon_0 x} & \text{if } x > L \end{cases} \tag{3.1}$$

in the limit

$$E \ll \frac{Z e^2}{4 \pi \epsilon_0 L} \quad (3.2)$$

is

$$T \propto e^{-\frac{\pi Z e^2}{4 \pi \epsilon_0 \hbar} \sqrt{\frac{2m}{E}}} = e^{-\frac{Z e^2}{2 \epsilon_0 \hbar v}} \quad (3.3)$$

Solution:

Let us compute the integral

$$\int_L^{\frac{Z e^2}{4 \pi \epsilon_0 E}} dx \sqrt{\frac{Z e^2}{4 \pi \epsilon_0 x} - E} = \frac{Z e^2}{4 \pi \epsilon_0 \sqrt{E}} \int_{\frac{4 \pi \epsilon_0 L E}{Z e^2}}^1 \frac{dy}{\sqrt{y}} \sqrt{1-y} \quad (3.4)$$

In the limit (3.2)

$$\int_{\frac{4 \pi \epsilon_0 L E}{Z e^2}}^1 \frac{dy}{\sqrt{y}} \sqrt{1-y} \rightarrow \int_0^1 \frac{dy}{\sqrt{y}} \sqrt{1-y} = \int_0^1 2 d\xi \sqrt{1-\xi^2} = \frac{\pi}{2} \quad (3.5)$$

Hence

$$T \propto e^{-2 \sqrt{\frac{2m}{\hbar^2}} \frac{Z e^2}{4 \pi \epsilon_0 \sqrt{E}} \frac{\pi}{2}} = e^{-\pi \sqrt{\frac{2m}{E}} \frac{Z e^2}{4 \pi \epsilon_0 \hbar}} = e^{-\frac{Z e^2}{2 \epsilon_0 \hbar v}} \quad (3.6)$$

Problem 5. Find the reflection and transmission coefficients R and T for the rectangular potential barrier for $E < V_0$, in the limit in which $L \rightarrow 0$, $V_0 \rightarrow +\infty$ and $V_0 L = \mathcal{V}$ constant. (This is the so-called “thin barrier” limit.)

Solution:

In this limit

$$L \rightarrow 0 \quad L k' \rightarrow \frac{\sqrt{2m\mathcal{V}}}{\hbar} \sqrt{L} \rightarrow 0 \quad (k')^2 L \rightarrow \frac{2m\mathcal{V}}{\hbar^2} \quad (3.7)$$

Then

$$\begin{aligned} T &= \frac{16 k^2 |k'|^2}{\left| (k + i |k'|)^2 e^{-|k'|L} - (k - i |k'|)^2 e^{|k'|L} \right|^2} = \\ &= \frac{16 k^2 |k'|^2}{\left| (k^2 - |k'|^2) (e^{-|k'|L} - e^{|k'|L}) + 2 i k |k'| (e^{-|k'|L} + e^{|k'|L}) \right|^2} \\ &\rightarrow \frac{16 k^2 |k'|^2}{\left| |k'|^2 2 |k'| L + 2 i k |k'| 2 \right|^2} = \frac{4 k^2}{\left| |k'|^2 L + 2 i k \right|^2} \rightarrow \\ &\rightarrow \frac{k^2}{\left| \frac{m\mathcal{V}}{\hbar^2} + i k \right|^2} = \frac{\hbar^2 k^2}{\frac{m^2 \mathcal{V}^2}{\hbar^2} + \hbar^2 k^2} = \frac{p^2}{\frac{m^2 \mathcal{V}^2}{\hbar^2} + p^2} \end{aligned} \quad (3.8)$$

Problem 6. Determine the discrete levels and the energy eigenfunctions of an unidimensional particle moving in the potential well:

$$V(x) = \begin{cases} 0 & \text{if } |x| > \frac{a}{2}, \\ V_0 & \text{if } |x| \leq \frac{a}{2}. \end{cases} \quad (3.9)$$

for $V_0 < 0$.

Solution: Discrete states exists only if

$$V_0 < E < 0 \quad (3.10)$$

Wave functions of discrete eigenstates are either even or odd under reflection $x \rightarrow -x$. Let us denote even (odd) energy eigenfunctions with $\psi_E^+(x)$ ($\psi_E^-(x)$).

$$\psi_E^+(x) = \begin{cases} A_+ \cos k' x & |x| < \frac{a}{2} \\ B_+ e^{-kx} & x > \frac{a}{2} \\ B_+ e^{+kx} & x < -\frac{a}{2} \end{cases} \quad (3.11)$$

and

$$\psi_E^-(x) = \begin{cases} A_- \sin k' x & |x| < \frac{a}{2} \\ B_- e^{-kx} & x > \frac{a}{2} \\ -B_- e^{+kx} & x < -\frac{a}{2} \end{cases} \quad (3.12)$$

where

$$k = \frac{\sqrt{2m|E|}}{\hbar} \quad k' = \frac{\sqrt{2m(E - V_0)}}{\hbar} \quad (3.13)$$

Continuity of wave function and of its first derivative at $x = \frac{a}{2}$ implies

$$\begin{aligned} A_+ \cos \frac{k' a}{2} &= B_+ e^{-\frac{k a}{2}} \\ -k' A_+ \sin \frac{k' a}{2} &= -k B_+ e^{-\frac{k a}{2}} \end{aligned} \quad (3.14)$$

and

$$\begin{aligned} A_- \sin \frac{k' a}{2} &= B_- e^{-\frac{k a}{2}} \\ k' A_- \cos \frac{k' a}{2} &= -k B_- e^{-\frac{k a}{2}} \end{aligned} \quad (3.15)$$

We get therefore the eigenvalue equation for E , for

$$\begin{aligned} k' \tan \frac{k' a}{2} = k & \quad \text{for} \quad \psi_E^+ \\ k' \cot \frac{k' a}{2} = -k & \quad \text{for} \quad \psi_E^- \end{aligned} \quad (3.16)$$

Introducing the adimensional variables

$$\xi = \frac{k' a}{2} \quad \eta = \frac{k a}{2} \quad (3.17)$$

the equations (3.16) become

$$\begin{aligned} \eta = \xi \tan \xi & \quad \text{for} \quad \psi_E^+ \\ \eta = -\xi \cot \xi & \quad \text{for} \quad \psi_E^- \end{aligned} \quad (3.18)$$

Moreover we have the relationship between ξ and η

$$\xi^2 + \eta^2 = \frac{a^2 m |V_0|}{2 \hbar^2} \quad (3.19)$$

and the Eq. (3.10) means that

$$0 < \xi < \frac{a^2 m |V_0|}{2 \hbar^2} \quad 0 < \eta < \frac{a^2 m |V_0|}{2 \hbar^2} \quad (3.20)$$

The eigenvalues E are determined therefore by the intersections of the two curves

$$\begin{aligned} \eta = \xi \tan \xi & \quad \text{for} \\ \xi^2 + \eta^2 = \frac{a^2 m |V_0|}{2 \hbar^2} & \quad \psi_E^+ \end{aligned} \quad (3.21)$$

and

$$\begin{aligned} \eta = -\xi \cot \xi & \quad \text{for} \\ \xi^2 + \eta^2 = \frac{a^2 m |V_0|}{2 \hbar^2} & \quad \psi_E^- \end{aligned} \quad (3.22)$$

which lie in the first quadrant of (ξ, η) plane.

By drawing the graphs of the curves (3.21), we see that the solutions $\{\xi_1, \xi_3, \xi_5 \dots\}$ corresponding to the energy eigenvalues E_1, E_3, E_5, \dots of the even wave functions satisfy

$$0 < \xi_1 < \frac{\pi}{2} \quad \pi < \xi_3 < \frac{3\pi}{2} \quad 2\pi < \xi_5 < \frac{5\pi}{2} \quad (3.23)$$

Similarly, the solutions $\{\xi_2, \xi_4, \xi_6 \dots\}$ corresponding to the energy eigenvalues E_2, E_4, E_6, \dots of the even wave functions satisfy

$$\frac{\pi}{2} < \xi_2 < \pi \quad \frac{3\pi}{2} < \xi_4 < 2\pi \quad \frac{5\pi}{2} < \xi_6 < 3\pi \quad (3.24)$$

The number n of bound states is therefore the highest positive integer such that

$$(n-1) \frac{\pi}{2} \leq \sqrt{\frac{a^2 m |V_0|}{2 \hbar^2}} \quad (3.25)$$

In particular we have always at least 1 bound state,

$$0 < \xi_1 < \frac{\pi}{2} \quad (3.26)$$

for which

$$0 < E_1 - V_0 < \frac{\pi^2 \hbar^2}{2m a^2} \quad (3.27)$$

The *un-normalized* wave functions of such bound states are obtained by replacing (3.14) and (3.15) into (3.11) and (3.12)

$$\psi_E^+(x) = \begin{cases} \cos k' x & |x| < \frac{a}{2} \\ \cos \frac{k'a}{2} e^{k(\frac{a}{2}-x)} & x > \frac{a}{2} \\ \cos \frac{k'a}{2} e^{k(\frac{a}{2}+x)} & x < -\frac{a}{2} \end{cases} \quad (3.28)$$

and

$$\psi_E^-(x) = \begin{cases} \sin k' x & |x| < \frac{a}{2} \\ \sin \frac{k'a}{2} e^{k(\frac{a}{2}-x)} & x > \frac{a}{2} \\ -\sin \frac{k'a}{2} e^{k(\frac{a}{2}+x)} & x < -\frac{a}{2} \end{cases} \quad (3.29)$$

Problem 7. Determine the discrete levels of an unidimensional particle moving in the potential well

$$V(x) = \begin{cases} +\infty & \text{if } x < 0 \\ -V_0 & \text{if } 0 < x < L, \\ 0 & \text{if } x > L. \end{cases} \quad (3.30)$$

for $V_0 > 0$. Find the value of V_0 for which there is one single bound state.

