



MR301: Concepts in Materials Science I

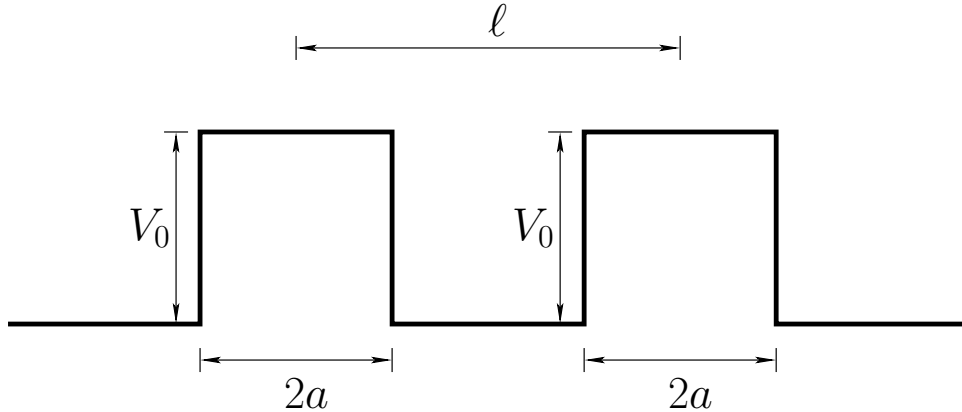
Materials Research Centre, IISc Bangalore

Semester I, 2005–2006

PROBLEM SET 3

- 3/1. **Review Time!** Look at the slide 1 of “Quantum Mechanics Basics” notes. There is a list of things that motivate the need for quantum mechanics. For each of these, write two to three sentences explaining how classical mechanics fails.
- 3/2. **Don’t be Stern on Gerlach!** Why do you need an inhomogeneous magnetic field for Stern-Gerlach experiment? Give a detailed justification.
- 3/3. **Cast the Die!** For a fair die, find the mean value and standard deviation.
- 3/4. **Self Test!** State if each of the following are true or false. Give reason(s).
- (a) The description of the state of a quantum mechanical particle *always* requires a continuous complex valued function.
 - (b) The state of a particle is determined by a *unique* continuous complex valued function.
 - (c) Consider particle in a box: On a particular system, a single measurement of position is performed at time $t = 0$ obtains $x = \ell/2$ (ℓ is the length of the box). If a second measurement of position is performed at $t = 1\text{sec}$ on the same system, the result will be equal to $\ell/2$ again.
 - (d) It is known that at time $t = 0$, a particle is in the eigenstate of the operator A with eigenvalue a . An experiment to measure A gives a result of a with no uncertainty at time $t = 0$. It will also give a result of a at all times with no uncertainty.
 - (e) Every Hermitian operator commutes with the Hamiltonian operator.
 - (f) The position operator for the particle in a box commutes with the Hamiltonian operator.
 - (g) For the particle in a box, a single measurement of the energy at time $t = 0$ gives $E = E_0$ (E_0 defined in notes). This necessarily means that the state of the particle is the ground state.
 - (h) For the particle in a box, a single measurement of the energy at time $t = 0$ gives $E = 4E_0$ (E_0 defined in notes). A single measurement of the energy of the particle in the same box at time $t = 2$ can possibly give a value of $E = E_0$.
 - (i) The expected value of momentum for *any* state for the particle in a box is zero.
 - (j) Momentum of a particle in a box is conserved since the momentum operator commutes with the Hamiltonian.
- 3/5. **A Carcinogenic Question!** Use the particle in a box to estimate the HOMO-LUMO gap of Benzene. How does it compare with experiment?
- 3/6. **Is Ehrenfest Correct?** Prove or disprove Ehrenfest.

- 3/7. **Periodic Box!** Consider a box of length ℓ with no external potential, but with periodic boundary conditions. Find the stationary states and energy eigenvalues. What is the main difference between this solution and the solution obtained in class for the non-periodic box? Comment on the *physics*.
- 3/8. **Power and Position?** An electron is in the state $\frac{12}{13}|1\rangle + \frac{5}{13}|2\rangle$ of the particle in a box of length ℓ at time $t = 0$. Find $\langle X \rangle(t)$. Make a connection (a rough argument) with emitted/absorbed radiation.
- 3/9. **Dirac here too?** Show that $\langle x|P|\psi\rangle = -i\hbar \frac{\partial \psi}{\partial x}$.
- 3/10. **Double Barrier!** Consider the double barrier potential shown in the figure below. Our goal is to understand the physics as a function of the barrier separation ℓ .



- Is $E < 0$ energy eigenstates possible in this scenario?
- What are the different lengths scales in the problem? How do you expect the physics to differ for different regimes of the length scales? What we are trying to do in this part is to figure out everything about the solution without actually solving anything explicitly.
- Use Schrodinger recipe and find the transmission coefficient T as a function of the electron wavevector k (Just as was done in class; write wavefunctions in different segments, do boundary condition matching). Make a plot of $|T|^2$ as a function of k for different values of ℓ . Comment on any resonances etc., that you find. You may wish to use Mathematica or some such thing to make your life simpler.
- There is another way of solving this problem, which is perhaps much simpler, requiring a bit more thought. Use the solution of a *single* barrier to derive the result that you found in part 3/10c.
- Recall that we had derived an expression for T for the single barrier in class; call this T_1 . Is T that you derived in part 3/10c equal to T_1^2 ? If no, why? If yes, under what conditions?

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