Homework # 2

Exercise 1 – Particle in a 1D-box

In 1960 Avakian and Smakula showed that the coloration in cesium halides is due to electrons and holes trapped in lattice vacancies [1]. In particular, an F center or Farbe center is a type of crystallographic defect in which an anionic vacancy in a crystal lattice is occupied by one or more unpaired electrons. Basically, it's an electron in a three-dimensional box. Electrons in such a vacancy in a crystal lattice tend to absorb light in the visible spectrum such that a material that is usually transparent becomes colored.

Consider an electron confined in a one-dimensional box of length a ($0 < x < a$) with infinitely high walls. Consider the time-dependent Schrödinger equation:

$$i\hbar \frac{\partial \Phi_n(x,t)}{\partial t} = \hat{H}\Phi_n(x,t). \tag{1}$$

1. Show that $\Phi_n(x,t) = e^{-\frac{i}{\hbar}Et}\psi_n(x)$ is a solution if $\psi_n(x)$ is an eigenfunction of $\hat{H}$. What is E from the physical point of view? And from the mathematical?

We saw during the lectures that the eigenfunctions $\psi_n(x)$ have the following expression:

$$\psi_n(x) = C_n \sin\left(\frac{n\pi x}{a}\right), \qquad n = 1, 2, 3, ... \tag{2}$$

2. Imposing the normalization condition $1 = \int_0^a dx|\psi_n(x)|^2$ for the eigenfunctions compute the coefficients C_n (assume C_n is real).

   Hint: $\int dx \sin^2(x) = \frac{x}{2} - \frac{\sin(2x)}{4}$. What is the physical motivation for imposing such condition? Why is the $n = 0$ solution not acceptable?

3. Derive the expression for E_n as the expectation value of the Hamiltonian operator $\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$ for the eigenfunctions $\psi_n(x)$. What is the minimum-energy level for this system? Is this what you would expect for an equivalent classical system?

Exercise 2 – Scanning Tunnelling Microscope (STM)

A scanning tunneling microscope (STM) is a type of microscope used for imaging surfaces at the atomic level, developed in 1981 by Gerd Binnig and Heinrich Rohrer at IBM Zürich. STM senses the surface by using a conducting tip that can distinguish features smaller than 0.1 nm. STM is based on the concept of quantum tunneling [2].

Let's consider a metallic-surface step-like potential of the form $V(x) = V_0\ \theta(x)$, with $\theta(x) = 1,\ x \geq 0$ and 0 otherwise.

1. Since for time-independent potential the time-dependent solution of the Schrödinger equation can be recast into an eigenvalue problem, write directly the time-independent Schrödinger equation with the potential explicit.

[1] P. Avakian and A. Smakula, Phys. Rev. **120**, 2007 (1960)
[2] G. Binnig, H. Rohrer, Ch. Gerber, and E. Weibel, Phys. Rev. Lett. **49**, 57 (1982)

2. A particular eigensolution for this problem can be written in the form:

$$\psi(x) = \left(Ae^{ikx} + Be^{-ikx}\right)\theta(-x) + \left(Ce^{iKx}\right)\theta(x), \tag{3}$$

with $k = \sqrt{\frac{2mE}{\hbar^2}}$ and $K = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$ and A, B, C constants different from 0 that assure continuity in 0 and correct normalization. What happens if $E < V_0$?

3. For the case $E < V_0$ show that there is a non zero probability of finding the particle in the interval $[\frac{a_b}{2}, a_b]$ (a_b is the Bohr radius). Why is this a non classical phenomenon? With such potential what would a classical particle coming from the left do?