Solution: Bound states are possible only for $-V_0 < E < 0$. The eigenfunctions have the form

$$\psi_E(x) = \begin{cases} A e^{\frac{i}{\hbar} p' x} + B e^{-\frac{i}{\hbar} p' x} & \text{if } 0 < x < L \\ A' e^{\frac{1}{\hbar} p x} + B' e^{-\frac{1}{\hbar} p x} & \text{if } x > L \end{cases} \quad (3.31)$$

where

$$p' = \sqrt{2m(E + V_0)} \quad p = \sqrt{2m|E|} = \sqrt{-2mE} \quad (3.32)$$

Since the particle is bound to be in the region $x > 0$, we have the boundary condition of the wave function

$$\psi_E(0) = 0 \quad (3.33)$$

Moreover the wave function of a bound state must vanish for $x \rightarrow +\infty$. Therefore

$$\psi_E(x) = \begin{cases} A [e^{\frac{i}{\hbar} p' x} - e^{-\frac{i}{\hbar} p' x}] & \text{if } 0 < x < L \\ B' e^{-\frac{1}{\hbar} p x} & \text{if } x > L \end{cases} \quad (3.34)$$

The continuity conditions at $x = L$ are

$$\begin{aligned} 2iA \sin \frac{p' L}{\hbar} &= B' e^{-\frac{pL}{\hbar}} \\ 2 \frac{i}{\hbar} p' A \cos \frac{p' L}{\hbar} &= -B' \frac{p}{\hbar} e^{-\frac{pL}{\hbar}} \end{aligned} \quad (3.35)$$

Dividing the second equation by the first we obtain the necessary and sufficient condition for this linear homogenous system to have a solution:

$$p = -p' \cot \frac{p' L}{\hbar} \quad (3.36)$$

Energy eigenvalues are therefore determined by the intersections of the two curves in the positive quadrant of the (p', p) plane

$$\begin{aligned} p &= -p' \cot \frac{p' L}{\hbar} \\ p'^2 + p^2 &= 2 m V_0 \\ p > 0 \quad p' > 0 \end{aligned} \quad (3.37)$$

Introducing the adimensional variables

$$\xi = \frac{p' L}{\hbar} \quad \eta = \frac{p L}{\hbar} \quad \alpha^2 \equiv \frac{2 m V_0 L^2}{\hbar^2} \quad (3.38)$$

the equations of the curves become

$$\begin{aligned} \eta &= -\xi \cot \xi \\ \xi^2 + \eta^2 &= \alpha^2 \\ \eta > 0 \quad \xi > 0 \end{aligned} \quad (3.39)$$

Drawing the graphs of the two curves we see that minimal α for which an intersection in the *positive* quadrant exists is for $\alpha = \frac{\pi}{2}$

$$\alpha = \frac{\pi}{2} \quad \xi = \frac{\pi}{2} \quad \eta = 0 \quad (3.40)$$

Thus the minimal value of V_0 for which there is a bound state is

$$V_0^{min} = \frac{\hbar^2 \pi^2}{8 m L^2} \quad (3.41)$$

When α increases and

$$\frac{\pi}{2} < \alpha < \frac{3\pi}{2} \quad (3.42)$$

there is one single intersection in the positive quadrant. Thus for

$$\frac{\hbar^2 \pi^2}{8 m L^2} < V_0 < \frac{9 \hbar^2 \pi^2}{8 m L^2} \quad (3.43)$$

there is a single bound state with

$$E_0 = \frac{\hbar^2 \xi^2}{2 m L^2} - V_0 \quad \frac{\pi}{2} < \xi < \pi \quad (3.44)$$

More generally when α reaches the values

$$\alpha_n = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, \dots \quad (3.45)$$

new solutions with $\eta = 0$ appear, in correspondence with new bound states. The new bound states starts at $E = 0$ for $\alpha = \alpha_n$, and, as α goes from α_n to α_{n+1} , its energy becomes more negative and lies in the range

$$\frac{\alpha_n^2 \hbar^2}{2mL^2} - V_0 < E < \frac{\alpha_{n+1}^2 \hbar^2}{2mL^2} - V_0 \quad (3.46)$$

When $V_0 \rightarrow \infty$ the numbers of bound states increases. The ground state level E_0 tends to the limiting value

$$E_0 = \frac{\hbar^2 \xi}{2mL^2} - V_0 \rightarrow \frac{\hbar^2 \pi^2}{2mL^2} - V_0 \quad (3.47)$$

Problem 8. Determine the discrete levels of an unidimensional particle moving in the potential well by using the expression obtained for the transfer matrix for the potential barrier

$$\mathcal{T} = \frac{1}{4} \times \begin{pmatrix} \frac{(k+k')^2}{kk'} e^{i(k-k')L} - \frac{(k-k')^2}{kk'} e^{i(k+k')L} & \frac{k^2-(k')^2}{kk'} (e^{-i(k-k')L} - e^{-i(k+k')L}) \\ \frac{k^2-(k')^2}{kk'} (e^{i(k-k')L} - e^{i(k+k')L}) & \frac{(k+k')^2}{kk'} e^{-i(k-k')L} - \frac{(k-k')^2}{kk'} e^{-i(k+k')L} \end{pmatrix}$$

Solution:

We must put in this case

$$k = \frac{\sqrt{2mE}}{\hbar} = i \frac{\sqrt{2m|E|}}{\hbar} = i|k| \quad k' = \frac{\sqrt{2m(E+V_0)}}{\hbar} \quad (3.48)$$

Moreover we should impose

$$A = B'' = 0 \quad A'' = 1 \quad (3.49)$$

in the equation

$$\begin{pmatrix} A \\ B \end{pmatrix} = \mathcal{T} \begin{pmatrix} A'' \\ B'' \end{pmatrix} \quad (3.50)$$

Hence the equation which determine the energy levels is

$$\mathcal{T}_{11} = \frac{(i|k| + k')^2}{k k'} e^{i(k-k')L} - \frac{(i|k| - k')^2}{k k'} e^{i(k+k')L} = 0 \quad (3.51)$$

from which

$$\frac{(i|k| + k')^2}{(i|k| - k')^2} = e^{2ik'L} \quad (3.52)$$

Let us put

$$i|k| + k' = |i|k| + k'| e^{i\theta_E} \quad \tan \theta_E = \frac{|k|}{k'} \quad (3.53)$$

Thus

$$\frac{(i|k| + k')^2}{(i|k| - k')^2} = e^{4i\theta_E} \quad (3.54)$$

The equations for the eigenvalues becomes therefore

$$4\theta_E = 2k'L + 2n\pi \quad n = 0, \pm 1, \pm 2, \dots \quad (3.55)$$

i.e.

$$\theta_E = \frac{k'L}{2} + \frac{n\pi}{2} \quad \Rightarrow \tan \theta_E = \frac{|k|}{k'} = \tan\left(\frac{k'L}{2} + \frac{n\pi}{2}\right) \quad (3.56)$$

For n even

$$\frac{|k|}{k'} = \tan\left(\frac{k'L}{2}\right) \quad (3.57)$$

and for n odd

$$-\frac{|k|}{k'} = \cot\left(\frac{k'L}{2}\right) \quad (3.58)$$

in agreement with (3.16).

Problem 9. Determine the energy eigenfunctions for the potential barrier

$$V(x) = \begin{cases} 0 & \text{if } |x| > \frac{a}{2}, \\ V_0 & \text{if } |x| \leq \frac{a}{2}. \end{cases} \quad (3.59)$$

with $V_0 > 0$ and $0 < E < V_0$ which are also eigenstates of the spatial inversion operator $I : \psi(x) \rightarrow \psi(-x)$. Derive the transmission matrix for this barrier.

Solution:

The even and odd energy eigenfunctions with $0 < E < V_0$ have the form:

$$\psi_E^+(x) = \begin{cases} e^{+ikx} + B_+ e^{-ikx} & x < -\frac{a}{2} \\ A_+ \cosh k'x & |x| < \frac{a}{2} \\ B_+ e^{ikx} + e^{-ikx} & x > \frac{a}{2} \end{cases} \quad (3.60)$$

and

$$\psi_E^-(x) = \begin{cases} e^{+ikx} + B_- e^{-ikx} & x < -\frac{a}{2} \\ A_- \sinh k'x & |x| < \frac{a}{2} \\ -B_- e^{ikx} - e^{-ikx} & x > \frac{a}{2} \end{cases} \quad (3.61)$$

where

$$k = \frac{\sqrt{2mE}}{\hbar} \quad k' = \frac{\sqrt{2m|V_0 - E|}}{\hbar} \quad (3.62)$$

Continuity of the wave-functions and of their first derivative at $x = \pm \frac{a}{2}$ gives

$$\begin{aligned} B_+ e^{+i\frac{ka}{2}} + e^{-i\frac{ka}{2}} &= A_+ \cosh \frac{k'a}{2} \\ ik (B_+ e^{i\frac{ka}{2}} - e^{-i\frac{ka}{2}}) &= A_+ k' \sinh \frac{k'a}{2} \\ B_- e^{i\frac{ka}{2}} + e^{-i\frac{ka}{2}} &= -A_- \sinh \frac{k'a}{2} \\ -ik (B_- e^{i\frac{ka}{2}} - e^{-i\frac{ka}{2}}) &= A_- k' \cosh \frac{k'a}{2} \end{aligned} \quad (3.63)$$

