M1 "Sciences et Génies des Matériaux" & M1 franco-allemand "Polymères"

Quantum Mechanics course

Two-hour exam, **session 1**, January 2025 – Lecturer: *E. Fromager*

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1. Questions on the lectures [12 points]

a) [**4 pts**] Which mathematical functions are used for describing the state of a particle moving along the x axis in classical Newton and quantum mechanics, respectively? Write the fundamental time-dependent equations that these functions are supposed to fulfill.

b) [**2 pts**] What is the general idea behind perturbation theory? How do we technically derive the perturbation expansion of the energies for a given Hamiltonian $\hat{H}$?

c) [**6 pts**] Let $\hat{H}$ denote the Hamiltonian operator of a quantum system and $\hat{U}(t) = e^{-\mathrm{i}\hat{H}t/\hbar}$, where t denotes the time and $\mathrm{i}^2 = -1$. We recall that, for any quantum operator $\hat{A}$, the exponential of $\hat{A}$ reads $e^{\hat{A}} \equiv \sum_{n=0}^{+\infty} \dfrac{\hat{A}^n}{n!}$. We consider an orthonormal basis $\{|\Psi_j\rangle\}$ of eigenvectors of $\hat{H}$ and denote $\{E_j\}$ the associated energies. Show that $\hat{H} = \hat{H}\hat{\mathbb{1}} = \sum_k E_k |\Psi_k\rangle \langle\Psi_k|$ and $\hat{U}(t) = \hat{U}(t)\hat{\mathbb{1}} = \sum_j e^{-\mathrm{i}E_j t/\hbar} |\Psi_j\rangle \langle\Psi_j|$. Deduce that $\hat{H}\hat{U}(t) = \mathrm{i}\hbar \dfrac{d\hat{U}(t)}{dt}$ and conclude that $|\Psi(t)\rangle = \hat{U}(t)\,|\Psi(t=0)\rangle$ is the quantum state of the system at time t if, at time $t = 0$, it is in the state $|\Psi(t=0)\rangle$. Why is $\hat{U}(t)$ referred to as time evolution operator? Why are the eigenvectors of $\hat{H}$ referred to as stationary states?

2. Exercise: Generalization of the Heisenberg inequality (9 points)

Let A and B be two observables to which we associate the Hermitian quantum operators $\hat{A}$ and $\hat{B}$, respectively. The purpose of the exercise is to show that, for any normalized quantum state $|\Psi\rangle$, the following inequality is fulfilled,

$$\left(\Delta A\right)_{\Psi}\left(\Delta B\right)_{\Psi} \geq \frac{1}{2}\left|\langle\Psi|[\hat{A},\hat{B}]|\Psi\rangle\right|, \tag{1}$$

where $\left(\Delta A\right)_{\Psi} = \sqrt{\left\langle\Psi\middle|\left(\hat{A} - \langle\Psi|\hat{A}|\Psi\rangle \times \hat{\mathbb{1}}\right)^2\middle|\Psi\right\rangle}$ and $\left(\Delta B\right)_{\Psi} = \sqrt{\left\langle\Psi\middle|\left(\hat{B} - \langle\Psi|\hat{B}|\Psi\rangle \times \hat{\mathbb{1}}\right)^2\middle|\Psi\right\rangle}$ are the standard deviations for the measurement of A and B, respectively. The operator $[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ is the commutator of $\hat{A}$ and $\hat{B}$, and $\hat{\mathbb{1}}$ is the identity operator.

a) **[3 pts]** Let α be a ***real*** number that we use to construct the α-dependent quantum state

$$|\Psi(\alpha)\rangle = \left[\left(\hat{A} - \langle\Psi|\hat{A}|\Psi\rangle \times \hat{\mathbb{1}}\right) + \mathrm{i}\alpha\left(\hat{B} - \langle\Psi|\hat{B}|\Psi\rangle \times \hat{\mathbb{1}}\right)\right]|\Psi\rangle, \tag{2}$$

where $\mathrm{i}^2 = -1$. Show that the square norm of $|\Psi(\alpha)\rangle$, that we denote $N(\alpha) = \langle\Psi(\alpha)|\Psi(\alpha)\rangle$, can be written as

$$N(\alpha) = \left(\Delta A\right)^2_\Psi + \left(\Delta B\right)^2_\Psi \alpha^2 + \alpha\, C_\Psi, \quad \text{where} \;\; C_\Psi = \langle\Psi|\hat{C}|\Psi\rangle \;\; \text{and} \;\; \hat{C} = \mathrm{i}[\hat{A}, \hat{B}]. \tag{3}$$

b) **[2 pts]** Explain why we expect C_Ψ to be a real number. Prove it by showing that $\hat{C}$ is Hermitian.

c) **[1 pt]** Show that $N(\alpha) = \left(\Delta B\right)^2_\Psi \left[\left(\alpha + \dfrac{C_\Psi}{2\left(\Delta B\right)^2_\Psi}\right)^2 + \dfrac{1}{\left(\Delta B\right)^2_\Psi}\left(\left(\Delta A\right)^2_\Psi - \dfrac{C_\Psi^2}{4\left(\Delta B\right)^2_\Psi}\right)\right]$.

d) **[1 pt]** Explain why $N(\alpha)$ should be positive for any value of α [**Hint:** see its definition in question 2. a)]. Show that the generalized Heisenberg inequality in Eq. (1) is recovered when $\alpha = -\dfrac{C_\Psi}{2\left(\Delta B\right)^2_\Psi}$.

e) **[2 pts]** Conclude that the commutator of two operators determines if the corresponding observables can be measured simultaneously or not. Show that the famous inequality of Heisenberg is recovered from Eq. (1) when $\hat{A}$ and $\hat{B}$ are the position $\hat{x} \equiv x\times$ and momentum $\hat{p}_x \equiv -\mathrm{i}\hbar\partial/\partial x$ operators, respectively.