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

Quantum Mechanics course

Two-hour exam, **session 1**, December 2023 – 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: The Heisenberg inequality and the harmonic oscillator (10 points)

According to the Heisenberg inequality, the standard deviations $\Delta x = \sqrt{\langle\Psi|\hat{x}^2|\Psi\rangle - \langle\Psi|\hat{x}|\Psi\rangle^2}$ *and* $\Delta p_x = \sqrt{\langle\Psi|\hat{p}_x^2|\Psi\rangle - \langle\Psi|\hat{p}_x|\Psi\rangle^2}$ *for the position* x *and momentum* p_x *of a particle described by a quantum state* $|\Psi\rangle$ *are such that*

$$\Delta x\, \Delta p_x \geq \hbar/2. \tag{1}$$

In this exercise, we consider a particle with mass m *attached to a spring of constant* k *moving along the* x *axis. The corresponding (so-called one-dimensional harmonic oscillator) Hamiltonian reads*

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2, \tag{2}$$

where $\omega = \sqrt{\dfrac{k}{m}}$*. It can be shown that, by introducing the so-called annihilation operator* $\hat{a}$ *defined as follows,*

$$\hat{a} = \frac{1}{\sqrt{2}} \left(\sqrt{\frac{m\omega}{\hbar}} \hat{x} + \frac{\mathrm{i}}{\sqrt{m\hbar\omega}} \hat{p}_x \right), \quad \textit{where} \quad \mathrm{i}^2 = -1, \tag{3}$$

and its adjoint $\hat{a}^\dagger$ (referred to as creation operator), the Hamiltonian in Eq. (2) can be rewritten as

$$\hat{H} = \hbar\omega\left(\hat{N} + \frac{1}{2}\right), \tag{4}$$

where $\hat{N} = \hat{a}^\dagger\hat{a}$ is the so-called counting operator. By using the commutation rule $\left[\hat{a}, \hat{a}^\dagger\right] = \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} = 1$, it can finally be shown that the eigenvalues n of the counting operator $\hat{N}$ are integers ($n = 0, 1, 2, \ldots$), and that the associated orthonormalized eigenvectors $\left\{|\Psi_n\rangle\right\}_{n=0,1,2,\ldots}$ are connected through the relation

$$\hat{a}^\dagger|\Psi_n\rangle = \sqrt{n+1}|\Psi_{n+1}\rangle. \tag{5}$$

a) **[1 pt]** Show that

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}^\dagger + \hat{a}\right) \quad \text{and} \quad \hat{p}_x = \mathrm{i}\sqrt{\frac{m\hbar\omega}{2}}\left(\hat{a}^\dagger - \hat{a}\right). \tag{6}$$

Conclude from Eq. (5) that $\langle\Psi_n|\hat{x}|\Psi_n\rangle = 0 = \langle\Psi_n|\hat{p}_x|\Psi_n\rangle$.

b) **[0.5 pt]** Explain why, according to Eq. (4), the energies of the one-dimensional harmonic oscillator are $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$ and the corresponding eigenstates are $|\Psi_n\rangle$ with $n = 0, 1, 2, \ldots$

c) **[1 pt]** Explain why $E_n = \langle\Psi_n|\hat{H}|\Psi_n\rangle$ and deduce from question 2. b) and Eq. (2) that, for a given eigenstate $|\Psi_n\rangle$, the expectation value of $\hat{p}_x^2$ is obtained from that of $\hat{x}^2$ as follows, $\langle\Psi_n|\hat{p}_x^2|\Psi_n\rangle = m\hbar\omega(2n+1) - m^2\omega^2\langle\Psi_n|\hat{x}^2|\Psi_n\rangle$.

d) **[0.5 pt]** In order to determine the expectation value of $\hat{x}^2$ for $|\Psi_n\rangle$, we introduce a real parameter λ and construct the following λ-dependent Hamiltonian:

$$\hat{H}(\lambda) = \frac{\hat{p}_x^2}{2m} + \frac{\lambda}{2}m\omega^2\hat{x}^2. \tag{7}$$

Its normalized eigenvectors and associated eigenvalues are denoted $|\Psi_n(\lambda)\rangle$ and $E_n(\lambda)$, respectively. For which value of λ do we recover from $\hat{H}(\lambda)$ the problem we are interested in?

e) **[2 pts]** Explain why $E_n(\lambda) = \left\langle\Psi_n(\lambda)\middle|\hat{H}(\lambda)\middle|\Psi_n(\lambda)\right\rangle$. Prove the Hellmann–Feynman theorem, $\dfrac{\mathrm{d}E_n(\lambda)}{\mathrm{d}\lambda} = \left\langle\Psi_n(\lambda)\middle|\dfrac{\partial\hat{H}(\lambda)}{\partial\lambda}\middle|\Psi_n(\lambda)\right\rangle$, and conclude that $\langle\Psi_n(\lambda)|\hat{x}^2|\Psi_n(\lambda)\rangle = \dfrac{2}{m\omega^2}\dfrac{\mathrm{d}E_n(\lambda)}{\mathrm{d}\lambda}$.

f) **[1 pt]** Explain why, according to Eqs. (2) and (7), $E_n(\lambda) = \sqrt{\lambda}\hbar\omega\left(n + \frac{1}{2}\right)$. **Hint**: Introduce the λ-dependent frequency $\omega(\lambda) = \omega\sqrt{\lambda}$, rewrite $\hat{H}(\lambda)$ in terms of $\omega(\lambda)$, and compare the resulting expression with that of Eq. (2). Conclude from question 2. b).

g) **[1 pt]** Conclude from questions 2. d), e), and f) that $\langle\Psi_n|\hat{x}^2|\Psi_n\rangle = \dfrac{\hbar}{m\omega}\left(n + \frac{1}{2}\right)$.

h) **[1 pt]** Deduce from questions 2. c) and g) that $\langle\Psi_n|\hat{p}_x^2|\Psi_n\rangle = m\hbar\omega\left(n + \frac{1}{2}\right)$.

i) **[2 pts]** Verify from questions 2. a), g) and h) that the solutions to the Schrödinger equation for the one-dimensional harmonic oscillator fulfill the Heisenberg inequality in Eq. (1). What is remarkable about the ground state $|\Psi_0\rangle$?