From this

$$\begin{aligned} \frac{B_+ - e^{-ika}}{B_+ + e^{-ika}} &= -i \frac{k'}{k} \tanh \frac{k'a}{2} \\ \frac{B_- - e^{-ika}}{B_- + e^{-ika}} &= -i \frac{k'}{k} \coth \frac{k'a}{2} \end{aligned} \quad (3.64)$$

and

$$\begin{aligned} B_+ &= \frac{1 + i \frac{k'}{k} \tanh \frac{k'a}{2}}{1 - i \frac{k'}{k} \tanh \frac{k'a}{2}} e^{-ika} = e^{2i\theta_+(E)} e^{-ika} \\ B_- &= \frac{1 + i \frac{k'}{k} \coth \frac{k'a}{2}}{1 - i \frac{k'}{k} \coth \frac{k'a}{2}} e^{-ika} = e^{2i\theta_-(E)} e^{-ika} \end{aligned} \quad (3.65)$$

where

$$\begin{aligned}\tan \theta_+(E) &= \frac{k'}{k} \tanh \frac{k' a}{2} \\ \tan \theta_-(E) &= \frac{k'}{k} \coth \frac{k' a}{2}\end{aligned}\quad (3.66)$$

Hence

$$\begin{aligned}A_+ &= e^{+i \frac{k a}{2}} \frac{B_+ + e^{-i k a}}{\cosh \frac{k' a}{2}} = e^{-i \frac{k a}{2}} \frac{1 + e^{2i \theta_+(E)}}{\cosh \frac{k' a}{2}} = \\ A_- &= -e^{+i \frac{k a}{2}} \frac{B_- + e^{-i k a}}{\sinh \frac{k' a}{2}} = -e^{-i \frac{k a}{2}} \frac{1 + e^{2i \theta_-(E)}}{\sinh \frac{k' a}{2}}\end{aligned}\quad (3.67)$$

The relation that defines the transfer matrix is

$$\begin{pmatrix} A_+ \\ B_+ \end{pmatrix} = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \begin{pmatrix} A_- \\ B_- \end{pmatrix}\quad (3.68)$$

where $\{A_+, B_+\}$ ($\{A_-, B_-\}$) are the coefficients of the right-moving and left-moving plane waves to which the energy eigenfunction reduces for $x \rightarrow +\infty$ ($x \rightarrow -\infty$). By comparing with (3.60) and (3.61) we deduce

$$\begin{aligned}\begin{pmatrix} B_+ \\ 1 \end{pmatrix} &= \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \begin{pmatrix} 1 \\ B_+ \end{pmatrix} \\ \begin{pmatrix} -B_- \\ -1 \end{pmatrix} &= \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \begin{pmatrix} 1 \\ B_- \end{pmatrix}\end{aligned}\quad (3.69)$$

and hence

$$\begin{aligned}\begin{pmatrix} B_+ - B_- \\ 0 \end{pmatrix} &= \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \begin{pmatrix} 2 \\ B_+ + B_- \end{pmatrix} \\ \begin{pmatrix} B_+ + B_- \\ 2 \end{pmatrix} &= \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix} \begin{pmatrix} 0 \\ B_+ - B_- \end{pmatrix}\end{aligned}\quad (3.70)$$

The reflection and transmission coefficients are therefore

$$\begin{aligned}R &= \left| \frac{B_+ + B_-}{2} \right|^2 = \frac{1}{4} \left| e^{2i \theta_+(E)} + e^{2i \theta_-(E)} \right|^2 = \\ &= \frac{1 + \cos 2(\theta_+(E) - \theta_-(E))}{2} = \cos^2(\theta_+(E) - \theta_-(E)) \\ T &= \left| \frac{B_+ - B_-}{2} \right|^2 = \frac{1}{4} \left| e^{2i \theta_+(E)} - e^{2i \theta_-(E)} \right|^2 = \\ &= \frac{1 - \cos 2(\theta_+(E) - \theta_-(E))}{2} = \sin^2(\theta_+(E) - \theta_-(E))\end{aligned}\quad (3.71)$$

which shows that

$$R + T = 1 \quad (3.72)$$

We can also express the elements of the transfer matrix in terms of $\theta_{\pm}(E)$

$$\begin{aligned} T_{22} &= \frac{2}{B_+ - B_-} = e^{i k a} \left(\cosh(k'a) + \frac{i(k^2 - (k')^2)}{2 k k'} \sinh(k'a) \right) \\ T_{12} &= -T_{21} = \frac{B_+ + B_-}{B_+ - B_-} = \frac{i(k^2 + (k')^2)}{2 k k'} \sinh(k'a) \\ T_{11} &= -\frac{2 B_+ B_-}{B_+ - B_-} = \\ &= e^{-i k a} \left(\cosh(k'a) - \frac{i(k^2 - (k')^2)}{2 k k'} \sinh(k'a) \right) \end{aligned} \quad (3.73)$$

and the transmission coefficient

$$\begin{aligned} T &= \frac{1}{|T_{22}|^2} = \frac{1}{\cosh^2(k'a) + \frac{(k^2 - (k')^2)^2}{4 k^2 (k')^2} \sinh^2(k'a)} = \\ &= \frac{1}{\cosh^2(g \sqrt{1 - \epsilon}) + \frac{(1 - 2\epsilon)^2}{4\epsilon(1 - \epsilon)} \sinh^2(g \sqrt{1 - \epsilon})} \end{aligned} \quad (3.74)$$

where

$$\epsilon \equiv \frac{E}{V_0} \quad g \equiv \sqrt{\frac{2 m a^2 V_0}{\hbar^2}} \quad (3.75)$$

in agreement with the result obtained in the main text. In the limit of “high” barrier

$$k' a \gg 1 \Rightarrow g \sqrt{1 - x} \gg 1 \quad (3.76)$$

we obtain

$$T \approx 4 e^{-2k'a} \frac{4 k^2 (k')^2}{(k^2 + (k')^2)^2} = 16 \frac{E}{V_0} \left(1 - \frac{E}{V_0} \right) e^{-2k'a} \quad (3.77)$$

When the energy tends to the threshold value $E \rightarrow V_0^-$, the transmission coefficient tends to the value

$$\lim_{E \rightarrow V_0^-} T = \frac{1}{1 + \frac{m V_0 L^2}{2 \hbar^2}} \quad (3.78)$$

For $E > V_0$ we derive analogously

$$\begin{aligned}
 T &= \frac{1}{\cos^2(|k'|a) + \frac{(k^2+|k'|^2)^2}{4k^2|k'|^2} \sin^2(|k'|a)} = \\
 &= \frac{1}{\cos^2(g\sqrt{\epsilon-1}) + \frac{(1-2\epsilon)^2}{4\epsilon(\epsilon-1)} \sin^2(g\sqrt{\epsilon-1})} \quad (3.79)
 \end{aligned}$$

Problem 10.

A 1-dimensional particle moves on the half line $x > 0$ in the potential

$$V(x) = \begin{cases} +\infty & \text{if } x < 0, \\ 0 & \text{if } 0 < x < L. \\ V_0 & \text{if } L < x < L + a. \\ 0 & \text{if } L + a < x. \end{cases} \quad (3.80)$$

with $V_0 > 0$. Determine the energy eigenfunctions.

Solution:

The spectrum is continuous and not-degenerate for $E > 0$. For $0 < E < V_0$ the energy eigenfunctions have the form

$$\psi_E(x) = \begin{cases} \sin kx & 0 < x < L \\ A' e^{k'x} + B' e^{-k'x} & L < x < L + a \\ A e^{ikx} + B e^{-ikx} & x > L + a \end{cases} \quad (3.81)$$

where

$$k = \frac{\sqrt{2mE}}{\hbar} \quad k' = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \quad (3.82)$$

Continuity of the wave function and of its first derivative at $x = L$ gives

$$\begin{aligned}
 \sin kL &= A' e^{k'L} + B' e^{-k'L} \\
 \frac{k}{k'} \cos kL &= A' e^{k'L} - B' e^{-k'L} \quad (3.83)
 \end{aligned}$$

From this we obtain

$$\begin{aligned}
 A' &= \frac{1}{2} e^{-k'L} \left(\sin kL + \frac{k}{k'} \cos kL \right) \\
 B' &= \frac{1}{2} e^{k'L} \left(\sin kL - \frac{k}{k'} \cos kL \right) \quad (3.84)
 \end{aligned}$$

Continuity of the wave function and of its first derivative at $x = L + a$ gives

$$\begin{aligned}
A e^{i k(L+a)} + B e^{-i k(L+a)} &= A' e^{k'(L+a)} + B' e^{-k'(L+a)} = \\
&= \frac{1}{2} \left(\sin k L + \frac{k}{k'} \cos k L \right) e^{k' a} + \frac{1}{2} \left(\sin k L - \frac{k}{k'} \cos k L \right) e^{-k' a} = \\
&= \sin(k L) \cosh(k' a) + \frac{k}{k'} \cos(k L) \sinh(k' a) \\
A e^{i k(L+a)} - B e^{-i k(L+a)} &= \frac{k'}{i k} \left(A' e^{k'(L+a)} - B' e^{-k'(L+a)} \right) = \\
&= -i \frac{k'}{k} \sin(k L) \sinh(k' a) - i \cos(k L) \cosh(k' a) \tag{3.85}
\end{aligned}$$

From this we obtain

$$\begin{aligned}
A &= \frac{1}{2} e^{-i k(L+a)} \left[\sin(k L) \cosh(k' a) + \frac{k}{k'} \cos(k L) \sinh(k' a) + \right. \\
&\quad \left. -i \cos(k L) \cosh(k' a) - i \frac{k'}{k} \sin(k L) \sinh(k' a) \right] \\
B &= A^* \tag{3.86}
\end{aligned}$$

Problem 11. Compute the averages of \hat{x}^2 and of \hat{p}^2 on the ground state $|0\rangle$ of the harmonic oscillator. (*Hint:* write \hat{x} and \hat{p} in terms of a and a^\dagger .)

