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

Quantum Mechanics course

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The following questions are meant to help the students in reviewing their lecture notes.

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1. 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.

2. Let $\left[\hat{A}\right] \equiv \{A_{ij}\}_{1\leq i,j\leq N}$ be the matrix representation of a *linear* quantum operator $\hat{A}$ in a given basis $\{|u_i\rangle\}_{1\leq i\leq N}$. Show that, according to the linearity of $\hat{A}$, we can deduce from $\left[\hat{A}\right]$ the quantum state $\hat{A}\,|\Psi\rangle$ that is obtained by applying $\hat{A}$ to *any* state $|\Psi\rangle = \sum_{j=1}^{N} C_j\,|u_j\rangle$. Show that, if $\{|u_i\rangle\}_{1\leq i\leq N}$ is orthonormal, then $C_i = \langle u_i|\Psi\rangle$ and $A_{kj} = \langle u_k|\hat{A}|u_j\rangle$. Deduce that the identity operator reads $\hat{\mathbb{1}} = \sum_{j=1}^{N} |u_j\rangle\,\langle u_j|$ and that $\hat{A} = \hat{\mathbb{1}}\hat{A}\hat{\mathbb{1}} = \sum_{i,j=1}^{N} A_{ij}\,|u_i\rangle\,\langle u_j|$.

3. How does the wave function $\Psi(\vec{r})$, where $\vec{r} \equiv (x,y,z)$ denotes a position that the particle under study could have in the three-dimensional real space, relate to the quantum state $|\Psi\rangle$ of that particle? Explain the notation $\Psi(\vec{r}\,') = \langle\vec{r}\,'|\Psi\rangle$, where $\vec{r}\,' \equiv (x',y',z')$ is some given fixed position. Let $\hat{x}$ denote the x coordinate position operator. Why, according to the postulates of quantum mechanics, should we expect the following equality to be fulfilled: $\hat{x}\,|\vec{r}\,'\rangle = x'\,|\vec{r}\,'\rangle$? Deduce that $(\hat{x}\Psi)(\vec{r}\,') = \langle\vec{r}\,'|\hat{x}|\Psi\rangle = x' \times \Psi(\vec{r}\,')$.

4. Let $\hat{\mathcal{O}}$ denote a Hermitian quantum operator and $|\Psi_{o_i}\rangle$ an eigenvector of $\hat{\mathcal{O}}$ associated to the eigenvalue o_i (which is indexed with i). Show that o_i is a real number (*i.e.*, it is equal to its complex conjugate). Show that, if $\left|\Psi_{o_j}\right\rangle$ is another eigenvector of $\hat{\mathcal{O}}$ associated to a different eigenvalue $o_j \neq o_i$, then $\left|\Psi_{o_j}\right\rangle$ and $|\Psi_{o_i}\rangle$ are orthogonal. On the basis of these mathematical properties, explain why, in quantum mechanics, we associate to any observable $\mathcal{O}$ a Hermitian operator $\hat{\mathcal{O}}$. We assume that, just before measuring $\mathcal{O}$, the system under study is in the quantum state $|\Psi\rangle = \sum_k C_k\,|\Psi_{o_k}\rangle$. What is the probability of measuring o_i? Why should we always verify that $|\Psi\rangle$ is normalized before evaluating that probability? If $|\Psi\rangle$ is not normalized, how can we construct a normalized quantum state that is equivalent to $|\Psi\rangle$?

5. Let $\hat{A}$ and $\hat{B}$ be two Hermitian operators. We assume that they share a *common* orthonormal basis of eigenvectors $\{|u_i\rangle\}$. We denote a_i and b_i the eigenvalues of $\hat{A}$ and $\hat{B}$, respectively, that are associated to $|u_i\rangle$. Show that $\hat{A}$ and $\hat{B}$ commute, *i.e.*, $\left[\hat{A}, \hat{B}\right]|u_i\rangle = 0$ for any basis vector $|u_i\rangle$. Explain why, in this case, the observables A and B (that are associated to $\hat{A}$ and $\hat{B}$, respectively) can be measured simultaneously. If the value a_j is measured for A, which value will then be measured for B?

6. We represent the Hamiltonian of a quantum student in the two-state orthonormal basis $\{|☺\rangle, |☹\rangle\}$ of "happy" and " not happy" states as follows: $\left[\hat{H}\right] = \begin{bmatrix} \alpha & \beta \\ \beta & \alpha \end{bmatrix}$, where $\beta < 0$. Are $|☺\rangle$ and $|☹\rangle$ stationary states? Verify that the normalized eigenvectors of $\hat{H}$ read $\dfrac{1}{\sqrt{2}}(|☺\rangle + |☹\rangle)$ and $\dfrac{1}{\sqrt{2}}(|☺\rangle - |☹\rangle)$. What is the probability of being happy for a quantum student that stands in its ground state?

7. 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?

8. What is the general idea behind perturbation theory? How do we technically derive the perturbation expansion of the energies for a given Hamiltonian $\hat{H}$?

9. Let $\hat{H}_0$ and $\hat{H}$ be two different Hamiltonian operators. We denote $\hat{W} = \hat{H} - \hat{H}_0$ and introduce the α-dependent Hamiltonian $\hat{H}(\alpha) = \hat{H}_0 + \alpha\hat{W}$, where α is a real number. Verify that $\hat{H}(\alpha)$ is Hermitian. We denote $E_i(\alpha)$ the eigenvalue of $\hat{H}(\alpha)$ associated to the eigenvector $|\Psi_i(\alpha)\rangle$ which is *normalized* for any value of α. Prove the Hellmann–Feynman theorem: $\dfrac{dE_i(\alpha)}{d\alpha} = \left\langle \Psi_i(\alpha) \middle| \dfrac{\partial \hat{H}(\alpha)}{\partial \alpha} \middle| \Psi_i(\alpha) \right\rangle$. Deduce that, in perturbation theory, the first-order correction to the energy is determined solely from the perturbation operator $\hat{W}$ and the unperturbed quantum state $|\Psi_i(\alpha = 0)\rangle$.