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

Exam in quantum mechanics

December 2018

two-hour exam

Neither documents nor calculators are allowed.

The grading scale might be changed.

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1. Questions on the lecture material (4 points)

a) **[2 pts]** What is the key difference between the (so-called Rayleigh–Ritz) variational principle and the stationarity condition of the energy in quantum mechanics ? How can they be used in practical electronic structure calculations ?

b) **[2 pts]** What is the purpose of both Hartree–Fock and Hückel methods ? What is the main advantage of the former over the latter ? Is the Hartree–Fock approach in principle exact ? Justify your answers.

2. Problem I: 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,

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

where $(\Delta A)_\Psi = \sqrt{\left\langle \Psi \middle| \left(\hat{A} - \langle \Psi | \hat{A} | \Psi \rangle \times \hat{\mathbb{1}} \right)^2 \middle| \Psi \right\rangle}$ and $(\Delta B)_\Psi = \sqrt{\left\langle \Psi \middle| \left(\hat{B} - \langle \Psi | \hat{B} | \Psi \rangle \times \hat{\mathbb{1}} \right)^2 \middle| \Psi \right\rangle}$ 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 $N(\alpha) = \langle \Psi(\alpha)|\Psi(\alpha)\rangle$ can be written as

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

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

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 $\alpha = -\dfrac{C_\Psi}{2(\Delta B)^2_\Psi}$.

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.

3. Problem II: Quantum mechanics with a non-hermitian Hamiltonian (9 points)

The time-dependent Schrödinger equation is traditionally written with a Hamiltonian operator that is hermitian. In this exercise ***we will assume that the Hamiltonian operator $\hat{\mathcal{H}}$ is not necessarily hermitian*** and we will try to understand what is the physical implication of such an assumption.

a) **[1 pt]** Let us consider a particle described by the time-dependent wave function $\Psi(\mathbf{r}, t)$ where $\mathbf{r} \equiv (x, y, z)$. Let $N(t) = \langle \Psi(t)|\Psi(t)\rangle = \displaystyle\int_{\mathbb{R}^3} \mathrm{d}\mathbf{r} \, |\Psi(\mathbf{r}, t)|^2$ where $\mathrm{d}\mathbf{r} = \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}z$. What is the physical meaning of $N(t)$?

b) **[2 pts]** Show that, according to the time-dependent Schrödinger equation,

$$\frac{\mathrm{d}N(t)}{\mathrm{d}t} = \frac{1}{\mathrm{i}\hbar} \left\langle \Psi(t) \middle| \left(\hat{\mathcal{H}} - \hat{\mathcal{H}}^\dagger \right) \middle| \Psi(t) \right\rangle. \tag{4}$$

c) **[2 pts]** Let us assume that $\hat{\mathcal{H}} = \hat{H} - (\mathrm{i}\hbar\gamma/2) \times \hat{\mathbb{1}}$ where $\gamma > 0$, $\hat{\mathbb{1}}$ is the identity operator, and $\hat{H}$ is a "regular" ***hermitian*** Hamiltonian operator. Verify that $\hat{\mathcal{H}}$ is indeed ***not*** hermitian. Give an explicit expression for $\hat{H}$ if the system under study is the hydrogen atom.

d) **[2 pts]** We assume that $N(0) = 1$. Show that, according to questions 3.b) and 3.c), $N(t)$ varies as $N(t) = e^{-\gamma t}$ for $t \geq 0$. Explain why $1/\gamma$ can be interpreted as the lifetime of the system.

e) **[2 pts]** Explain why, in the light of question 3.d), the use of non-hermitian Hamiltonians is often connected to the description of open quantum systems. In the particular case of the hydrogen atom, what kind of physical process is described when adding the non-hermitian contribution $-(\mathrm{i}\hbar\gamma/2)\times\hat{\mathbb{1}}$ to the Hamiltonian $\hat{H}$?