Solution:

$$\hat{x} = i \lambda (a - a^\dagger) \quad \hat{p} = \frac{\hbar}{2 \lambda} (a + a^\dagger) \tag{3.87}$$

Therefore

$$\langle 0 | \hat{x} | 0 \rangle = 0 \quad \langle 0 | \hat{p} | 0 \rangle = 0 \tag{3.88}$$

Moreover

$$\begin{aligned}
\hat{x}^2 &= -\lambda^2 (a^{\dagger 2} + a^2 - a^\dagger a - a a^\dagger) \\
\hat{p}^2 &= \frac{\hbar^2}{4 \lambda^2} (a^{\dagger 2} + a^2 + a^\dagger a + a a^\dagger) \tag{3.89}
\end{aligned}$$

Therefore

$$\begin{aligned}
\langle 0 | \hat{x}^2 | 0 \rangle &= -\lambda^2 \langle 0 | (a^{\dagger 2} + a^2 - a^\dagger a - a a^\dagger) | 0 \rangle = \lambda^2 \langle 0 | a a^\dagger | 0 \rangle = \lambda^2 \\
\langle 0 | \hat{p}^2 | 0 \rangle &= \frac{\hbar^2}{4 \lambda^2} \langle 0 | (a^{\dagger 2} + a^2 + a^\dagger a + a a^\dagger) | 0 \rangle = \frac{\hbar^2}{4 \lambda^2} \langle 0 | a a^\dagger | 0 \rangle = \\
&= \frac{\hbar^2}{4 \lambda^2} \tag{3.90}
\end{aligned}$$

In conclusion

$$\begin{aligned}\Delta x^2 &= \langle 0|\hat{x}^2|0\rangle - (\langle 0|\hat{x}|0\rangle)^2 = \lambda^2 \\ \Delta p^2 &= \langle 0|\hat{p}^2|0\rangle - (\langle 0|\hat{p}|0\rangle)^2 = \frac{\hbar^2}{4\lambda^2}\end{aligned}\quad (3.91)$$

and thus

$$\Delta x \Delta p = \frac{\hbar}{2} \quad (3.92)$$

The ground state is therefore a state of minimal uncertainty.

Problem 12. Consider the state ψ of an harmonic oscillator of frequency ω and mass m which satisfies the equation

$$a\psi = \alpha\psi \quad (3.93)$$

where α is a *complex number*.

- a) Find the *normalized* wave function of ψ in the Schrödinger representation.
- b) Compute Δx and Δp on the state ψ and show it is a state of minimal indeterminacy.
- c) Consider the state

$$\tilde{\psi} = \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \quad (3.94)$$

where $|n\rangle$ with $n = 0, 1, 2, \dots$ are the normalized eigenstates of the harmonic oscillator Hamiltonian. Show that $\tilde{\psi}$ satisfies (3.93).

- d) Compute the norm of $\tilde{\psi}$.
- e) Let $\hat{\psi}$ be a normalized vector corresponding to $\tilde{\psi}$. By comparing the wave function in the Schrödinger representation of $\hat{\psi}$ with the normalized wave-function computed in a), derive an explicit formula for the Hermite polynomials for any n .

Solution:

- a) The wave-function $\psi(x)$ satisfies the differential equation

$$-i\hbar\psi'(x) - im\omega x\psi(x) = \frac{\hbar\alpha}{\lambda}\psi(x) \quad (3.95)$$

that is

$$\frac{\psi'(x)}{\psi(x)} = \frac{i\alpha}{\lambda} - \frac{x}{2\lambda^2} \quad (3.96)$$

The solution is

$$\psi(x) = C e^{i\alpha \frac{x}{\lambda} - \frac{x^2}{4\lambda^2}} \quad (3.97)$$

The normalized wave-function is obtained by imposing

$$\begin{aligned} 1 = \langle \psi, \psi \rangle &= |C|^2 \int_{-\infty}^{\infty} dx e^{i(\alpha - \bar{\alpha}) \frac{x}{\lambda} - \frac{x^2}{2\lambda^2}} = |C|^2 \lambda \int_{-\infty}^{\infty} dy e^{i(\alpha - \bar{\alpha}) y - \frac{y^2}{2}} = \\ &= |C|^2 \lambda \sqrt{2\pi} e^{-\frac{(\alpha - \bar{\alpha})^2}{2}} \end{aligned} \quad (3.98)$$

Hence

$$\psi(x) = \frac{1}{(2\pi)^{\frac{1}{4}}} \frac{1}{\lambda^{\frac{1}{2}}} e^{\frac{(\alpha - \bar{\alpha})^2}{4}} e^{i\alpha \frac{x}{\lambda} - \frac{x^2}{4\lambda^2}} \quad (3.99)$$

b) Let us compute Δx by making use of the Schrödinger representation:

$$\begin{aligned} \langle \psi, \hat{x} \psi \rangle &= |C|^2 \int_{-\infty}^{\infty} dx x e^{i(\alpha - \bar{\alpha}) \frac{x}{\lambda} - \frac{x^2}{2\lambda^2}} = |C|^2 \lambda^2 \int_{-\infty}^{\infty} dy y e^{i(\alpha - \bar{\alpha}) y - \frac{y^2}{2}} = \\ &= -i |C|^2 \lambda^2 \sqrt{2\pi} \frac{\partial}{\partial(\alpha - \bar{\alpha})} e^{-\frac{(\alpha - \bar{\alpha})^2}{2}} = \\ &= i |C|^2 \lambda^2 \sqrt{2\pi} (\alpha - \bar{\alpha}) e^{-\frac{(\alpha - \bar{\alpha})^2}{2}} = i (\alpha - \bar{\alpha}) \lambda \end{aligned} \quad (3.100)$$

and

$$\begin{aligned} \langle \psi, \hat{x}^2 \psi \rangle &= |C|^2 \int_{-\infty}^{\infty} dx x^2 e^{i(\alpha - \bar{\alpha}) \frac{x}{\lambda} - \frac{x^2}{2\lambda^2}} = |C|^2 \lambda^3 \int_{-\infty}^{\infty} dy y^2 e^{i(\alpha - \bar{\alpha}) y - \frac{y^2}{2}} = \\ &= -|C|^2 \lambda^3 \sqrt{2\pi} \frac{\partial^2}{\partial(\alpha - \bar{\alpha})^2} e^{-\frac{(\alpha - \bar{\alpha})^2}{2}} = \\ &= |C|^2 \lambda^3 \sqrt{2\pi} (1 - (\alpha - \bar{\alpha})^2) e^{-\frac{(\alpha - \bar{\alpha})^2}{2}} = \lambda^2 (1 - (\alpha - \bar{\alpha})^2) \end{aligned} \quad (3.101)$$

Thus

$$\Delta x^2 = \lambda^2 [1 - (\alpha - \bar{\alpha})^2 + (\alpha - \bar{\alpha})^2] = \lambda^2 \quad (3.102)$$

For Δp , let us show how to perform the computation by using raising and lowering operators together with Eq. (3.93). As a matter of fact, this method is simpler:

$$\begin{aligned}\langle \psi, \hat{p} \psi \rangle &= \frac{\hbar}{2\lambda} \langle \psi, (a + a^\dagger) \psi \rangle = \frac{\hbar}{2\lambda} \langle \psi, (\alpha + a^\dagger) \psi \rangle = \\ &= \frac{\hbar}{2\lambda} (\alpha + \langle a \psi, \psi \rangle) = \frac{\hbar}{2\lambda} (\alpha + \bar{\alpha})\end{aligned}\quad (3.103)$$

And

$$\begin{aligned}\langle \psi, \hat{p}^2 \psi \rangle &= \frac{\hbar^2}{4\lambda^2} \langle (a + a^\dagger) \psi, (a + a^\dagger) \psi \rangle = \\ &= \frac{\hbar^2}{4\lambda^2} [|\alpha|^2 + \langle a^\dagger \psi, a^\dagger \psi \rangle + \alpha^2 + \bar{\alpha}^2] = \\ &= \frac{\hbar^2}{4\lambda^2} [|\alpha|^2 + |\alpha|^2 + 1 + \alpha^2 + \bar{\alpha}^2] = \\ &= \frac{\hbar^2}{4\lambda^2} [2|\alpha|^2 + 1 + \alpha^2 + \bar{\alpha}^2]\end{aligned}\quad (3.104)$$

Hence

$$\Delta p^2 = \frac{\hbar^2}{4\lambda^2} [2|\alpha|^2 + 1 + \alpha^2 + \bar{\alpha}^2 - \alpha^2 - \bar{\alpha}^2 - 2|\alpha|^2] = \frac{\hbar^2}{4\lambda^2} \quad (3.105)$$

