August 26, 2021

Homework 1
OPTI 507
(due September 2, 2021)

The following problems are designed to help you review your knowledge of basic quantum mechanics. Such knowledge is a prerequisite for the understanding of electronic and optical properties of solids.

Problem 1
(i) In quantum mechanics, the position of a particle is associated with the position operator, $\hat{\vec{r}}$, and its momentum with the momentum operator $\hat{\vec{p}} = -i\hbar\vec{\nabla}$. Determine the commutators of the cartesian components of those two operators, $[\hat{r}_i, \hat{p}_j]$, for all $i, j = \{x, y, z\}$.
(ii) In general, a physical quantity associated with an operator $\hat{A}$ has a well-defined value if the wave function ϕ is an eigenfunction of $\hat{A}$, i.e. $\hat{A}\phi = a\phi$ where "a" is a real number. The eigenvalue "a" corresponds to the outcome of a measurement of the quantity associated with $\hat{A}$. Assuming that there exists a complete set of functions ψ_n that are eigenfunctions of two different operators $\hat{A}$ and $\hat{B}$, i.e. $\hat{A}\psi_n = a_n\psi_n$ and $\hat{B}\psi_n = b_n\psi_n$, show that $\hat{A}\hat{B}\Psi = \hat{B}\hat{A}\Psi$ for any wave function Ψ that can be expressed as a linear combination of the eigenfunctions, i.e. $\Psi = \sum_n c_n\psi_n$.

(10 Points)

Problem 2
Let a quantum mechanical system be described by the time-dependent wave function $\psi(\vec{r}, t)$. Assuming the Hamiltonian $\hat{H}$ to be time-independent, show that there exist solutions that can be factorized as $\psi(\vec{r}, t) = f(t)\phi(\vec{r})$. Derive the equations of motion for $f(t)$ and $\phi(\vec{r})$ and determine $f(t)$ (using the initial condition $f(0) = 1$). (Note that the most general solution to the time-dependent Schroedinger equation is a superposition of the factorized solutions.)

(10 Points)

Problem 3
Consider the simple quantum mechanical problem of an electron in free space. Write down the Hamiltonian, the time-dependent and time-independent Schrödinger equations, and the (unnormalized) solutions of the time-independent Schrödinger equation (you can simply guess the solutions, which are two linearly independent functions, and show that they solve the equation; note that in free space physical arguments suggest plane-wave solutions). Plot the energy vs. the magnitude of the wave vector. Write the (wave vector dependent) eigenergy in analogy to the energy of a classical particle, i.e. in terms of the particle's momentum. Assuming we could use the concepts of the particle's position, momentum and velocity in quantum mechanics the same way we use them in classical mechanics (which is of course not true), determine the time t it would take for an electron with wave vector $k = 0.85 \times 10^9 \mathrm{m}^{-1}$ to travel a distance of 12μm.

(10 Points)

Problem 4
Consider a system with a Hamiltonian of the form $\hat{H} = \hat{H}_0 + \hat{H}'(t)$, and assume the solutions of the unperturbed system,

$$\hat{H}_0 \phi_m(\vec{r}) \quad = \quad \varepsilon_m \phi_m(\vec{r})$$

to be known. Expand the time-dependent wave function,

$$\psi(\vec{r}, t) = \sum_m a_m(t) \phi_m(\vec{r})$$

and derive a set of equations for the expansion coefficients $a_m(t)$.

(10 Points)