## A

## **Problems in Quantum Mechanics**

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- A1. Calculate the integral  $\int e^{-a(k-k_0)^2} e^{ikx} dk$  over the entire k-axis.
- A2. (For F0053T) Consider a particle in a one dimensional box. Calculate the force on the wall from the particle both in a classical and in a quantum mechanical description. Compare results.

Hint: (1) In classical mechanics the change in momentum is given by  $\int dt F$ . Use the average over time. (2) Use the Schrödinger equation and calculate the force as F = -dE/dL in the quantum mechanical case.

A3. A particle is coming from  $+\infty$  towards the potential step:

$$\begin{cases} V(x) = -V_0 & \text{for } x < 0 \\ V(x) = 0 & \text{for } x > 0, \end{cases}$$
(A.1)

where  $V_0 > 0$ . Calculate the transmission and reflection coefficients.

A4. A constant current of electrons with energy E = 1 eV are sent towards a potential given by

$$\begin{cases} V(x) = V_0 & \text{for} \quad 0 < x < a \\ V(x) = 0 & \text{otherwise,} \end{cases}$$
(A.2)

where  $V_0 = 2 \text{ eV}$  and a = 4 Å. Make a detailed plot of the time-independent particle density, i.e. the probability density.

- A5. A simple model of electrons in chemical bonds is obtained when the atomic potentials have the form of Dirac delta functions  $\delta(x)$ . The potential of an atom *i* at  $x_i$  is represented by  $V(x) = -b\delta(x x_i)$ .
  - (a) Calculate the ground state wave function  $\psi_i$  of an electron in the potential  $V(x) = -b\delta(x x_i)$ .

- (b) Consider two atoms, one at  $x_1 = a/2$  and the other at  $x_2 = -a/2$ , with potentials  $V_1(x) = -b\delta(x a/2)$  and  $V_2(x) = -b\delta(x + a/2)$ . Calculate the ground state wave function  $\psi_{12}$  of an electron in the potential from the two atoms, i.e.  $V(x) = -b\delta(x a/2) b\delta(x + a/2)$ .
- (c) Compare the ground state wave function  $\psi_{12}$  obtained in (b) with a sum of two wave functions of the form  $\psi_1(x)$  obtained in (a).
- A6. Estimate the probability for a particle with mass m to pass trough the barrier given by

$$V(x) = -\kappa x^2. \tag{A.3}$$

A7. In the linear complex vector space, the scalar product can be defined as

$$v^{+}v = |v_{1}|^{2} + |v_{2}|^{2} + |v_{3}|^{2} + \dots$$
(A.4)

The adjoint  $A^{\dagger}$  of a matrix or a vector is defined as  $(A^T)^*$ , where T is the transpose and \* is the complex conjugate. A matrix is Hermitian if it is equal to its adjoint, i.e.  $A^{\dagger} = A$ , so that  $A_{nm} = A_{mn}^*$ . Show that the expectation value  $v^{\dagger}Av$  is real, if v is a complex colon vector and A is Hermitian.

Hint:  $v^{\dagger}Av = \sum_{ij} v_i^* A_{ij} v_j$ 

A8. Show that the eigenvalues of a hermitian matrix A are real.

Hint: Lock at the expectation value of A using the eigenvector v.

- A9. (For F0053T) What is wave function of the ground state for a spherical harmonic oscillator with  $V(x, y, z) = \frac{1}{2}m\omega^2(x^2 + y^2 + z^2)$ . Express the wave function both in Cartesian and spherical coordinates.
- A10. Calculate the commutator  $[L_z, sin(\phi)]$ , where  $\phi$  is the spherical angle  $\phi = \arctan(y/x) + n\pi$ .
- A11. (For F0053T) Express the spherical harmonics  $Y_{0,0}$ ,  $Y_{1,-1}$ ,  $Y_{1,0}$ ,  $Y_{1,1}$ ,  $Y_{2,-2}$ ,  $Y_{2,-1}$ ,  $Y_{2,0}$ ,  $Y_{2,1}$ , and  $Y_{2,2}$  in terms of

$$\begin{cases} x = r \sin \theta \cos \phi \\ y = r \sin \theta \sin \phi \\ z = r \cos \theta \end{cases}$$
(A.5)

- A12. (For F0053T only a, not b and c) In three dimensions the parity operator is given by Pf(x, y, z) = f(-x, -y, -z).
  - (a) What happens when P operates on the spherical coordinates  $r, \theta, \varphi$ .
  - (b) What is the parity of the state  $Y_{ll}$
  - (c) Show that  $Y_{lm}$  for m < l has the same parity as  $Y_{ll}$ . Hint: First show that  $[L_i, P] = 0$ , for i = x, y.