We verified that the state is indeed a state of minimal indeterminacy

$$\Delta x \Delta p = \frac{\hbar}{2} \quad (3.106)$$

c)

$$\begin{aligned}a \tilde{\psi} &= \sum_{n=1}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \sqrt{n} |n-1\rangle = \sum_{n=0}^{\infty} \frac{\alpha^{n+1}}{\sqrt{(n+1)!}} \sqrt{n+1} |n\rangle = \\ &= \alpha \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle = \alpha \tilde{\psi}\end{aligned}\quad (3.107)$$

d)

$$\langle \tilde{\psi}, \tilde{\psi} \rangle = \sum_{n=0}^{\infty} \frac{\bar{\alpha}^n}{\sqrt{n!}} \frac{\alpha^n}{\sqrt{n!}} = \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!} = e^{|\alpha|^2} \quad (3.108)$$

e) From d) we deduce that the vector

$$\hat{\psi} = e^{-\frac{|\alpha|^2}{2}} \tilde{\psi} = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle \quad (3.109)$$

has unit norm. The wave function of $\hat{\psi}$ in the Schrödinger representation is

$$\hat{\psi}(x) = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \psi_n(x) = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} \frac{H_n\left(\frac{x}{\lambda}\right)}{(2\pi)^{\frac{1}{4}} \lambda^{\frac{1}{2}}} e^{-\frac{x^2}{4\lambda^2}} \quad (3.110)$$

Here the $\psi_n(x)$ are the wave-functions of the energy eigenstates of the harmonic oscillator and the polynomials $H_n(y)$ are defined according to

$$\psi_n(x) = \langle x|n\rangle = \frac{H_n\left(\frac{x}{\lambda}\right)}{(2\pi)^{\frac{1}{4}} \lambda^{\frac{1}{2}}} e^{-\frac{x^2}{4\lambda^2}} \quad (3.111)$$

$H_n(y)$ are polynomial of degree n , of parity $(-1)^n$, which are (simply related to) the so-called Hermite polynomials. In the following we will derive a closed expression for $H_n(x)$ by comparing Eq. (3.110) with the result obtained in a).

Both $\hat{\psi}(x)$ and $\psi(x)$ satisfy the equation (3.93) and they both have unit norm: hence, they can differ at most by a x -independent factor of unit norm

$$\hat{\psi}(x) = e^{i\phi(\alpha, \bar{\alpha})} \psi(x) \quad (3.112)$$

where $\phi(\alpha, \bar{\alpha})$ is a *real-valued* function of α and $\bar{\alpha}$. It must therefore be that

$$\frac{1}{(2\pi)^{\frac{1}{4}} \lambda^{\frac{1}{2}}} e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} H_n\left(\frac{x}{\lambda}\right) e^{-\frac{x^2}{4\lambda^2}} = \frac{e^{i\phi(\alpha, \bar{\alpha})}}{(2\pi)^{\frac{1}{4}} \lambda^{\frac{1}{2}}} e^{\frac{(\alpha - \bar{\alpha})^2}{4}} e^{i\alpha \frac{x}{\lambda} - \frac{x^2}{4\lambda^2}} \quad (3.113)$$

or, dividing by the common factors,

$$\sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} H_n(y) = e^{i\phi(\alpha, \bar{\alpha})} e^{\frac{\alpha^2}{4} + \frac{\bar{\alpha}^2}{4}} e^{i\alpha y} \quad (3.114)$$

where $y \equiv \frac{x}{\lambda}$. The LHS of this equation depends only on α . This means that the factor $e^{i\phi(\alpha, \bar{\alpha})}$ must cancel the dependence on $\bar{\alpha}$ of the RHS. In other words the combination

$$e^{i\phi(\alpha, \bar{\alpha})} e^{\frac{\bar{\alpha}^2}{4}} = F(\alpha) \quad (3.115)$$

must depend on α but not on $\bar{\alpha}$. Since $i\phi(\alpha, \bar{\alpha})$ is pure imaginary, we conclude that

$$e^{i\phi(\alpha, \bar{\alpha})} = e^{-\frac{\alpha^2}{4} + \frac{\alpha^2}{4} + ic} \quad (3.116)$$

where c is a *real* constant independent of both α and $\bar{\alpha}$. Then

$$\sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} H_n(y) = e^{ic} e^{\frac{\alpha^2}{2}} e^{i\alpha y} \quad (3.117)$$

The value of the real constant c is determined by taking $\alpha \rightarrow 0$ in both sides of this equation. In this limit the LHS reduces to $H_0(y) = 1$ and thus

$$c = 0 \quad (3.118)$$

We established therefore the identity

$$\sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} H_n(y) = e^{\frac{\alpha^2}{2}} e^{i\alpha y} \quad (3.119)$$

By expanding the RHS in powers of α , and by equating terms with the same power of α , we obtain the following formula for $H_n(x)$ ¹

$$H_n(y) = i^n \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{\sqrt{n!}}{2^k k! (n-2k)!} (-1)^k y^{n-2k} \quad (3.120)$$

4 Time evolution

Problem 1. Let E_+ and E_- the two energy eigenvalues of a 2-states system and $|+\rangle$ and $|-\rangle$ the two corresponding energy eigenstates. Suppose that at

¹The polynomials $H_n(y)$ defined in (3.111) are related to the Hermite polynomials $h_n(y)$ by the formula

$$H_n(y) = \frac{i^n}{\sqrt{n!} 2^n} h_n\left(\frac{y}{\sqrt{2}}\right)$$

The factors i^n stems from the fact that our definition for a^\dagger differs by a factor i from the conventional one. The factor $\frac{1}{\sqrt{n!} 2^n}$ is a factor which is included in the usual definition of the harmonic oscillator energy eigenfunctions (3.111).

the time $t = 0$ the system is in the state $\psi(0) = \frac{1}{\sqrt{2}} (|+\rangle + |-\rangle)$. What is the probability that at the time $t > 0$ the system is in the state $|+\rangle$?

Solution: The state $\psi(t)$ at the time t is

$$\begin{aligned}\psi(t) &= e^{-\frac{i}{\hbar}t\hat{H}}\psi(0) = e^{-\frac{i}{\hbar}t\hat{H}}\frac{1}{\sqrt{2}}(|+\rangle + |-\rangle) = \\ &= \frac{1}{\sqrt{2}}(e^{-\frac{i}{\hbar}tE_+}|+\rangle + e^{-\frac{i}{\hbar}tE_-}|-\rangle)\end{aligned}\quad (4.121)$$

The probability that at the time t the system is in the state $|+\rangle$ is

$$P_+(t) = |\langle +|\psi(t)\rangle|^2 = \left|\frac{e^{-\frac{i}{\hbar}E_+t}}{\sqrt{2}}\right|^2 = \frac{1}{2}\quad (4.122)$$

The probability that at the time t the system is in the state $\psi(0)$ is:

$$\begin{aligned}P_{\psi(0)}(t) &= |\langle \psi(0), \psi(t)\rangle|^2 = \left|\frac{e^{-\frac{i}{\hbar}E_+t}}{2} + \frac{e^{-\frac{i}{\hbar}E_-t}}{2}\right|^2 = \\ &= \frac{1}{4}\left(1 + 1 + 2\cos\frac{(E_+ - E_-)t}{\hbar}\right) = \frac{1}{2}\left(1 + \cos\frac{(E_+ - E_-)t}{\hbar}\right) = \\ &= \cos^2\frac{(E_+ - E_-)t}{2\hbar}\end{aligned}\quad (4.123)$$

Problem 2

An harmonic oscillator of frequency ω is, at time $t = 0$, in the state

$$\psi_0 = |0\rangle + |1\rangle + |2\rangle\quad (4.124)$$

- a) Compute the average of \hat{p} and \hat{p}^2 at the time t .
- b) Write the normalized wave function of the state at the time t in the Schrödinger representation.
- c) What is the probability that at the time $t > 0$ the system is still in the state ψ_0 ?

Solution: The state at the time t is

$$\psi(t) = e^{-i\frac{\omega t}{2}}[|0\rangle + e^{-i\omega t}|1\rangle + e^{-2i\omega t}|2\rangle]\quad (4.125)$$

- a) Therefore

$$\begin{aligned}
\langle \psi(t), \hat{p} \psi(t) \rangle &= \frac{\hbar}{2\lambda} \langle \psi(t), (a + a^\dagger) \psi(t) \rangle = \\
&= e^{-i\frac{\omega t}{2}} \frac{\hbar}{2\lambda} \langle \psi(t), [e^{-i\omega t} |0\rangle + e^{-2i\omega t} \sqrt{2} |1\rangle + \\
&+ |1\rangle + e^{-i\omega t} \sqrt{2} |2\rangle + e^{-2i\omega t} \sqrt{3} |3\rangle] \rangle = \\
&= \frac{\hbar}{2\lambda} [e^{-i\omega t} + e^{-i\omega t} \sqrt{2} + e^{i\omega t} + e^{i\omega t} \sqrt{2}] = \\
&= \frac{\hbar}{\lambda} (1 + \sqrt{2}) \cos(\omega t) \tag{4.126}
\end{aligned}$$

The average of \hat{p} is therefore

$$\bar{p}(t) = \frac{\langle \psi(t), \hat{p} \psi(t) \rangle}{\langle \psi(t), \psi(t) \rangle} = \frac{\hbar}{3\lambda} (1 + \sqrt{2}) \cos(\omega t) \tag{4.127}$$

- b) Moreover

$$\begin{aligned}
\langle \psi(t), \hat{p}^2 \psi(t) \rangle &= \langle \hat{p} \psi(t), \hat{p} \psi(t) \rangle = \\
&= \frac{\hbar^2}{4\lambda^2} \left| e^{-i\omega t} |0\rangle + (1 + \sqrt{2} e^{-2i\omega t}) |1\rangle + \right. \\
&+ \left. e^{-i\omega t} \sqrt{2} |2\rangle + e^{-2i\omega t} \sqrt{3} |3\rangle \right|^2 = \\
&= \frac{\hbar^2}{4\lambda^2} (1 + |1 + \sqrt{2} e^{-2i\omega t}|^2 + 2 + 3) = \\
&= \frac{\hbar^2}{4\lambda^2} (6 + (3 + 2\sqrt{2} \cos(2\omega t))) = \\
&= \frac{\hbar^2}{4\lambda^2} (9 + 2\sqrt{2} \cos(2\omega t)) \tag{4.128}
\end{aligned}$$

The average of \hat{p}^2 is therefore

$$\bar{p}^2(t) = \frac{1}{3} \langle \psi(t), \hat{p}^2 \psi(t) \rangle = \frac{\hbar^2}{12\lambda^2} (9 + 2\sqrt{2} \cos(2\omega t)) \tag{4.129}$$

- c) The probability that at the time $t > 0$ the system is still in the state

ψ_0 is

$$\begin{aligned}
P_{\psi_0 \rightarrow \psi_0}(t) &= \frac{1}{9} |\langle \psi_0, \psi(t) \rangle|^2 = \frac{1}{9} \left| \langle |0\rangle + |1\rangle + |2\rangle, \right. \\
&\quad \left. |0\rangle + e^{-i\omega t} |1\rangle + e^{-2i\omega t} |2\rangle \rangle \right|^2 = \frac{1}{9} \left| 1 + e^{-i\omega t} + e^{-2i\omega t} \right|^2 = \\
&= \frac{1}{9} (3 + 4 \cos(\omega t) + 2 \cos(2\omega t)) \tag{4.130}
\end{aligned}$$

Problem 4. Determine the time evolution of the *free* wave packet

$$v_{\bar{p}, \Delta_p}(x) = \frac{1}{(\pi)^{\frac{1}{4}} \Delta_p^{\frac{1}{2}}} \int dp e^{-\frac{(p-\bar{p})^2}{2\Delta_p^2}} \frac{e^{\frac{i}{\hbar} p x}}{\sqrt{2\pi\hbar}} \tag{4.131}$$

Solution: The wave function at the time t is

$$\begin{aligned}
v_{\bar{p}, \Delta_p}(x; t) &= e^{-\frac{i}{\hbar} \hat{H} t} v_{\bar{p}, \Delta_p}(x) = \frac{1}{(\pi)^{\frac{1}{4}} \Delta_p^{\frac{1}{2}}} \int dp e^{-\frac{(p-\bar{p})^2}{2\Delta_p^2}} \frac{e^{\frac{i}{\hbar} p x - \frac{i}{\hbar} \frac{p^2}{2m} t}}{\sqrt{2\pi\hbar}} = \\
&= \frac{e^{\frac{i}{\hbar} \bar{p} x - \frac{i}{\hbar} \frac{\bar{p}^2}{2m} t}}{(\pi)^{\frac{1}{4}} \sqrt{2\pi\hbar} \Delta_p^{\frac{1}{2}}} \int dp e^{-(1+i t \frac{\Delta_p^2}{m\hbar}) \frac{p^2}{2\Delta_p^2} + \frac{i}{\hbar} p (x - \frac{\bar{p}}{m} t)} = \\
&= \frac{e^{\frac{i}{\hbar} \bar{p} x - \frac{i}{\hbar} \frac{\bar{p}^2}{2m} t}}{(\pi)^{\frac{1}{4}} \sqrt{2\pi\hbar} \Delta_p^{\frac{1}{2}}} \frac{\sqrt{2\pi} \Delta_p}{\sqrt{\frac{i}{\hbar} \frac{\Delta_p^2}{m} t + 1}} e^{-\frac{\Delta_p^2 (x - \frac{\bar{p}}{m} t)^2}{2\hbar^2 (1+i t \frac{\Delta_p^2}{m\hbar})}} = \\
&= \frac{e^{\frac{i}{\hbar} \bar{p} x - \frac{i}{\hbar} \frac{\bar{p}^2}{2m} t}}{\hbar^{\frac{1}{2}} (\pi)^{\frac{1}{4}}} \frac{\Delta_p^{\frac{1}{2}}}{\sqrt{\frac{i \Delta_p^2}{m\hbar} t + 1}} e^{-\frac{\Delta_p^2 (x - \frac{\bar{p}}{m} t)^2}{2\hbar^2 (1+i t \frac{\Delta_p^2}{m\hbar})}} \tag{4.132}
\end{aligned}$$

Problem 5. Compute the uncertainties of \hat{x} and \hat{p} on the *free* wave packet (4.131) for $t > 0$. (*Hint:* Use the Heisenberg picture of time evolution.)

Solution: Since the particle is free, the time dependent operators $\hat{x}(t)$ and $\hat{p}(t)$ in the Heisenberg picture are

$$\hat{x}(t) = \hat{x} + \frac{\hat{p}}{m} t \quad \hat{p}(t) = \hat{p}(0) = \hat{p} \tag{4.133}$$

Therefore

$$\begin{aligned}
\hat{x}^2(t) &= \hat{x}^2 + \frac{\hat{p}^2}{m^2} t^2 + \frac{t}{m} (\hat{x} \hat{p} + \hat{p} \hat{x}) \\
\hat{p}^2(t) &= \hat{p}^2(0) = \hat{p}^2 \tag{4.134}
\end{aligned}$$

Denote by $|v\rangle$ the state described by the wave function (4.131):

$$v_{\bar{p}, \Delta_p}(x) = \frac{\sqrt{\Delta_p}}{(\pi)^{\frac{1}{4}} \sqrt{\hbar}} e^{-\frac{\Delta_p^2 x^2}{2\hbar^2}} e^{\frac{i}{\hbar} \bar{p} x} \quad (4.135)$$

Then

$$\begin{aligned} \langle v | \hat{x}^2(t) | v \rangle &= \langle v | \hat{x}^2 | v \rangle + \frac{t^2}{m^2} \langle v | \hat{p}^2 | v \rangle + \frac{t}{m} \langle v | (\hat{x} \hat{p} + \hat{p} \hat{x}) | v \rangle \\ (\langle v | \hat{x}(t) | v \rangle)^2 &= (\langle v | \hat{x} | v \rangle + \frac{t}{m} \langle v | \hat{p} | v \rangle)^2 = \\ &= \langle v | \hat{x} | v \rangle^2 + \frac{t^2}{m^2} \langle v | \hat{p} | v \rangle^2 + 2 \frac{t}{m} \langle v | \hat{p} | v \rangle \langle v | \hat{x} | v \rangle \\ &= \frac{t^2}{m^2} \bar{p}^2 \\ \langle v | \hat{p}^2(t) | v \rangle &= \langle v | \hat{p}^2 | v \rangle \\ \langle v | \hat{p} | v \rangle^2 &= \bar{p}^2 \end{aligned} \quad (4.136)$$

since

$$\langle v | \hat{p} | v \rangle = \bar{p} \quad \langle v | \hat{x} | v \rangle = 0 \quad (4.137)$$

The uncertainties on x and p at the time t are therefore

$$\begin{aligned} \Delta x^2(t) &= \Delta x^2 + \frac{t^2}{m^2} \Delta p^2 + \frac{2t}{m} \langle v | \hat{x} \hat{p} | v \rangle - \frac{i \hbar t}{m} \\ \Delta p^2(t) &= \Delta p^2 \end{aligned} \quad (4.138)$$

We are left with the computation of the matrix element

$$\begin{aligned} \langle v | \hat{x} \hat{p} | v \rangle &= \frac{\Delta_p}{\sqrt{\pi} \hbar} \int dx e^{-\frac{\Delta_p^2 x^2}{\hbar^2}} (x \bar{p} + i x^2 \frac{\Delta_p^2}{\hbar}) = \\ &= \frac{\Delta_p}{\sqrt{\pi} \hbar} \frac{i \Delta_p^2}{\hbar} \int dx e^{-\frac{\Delta_p^2 x^2}{\hbar^2}} x^2 = \frac{i \Delta_p^3}{\sqrt{\pi} \hbar^2} \frac{\sqrt{\pi} \hbar^3}{2 \Delta_p^3} = \\ &= \frac{i \hbar}{2} \end{aligned} \quad (4.139)$$

In conclusion

$$\begin{aligned} \Delta x(t) &= \sqrt{\Delta x^2 + \frac{t^2}{m^2} \Delta p^2} \\ \Delta p(t) &= \Delta p \end{aligned} \quad (4.140)$$

Problem 6. Estimate the speed at which the following free wave packets, of minimal indeterminacy at $t = 0$, spread for large t :

- An electron with $\Delta x \approx 10^{-8} \text{ cm}$.
- An electron with $\Delta x \approx 10^{-2} \text{ cm}$.
- A grain of sand of $m = 10^{-12} \text{ g}$, with $\Delta x = 10^{-5} \text{ cm}$.