- A13. Calculate the matrix elements  $\langle u_{100}|z|u_{200}\rangle$  and  $\langle u_{100}|z|u_{210}\rangle$ Hint: Use the spherical coordinates  $(r, \theta, \varphi)$  and calculate the angular integrals first.
- A14. Calculate the eigenstate of  $S_{\varphi} = \cos(\varphi)S_x + \sin(\varphi)S_y$ .
- A15. What is the probability to get the value  $+\hbar/2$ , when  $S_{\varphi}$  is measured on a particle with spin up with respect to the z-axis.
- A16. A proton is placed in a magnetic field with B = 5 T in the z-direction. The spin part of the Hamiltonian is given by  $-\frac{g_p eB}{2m_p}S_z$ , where  $g_p = 2.793$  is the proton gyromagnetic ratio and  $m_p$  is the proton mass. Calculate the time dependency.
- A17. (For F0053T) A 100-Mev photon collides with a proton that is at rest. What is the maximum possible energy loss for the photon?
- A18. If one assumes that in stationary state of the hydrogen atom the electron fits into a circular orbit with an integral number of wavelengths, one can reproduce the results of the Bohr theory. Work this out.
- A19. Given that  $A(k) = N/(k^2 + \alpha^2)$  in  $\Psi(x) = \int_{-\infty}^{\infty} dk A(k) e^{ikx}$ , calculate  $\Psi(x)$ . Plot A(k) and  $\Psi(x)$  and show that  $\Delta k \Delta x > 1$ , independent of the choice of  $\alpha$ .
- A20. Consider a wave function of the form

$$\psi(x) = Ae^{-\mu|x|}$$

Calculate the wave function in momentum space  $\phi(p)$ .

- A21. Consider the previous problem. Calculate A so that  $\psi(x)$  is properly normalized.
- A22. Make an estimate of the strength of the nuclear potential energy given the following fact: The "size" of the box that roughly describes the nuclear potential is  $10^{-15}$ m, and it takes 8 MeV to eject a particle from this potential well.
  - a) Use the uncertainty principle to estimate  $\langle p^2 \rangle$  for a nucleon in the box, and given the fact that the mass of the nucleon is  $M = 1.67 \cdot 10^{-27}$  kg, estimate the kinetic energy of the nucleon.
  - b) Since the potential that gives rise to the binding must more than compensate for this, what is the negative potential energy?
- A23. (For F0053T) Consider an electron of mass  $m = 0.9 \cdot 10^{-30}$ kg in an infinite box of dimension  $a = 1.0 \cdot 10^{-9}$ m.
  - a) What is the energy difference between the ground state and the first excited state? Express your answer in eV.
  - b) Suppose the transition from state n = 2 to the state n = 1 is accompanied by the emission of a photon, as given by the Bohr rule. What is the wavelength of the emitted photon?
- A24. (For F0053T) Consider an electron in a macroscopic box of size a = 2cm.

- a) What value of n corresponds to an energy of 1.5 eV ?
- b) What is the difference in energy between the state n and n + 1 in that energy region?
- A25. (For F0053T) A particle is known to be localized in the left half of a box with sides at  $x = \pm a/2$ , with wave function

$$\psi(x) \begin{cases} = \sqrt{\frac{2}{a}} & -\frac{a}{2} < x < 0 \\ = 0 & 0 < x < \frac{a}{2} \end{cases}$$

- a) Will the particle remain localized at later times?
- b) Calculate the probability that an energy measurement yields the ground state energy; the energy of the first excited state.
- A26. (For F0053T) The eigenfunctions for a potential of the form

$$V(x) \begin{cases} = \infty & x < 0 \ ; \ x > a \\ = 0 & 0 < x < a \end{cases}$$

are of the form

$$u_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$$

Suppose a particle in the preceding potential has an initial normalized wave function of the form

$$\psi(x,0) = A\left(\sin \frac{\pi x}{a}\right)^5$$

- a) What is the form of  $\psi(x, t)$ ?
- b) Calculate A without doing the integral  $\int d\theta \sin^{10} \theta$ .
- c) What is the probability that an energy measurement yields  $E_3$ , where  $E_n = n^2 \pi^2 \hbar^2 / 2ma^2$ ?
- A27. A particle in free space is initially in a wave packet described by

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

- a) What is the probability that its momentum is in the range (p, p + dp)?
- b) What is the expectation value of the energy? Can you give an rough argument based on the "size" of the wave function and the uncertainty principle, for why the answer should be roughly what it is?