Solution: The speed at which the packets of minimal indeterminacy spread is, according to the solution of the previous problem, is for large t

$$\frac{d\Delta x(t)}{dt} \approx \frac{\hbar}{2m\Delta x} \quad (4.141)$$

Recall that the electron Compton wavelength is

$$\lambda_c = \frac{\hbar}{mc} = 0.387 \times 10^{-12} \text{ m} \quad (4.142)$$

Therefore for an electron

$$\frac{d\Delta x(t)}{dt} \approx \frac{\lambda_c}{\Delta x} c \quad (4.143)$$

For $\Delta x = 10^{-8} \text{ cm} = 10^{-10} \text{ m}$

$$\frac{d\Delta x(t)}{dt} \approx \frac{1}{2} \times 0.387 \times 10^{-2} \times 3 \times 10^8 \text{ m/s} = 0.580 \times 10^6 \text{ m/s} \quad (4.144)$$

For $\Delta x = 10^{-2} \text{ cm} = 10^{-4} \text{ m}$

$$\frac{d\Delta x(t)}{dt} \approx \frac{1}{2} \times 0.387 \times 10^{-8} \times 3 \times 10^8 \text{ m/s} = 0.580 \text{ m/s} \quad (4.145)$$

For a grain of sand of mass

$$m = 10^{-12} \text{ g} = 10^{-15} \text{ kg} = 1.10 \times 10^{15} m_{\text{electron}} \quad (4.146)$$

and $\Delta x = 10^{-5} \text{ cm} = 10^{-7} \text{ m}$, we have

$$\frac{d\Delta x(t)}{dt} \approx \frac{1}{2} \times \frac{0.387 \times 10^{-5}}{1.10 \times 10^{15}} \times 3 \times 10^8 \text{ m/s} = 0.527 \times 10^{-12} \text{ m/s} \quad (4.147)$$

“Large” time t means

$$t \gg \frac{m\Delta x}{\Delta p} = \frac{m\Delta x^2}{\hbar} = \frac{\Delta x}{\frac{\hbar}{m\Delta x}} \quad (4.148)$$

that is

$$t \frac{\hbar}{m\Delta x} \gg \Delta x \quad (4.149)$$

5 Symmetries

Problem 4. A spin 1 system is in the state with $S_z = +1$. Find the probabilities that the measurement of \hat{S}_x gives the values $S_x = -1, 0, 1$.

Solution.

Let $\{|S_z\rangle, S_z = -1, 0, 1\}$ of eigenstates of \hat{S}_z be the states of eigenstates of \hat{S}_z . Let us determine the matrix which represents \hat{S}_x in such a basis. We have

$$\hat{S}_x = \frac{\hat{S}_+ + \hat{S}_-}{2} \quad \hat{S}_y = \frac{\hat{S}_+ - \hat{S}_-}{2i} \quad (5.1)$$

and

$$\begin{aligned} \hat{S}_+|1\rangle &= 0 & \hat{S}_+|0\rangle &= \sqrt{2}|1\rangle & \hat{S}_+|-1\rangle &= \sqrt{2}|0\rangle \\ \hat{S}_-|1\rangle &= \sqrt{2}|0\rangle & \hat{S}_-|0\rangle &= \sqrt{2}|-1\rangle & \hat{S}_-|-1\rangle &= 0 \end{aligned} \quad (5.2)$$

Therefore

$$\hat{S}_x|1\rangle = \frac{1}{\sqrt{2}}|0\rangle \quad \hat{S}_x|0\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |-1\rangle) \quad \hat{S}_x|-1\rangle = \frac{1}{\sqrt{2}}|0\rangle$$

The matrix which represents \hat{S}_x in the $\{|1\rangle, |0\rangle, |-1\rangle\}$ basis is therefore

$$\hat{S}_x = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix} \quad (5.3)$$

The eigenvalues of this matrix are given by the equation

$$\begin{aligned} 0 &= \det \begin{pmatrix} -m_x & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & -m_x & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & -m_x \end{pmatrix} = -m_x \left(m_x^2 - \frac{1}{2}\right) - \frac{1}{\sqrt{2}} \left(-\frac{m_x}{\sqrt{2}}\right) = \\ &= m_x (1 - m_x^2) \end{aligned} \quad (5.4)$$

and are, as expected, $m_x = 1, 0, -1$. The eigenstate (x, y, z) corresponding to the eigenvalue m_x satisfies

$$\begin{aligned} -m_x x + \frac{y}{\sqrt{2}} &= 0 \\ \frac{x}{\sqrt{2}} - m_x y + \frac{z}{\sqrt{2}} &= 0 \\ \frac{y}{\sqrt{2}} - m_x z &= 0 \end{aligned} \quad (5.5)$$

For $m_x = 1$ this gives

$$x = z = \frac{y}{\sqrt{2}} \quad (5.6)$$

Therefore the normalized eigenstate with $m_x = 1$ is

$$|S_x = 1\rangle = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{\sqrt{2}} \\ \frac{1}{2} \end{pmatrix} \quad (5.7)$$

When $m_x = 0$ we have

$$y = 0 \quad x = -z \quad (5.8)$$

from which one derives the normalized eigenstate with $m_x = 0$

$$|S_x = 0\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ -\frac{1}{\sqrt{2}} \end{pmatrix} \quad (5.9)$$

Finally, Eqs. (5.5) for $m_x = -1$ become

$$x = z = -\frac{y}{\sqrt{2}} \quad (5.10)$$

from which

$$|S_x = -1\rangle = \begin{pmatrix} \frac{1}{2} \\ -\frac{1}{\sqrt{2}} \\ \frac{1}{2} \end{pmatrix} \quad (5.11)$$

These equations rewrite in a representation independent form as follows

$$\begin{aligned} |S_x = 1\rangle &= \frac{1}{2}|1\rangle + \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{2}|-1\rangle \\ |S_x = 0\rangle &= \frac{1}{\sqrt{2}}|1\rangle - \frac{1}{\sqrt{2}}|-1\rangle \\ |S_x = -1\rangle &= \frac{1}{2}|1\rangle - \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{2}|-1\rangle \end{aligned} \quad (5.12)$$

The inverse relations are

$$\begin{aligned} |1\rangle &= \frac{1}{2}|S_x = 1\rangle + \frac{1}{\sqrt{2}}|S_x = 0\rangle + \frac{1}{2}|S_x = -1\rangle \\ |0\rangle &= \frac{1}{\sqrt{2}}|S_x = 1\rangle - \frac{1}{\sqrt{2}}|S_x = -1\rangle \\ |-1\rangle &= \frac{1}{2}|S_x = 1\rangle - \frac{1}{\sqrt{2}}|S_x = 0\rangle + \frac{1}{2}|S_x = -1\rangle \end{aligned} \quad (5.13)$$

We conclude that the probabilities to obtain $S_x = -1, 0, 1$ on the state $|1\rangle$ are

$$P(S_x = +1) = \frac{1}{4} \quad P(S_x = 0) = \frac{1}{2} \quad P(S_x = -1) = \frac{1}{4} \quad (5.14)$$

Problem 9. Find the basis $H_{n,m}(x)$, of harmonic polynomials of degree $n = 3$ and $n = 4$ which are eigenfunctions of L_3 with m .

Solution.

($n = 3$) We have

$$H_{3,\pm 3}(x) = x_{\pm}^3 \quad H_{3,\pm 2} = x_{\pm}^2 x_3 \quad (5.15)$$

Moreover, the eigenfunctions of L_z with eigenvalues $m = 0$ and $m = 1$ must have the form

$$H_{3,1} = x_+ x_3^2 + \alpha x_+^2 x_- \quad H_{3,0} = x_3^3 + \beta x_+ x_- x_3 \quad (5.16)$$

The condition that $H_{3,1}$ be harmonic gives

$$\vec{\nabla}^2 H_{3,1} = \left[\frac{\partial^2}{\partial x_3^2} + 4 \frac{\partial}{\partial x_+} \frac{\partial}{\partial x_-} \right] H_{3,1} = 2x_+ + 8\alpha x_+ \quad (5.17)$$

Hence

$$\alpha = -\frac{1}{4} \quad (5.18)$$

and

$$H_{3,1} = x_+ x_3^2 - \frac{1}{4} x_+^2 x_- \quad (5.19)$$

Therefore

$$H_{3,-1} = x_- x_3^2 - \frac{1}{4} x_-^2 x_+ \quad (5.20)$$

Analogously

$$\vec{\nabla}^2 H_{3,0} = (6 + 4\beta) x_3 \quad (5.21)$$

Hence

$$\beta = -\frac{3}{2} \quad (5.22)$$

and

$$H_{3,0} = x_3^3 - \frac{3}{2} x_+ x_- x_3 \quad (5.23)$$

Problem 10.

Consider a 3-dimensional particle of mass m moving in a harmonic potential

$$V(r) = \frac{1}{2} m \omega^2 r^2 \quad (5.24)$$

Show that:

- a) The energy levels are given by $E_n = \hbar (n + \frac{3}{2})$ with $n = 0, 1, 2, \dots$
- b) The ground state is non-degenerate and has $l = 0$. Find the *normalized* radial wave function $\chi_{E_0,0}(r)$ with $l = 0$.
- c) The first excited level E_1 has degeneracy 3 and $l = 1$. Find the *normalized* radial wave function $\chi_{E_1,1}(r)$ with $l = 1$.

(*Hint:* Since one can write the 3-dimensional hamiltonian $\hat{H} = \sum_{i=1}^3 \hat{H}_i$ where $\hat{H}_i = \frac{p_i^2}{2m} + \frac{1}{2} m \omega^2 x_i^2$ is the hamiltonian of the 1-dimensional harmonic oscillator, the energy eigenfunctions of the 3-dimensional oscillator are

$$\psi_{n_1, n_2, n_3}(\vec{x}) = \psi_{n_1}(x_1) \psi_{n_2}(x_2) \psi_{n_3}(x_3) \quad (5.25)$$

where $\psi_{n_i}(x_i)$ are the eigenfunctions of the 1-dimensional harmonic oscillators.)
Solution.

- a) The energy levels corresponding to the wave functions

$$\psi_{n_1, n_2, n_3}(\vec{x}) = \psi_{n_1}(x_1) \psi_{n_2}(x_2) \psi_{n_3}(x_3) \quad (5.26)$$

are

$$E_{n_1, n_2, n_3} = \sum_{i=1}^3 \hbar \omega \left(n_i + \frac{1}{2} \right) = \hbar \omega \left(n + \frac{3}{2} \right) \quad (5.27)$$

where

$$n \equiv n_1 + n_2 + n_3 \quad (5.28)$$

b) The ground state corresponds to

$$n = 0 = n_1 = n_2 = n_3 \quad (5.29)$$

It is non-degenerate and has wave function

$$\begin{aligned} \psi_{0,0,0}(\vec{x}) &= \psi_0(x_1) \psi_0(x_2) \psi_0(x_3) = \prod_{i=1}^3 \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar} x_i^2} = \\ &= \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{3}{4}} e^{-\frac{m\omega}{2\hbar} r^2} \end{aligned} \quad (5.30)$$

Since this level is non-degenerate, it necessarily has $l = 0$ and $m = 0$:

$$\psi_{0,0,0}(\vec{x}) = Y_{0,0}(\theta, \phi) R_{E_{0,0}}(r) \quad (5.31)$$

Therefore the *radial* wave function is

$$\chi_{E_{0,0}}(r) = r R_{E_{0,0}}(r) = \sqrt{4\pi} \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{3}{4}} r e^{-\frac{m\omega}{2\hbar} r^2} = \frac{2}{\pi^{\frac{1}{4}}} \left(\frac{m\omega}{\hbar} \right)^{\frac{3}{4}} r e^{-\frac{m\omega}{2\hbar} r^2} \quad (5.32)$$

c) The first excited level has $n = 1$ and therefore it corresponds to the three degenerate normalized wave functions

$$\begin{aligned} \psi_{1,0,0}(\vec{x}) &= \sqrt{\frac{2m\omega}{\hbar}} x_1 \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{3}{4}} e^{-\frac{m\omega}{2\hbar} r^2} \\ \psi_{0,1,0}(\vec{x}) &= \sqrt{\frac{2m\omega}{\hbar}} x_2 \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{3}{4}} e^{-\frac{m\omega}{2\hbar} r^2} \\ \psi_{0,0,1}(\vec{x}) &= \sqrt{\frac{2m\omega}{\hbar}} x_3 \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{3}{4}} e^{-\frac{m\omega}{2\hbar} r^2} \end{aligned} \quad (5.33)$$

The wave function $\psi_{0,0,1}$ can re-written as

$$\begin{aligned}\psi_{0,0,1}(\vec{x}) &= \sqrt{\frac{8\pi}{3}} Y_{1,0}(\theta, \phi) \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}} r \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{3}{4}} e^{-\frac{m\omega}{2\hbar} r^2} = \\ &= Y_{1,0}(\theta, \phi) R_{E_{1,1}}(r)\end{aligned}\quad (5.34)$$

where

$$R_{E_{1,1}}(r) = \sqrt{\frac{8}{3}} \frac{r}{\pi^{\frac{1}{4}}} \left(\frac{m\omega}{\hbar}\right)^{\frac{5}{4}} e^{-\frac{m\omega}{2\hbar} r^2} \quad (5.35)$$

Hence this is a state with $l = 1$ and $m = 0$ and the associated *radial* wave function is

$$\chi_{E_{1,1}}(r) = r R_{E_{1,1}}(r) = \frac{1}{\pi^{\frac{1}{4}}} \sqrt{\frac{8}{3}} r^2 \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{5}{4}} e^{-\frac{m\omega}{2\hbar} r^2} \quad (5.36)$$

The following linear combinations of the $\psi_{1,0,0}$ and $\psi_{0,1,0}$ are the wave functions of the states with $l = 1$ and $m = \pm 1$

$$\begin{aligned}\frac{1}{\sqrt{2}}(\psi_{1,0,0}(\vec{x}) \pm i\psi_{0,1,0}(\vec{x})) &= \frac{(x_1 \pm i x_2)}{\pi^{\frac{3}{4}}} \left(\frac{m\omega}{\hbar}\right)^{\frac{5}{4}} e^{-\frac{m\omega}{2\hbar} r^2} = \\ &= \pm i Y_{1,\pm 1}(\theta, \phi) \sqrt{\frac{8}{3}} \frac{r}{\pi^{\frac{1}{4}}} \left(\frac{m\omega}{\hbar}\right)^{\frac{5}{4}} e^{-\frac{m\omega}{2\hbar} r^2} = \\ &= \pm i Y_{1,\pm 1}(\theta, \phi) R_{E_{1,1}}(r)\end{aligned}\quad (5.37)$$

Problem 11.

Show that the radial wave function of the ground state of the hydrogenoid

$$\chi_{E,0}(r) = 2 \left(\frac{Z}{a_B}\right)^{\frac{3}{2}} r e^{-\frac{Zr}{a_B}} \quad (5.38)$$

has norm one.

Solution.

$$\begin{aligned}\int_0^\infty dr |\chi_{E,0}(r)|^2 &= 4 \left(\frac{Z}{a_B}\right)^3 \int_0^\infty dr r^2 e^{-\frac{2Zr}{a_B}} = \\ &= \frac{1}{2} \int_0^\infty d\rho \rho^2 e^{-\rho} = 1\end{aligned}\quad (5.39)$$

Problem 12. Find the normalized radial wave function of the first excited state with $l = 0$ of the hydrogenoid atom by looking for solutions of

$$\chi_{E,0}(\rho) = \rho (b_0 + b_1 \rho) e^{-c\rho} \quad c > 0 \quad (5.40)$$

Solution. We have

$$\begin{aligned} \chi'_{E,0}(\rho) &= \left[b_0 + 2b_1 \rho - c\rho (b_0 + b_1 \rho) \right] e^{-c\rho} = \\ &= \left[b_0 + (2b_1 - cb_0)\rho - cb_1 \rho^2 \right] e^{-c\rho} \\ \chi''_{E,0}(\rho) &= \left[(2b_1 - cb_0) - 2cb_1 \rho - cb_0 + \right. \\ &\quad \left. -c(2b_1 - cb_0)\rho + c^2 b_1 \rho^2 \right] e^{-c\rho} = \\ &= \left[(2b_1 - 2cb_0) + (c^2 b_0 - 4cb_1)\rho + c^2 b_1 \rho^2 \right] e^{-c\rho} \end{aligned} \quad (5.41)$$

Therefore

$$\begin{aligned} \frac{\chi''_{E,0}(\rho)}{\chi_{E,0}(\rho)} &= \frac{(2b_1 - 2cb_0) + (c^2 b_0 - 4cb_1)\rho + c^2 b_1 \rho^2}{\rho (b_0 + b_1 \rho)} = \\ &= -\frac{E}{Z^2 |E_1^H|} - \frac{2}{\rho} \end{aligned} \quad (5.42)$$

Equivalently

$$\begin{aligned} (2b_1 - 2cb_0) + (c^2 b_0 - 4cb_1)\rho + c^2 b_1 \rho^2 &= \\ = -\left(\rho \frac{E}{Z^2 |E_1^H|} + 2\right) (b_0 + b_1 \rho) &= \\ = -2b_0 - \left(2b_1 + b_0 \frac{E}{Z^2 |E_1^H|}\right) \rho - \rho^2 \frac{E}{Z^2 |E_1^H|} b_1 \end{aligned} \quad (5.43)$$

From this we obtain the equations

$$\begin{aligned} 2b_1 - 2cb_0 &= -2b_0 \\ -c^2 b_0 + 4cb_1 &= 2b_1 + b_0 \frac{E}{Z^2 |E_1^H|} \\ c^2 b_1 &= -\frac{E}{Z^2 |E_1^H|} b_1 \end{aligned} \quad (5.44)$$

From the third equation we obtain

$$c^2 = -\frac{E}{Z^2 |E_1^H|} \quad (5.45)$$

Replacing this in the second equation we conclude

$$(4c - 2)b_1 = 0 \quad (5.46)$$

If $c \neq \frac{1}{2}$, this would give $b_1 = 0$. Replacing this value in the first equation we would obtain

$$(c - 1)b_0 = 0 \quad (5.47)$$

Since $b_0 \neq 0$ (otherwise we would recover the trivial solution $b_0 = b_1 = 0$), then $c = 1$. But this is the ground state solution $\propto e^{-\rho}$. The excited state corresponds to choosing the solution with $b_1 \neq 0$, and therefore

$$c = \frac{1}{2} \quad (5.48)$$

The first equation gives then

$$b_1 = -\frac{1}{2}b_0 \quad (5.49)$$

In conclusion there is a normalizable solution, whose energy eigenvalue is

$$E_2 = \frac{Z^2 E_1}{4} \quad (5.50)$$

and whose radial wave function is

$$\chi_{E_2,0}(\rho) = b_0 \rho \left(1 - \frac{1}{2}\rho\right) e^{-\frac{\rho}{2}} \quad (5.51)$$

This is the $|2, 0, 0\rangle$ excited state of the hydrogenoid. The normalization factor is determined by

$$\begin{aligned} 1 &= \frac{a_B}{Z} \int_0^\infty d\rho |\chi_{E_2,0}(\rho)|^2 = \frac{a_B |b_0|^2}{Z} \int_0^\infty d\rho \rho^2 \left(1 - \frac{1}{2}\rho\right)^2 e^{-\rho} = \\ &= \frac{2|b_0|^2 a_B}{Z} \end{aligned} \quad (5.52)$$

Therefore

$$b_0 = \sqrt{\frac{Z}{2a_B}} \quad (5.53)$$