Mecânica Quântica Avançada
Lista 1

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List of Exercises

Exercise 1 (4.1)**.** *Show that a necessary and sufficient condition for $|\psi\rangle$ to be an eigenvector of a Hermitian operator A is that the dispersion (4.8) $\Delta_\psi A = 0$.*

Answer. Vamos iniciar mostrando que se $|\psi\rangle = 0$, então $\Delta_\psi A = 0$. Ora, por definição:

$$\Delta_\psi A = \langle\psi|A^2|\psi\rangle - \langle\psi|A|\psi\rangle^2 \tag{1}$$

É fácil ver que

$$\langle\psi|A^2|\psi\rangle = \langle\psi|A^\dagger|\,|A|\psi\rangle = a^2 \tag{2}$$

E também

$$\langle\psi|A|\psi\rangle^2 = (a)^2 = a^2 \tag{3}$$

Logo, é trivial que $\Delta_\psi A = 0$.

Agora vamos assumir que a dispersão é nula, ou seja, $\Delta A = 0$. Então ,por definição:

$$0 = \sqrt{\langle A^2\rangle - \langle A\rangle^2} \tag{4}$$

$$\Rightarrow \langle A^2\rangle = \langle A\rangle^2 \tag{5}$$

Exercise 2 (4.4.2 - 1)**.** *Let $|\psi\rangle$ be a vector (not normalized) in the Hilbert space of states and H be a Hamiltonian. The expectation value $\langle H\rangle_\psi$ is*

$$\langle\psi\rangle_\psi = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \tag{6}$$

Show that if the minimum of this expectation value is obtained for $|\psi\rangle = |\psi_m\rangle$ and the maximum for $|\psi\rangle = |\psi_M\rangle$, then

$$H|\psi_m\rangle = E_m|\psi_m\rangle\,, \qquad H|\psi_M\rangle = E_M|\psi_M\rangle \tag{7}$$

where E_m and E_M are the smallest and largest eigenvalues.

Answer. É evidente que

$$\langle H \rangle_{\psi_m} = \frac{\langle \psi_m | H | \psi_m \rangle}{\langle \psi_m | \psi_m \rangle} = E_m \tag{8}$$

Portanto, é evidente que se $\langle H \rangle_{\psi_m}$ for mínimo, então E_m também é. Vale um raciocínio análogo para $E_M = \langle H \rangle_{\psi_M}$.

Exercise 3 (4.4.2 - 2)**.** *We assume that the vector $|\varphi\rangle$ depends on a parameter $\alpha : |\varphi\rangle = |\varphi(\alpha)\rangle$. Show that if*

$$\left.\frac{\partial \langle H \rangle_{\varphi(\alpha)}}{\partial \alpha}\right|_{\alpha=\alpha_0} = 0, \tag{9}$$

then $E_m \leq \langle H \rangle_{\varphi(\alpha_0)}$ if α_0 corresponds to a minimum of $\langle H \rangle_{\varphi(\alpha)}$, and $\langle H \rangle_{\varphi(\alpha_0)} \leq E_M$ if α_0 corresponds to a maximum. This result forms the basis of an approximation method called the variational method (Section 14.1.4).

Answer. Vamos abrir a derivada:

$$\frac{\partial \langle H \rangle \varphi(\alpha)}{\partial \alpha} = \frac{1}{\langle \psi | \psi \rangle} \left(\langle \psi | H | \, \partial_\alpha \, |\psi\rangle + (\partial_\alpha \langle \psi |) \, |H|\psi\rangle \right) - \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle^2} \left((\partial_\alpha \langle \psi |) \, |\psi\rangle + \langle \psi | \, \partial_\alpha \, |\psi\rangle \right) \tag{10}$$

Então, em α_0

$$\langle \psi | H | \partial_\alpha \psi \rangle + \langle \partial_\alpha \psi | H | \psi \rangle = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \big(\langle \partial_\alpha \psi | \psi \rangle + \langle \psi | \partial_\alpha \psi \rangle \big) \tag{11}$$

Isolando a quantidade de interesse:

$$\langle H \rangle_{\varphi(\alpha_0)} = \frac{\langle \psi | H | \partial_\alpha \psi \rangle + \langle \partial_\alpha \psi | H | \psi \rangle}{\langle \partial_\alpha \psi | \psi \rangle + \langle \psi | \partial_\alpha \psi \rangle} \tag{12}$$

Podemos reescrever, usando que $H = H^\dagger$:

$$\langle H \rangle_{\varphi(\alpha_0)} = \frac{\langle \partial_\alpha \psi | H | \psi \rangle^\dagger + \langle \partial_\alpha \psi | H | \psi \rangle}{\langle \partial_\alpha \psi | \psi \rangle^\dagger + \langle \partial_\alpha \psi | \psi \rangle} \tag{13}$$

Podemos expandir qualquer estado usando os autokets do hamiltoniano, que são ortonormais:

$$|\psi\rangle = \sum c_j \, |\psi_j\rangle \tag{14}$$

De modo que

$$\partial_\alpha \, |\psi\rangle = \sum \frac{\partial c_j}{\partial \alpha} \, |\psi_j\rangle \tag{15}$$

Assim, vale que

$$\langle \partial_\alpha \psi | \psi \rangle = \sum c_j \frac{\partial c_j^*}{\partial \alpha} \tag{16}$$

E também

$$\langle \partial_\alpha \psi | H | \psi \rangle = \sum E_j c_j \frac{\partial c_j^*}{\partial \alpha} \tag{17}$$

Considere o denominador:

$$\begin{aligned}
\langle \partial_\alpha \psi | \psi \rangle^\dagger + \langle \partial_\alpha \psi | \psi \rangle &= \sum c_j \frac{\partial c_j^*}{\partial \alpha} + c_j^* \frac{\partial c_j}{\partial \alpha} \\
&= \sum \frac{\partial}{\partial \alpha} (c_j^* c_j) \\
&= \sum \partial_\alpha |c_j|^2 \\
&= \partial_\alpha \sum |c_j|^2
\end{aligned}$$

Considerando, enfim, o numerador e fazendo os mesmos cálculos:

$$\begin{aligned}
\langle \partial_\alpha \psi | H | \psi \rangle^\dagger + \langle \partial_\alpha \psi | H | \psi \rangle &= \sum E_j c_j \frac{\partial c_j^*}{\partial \alpha} + E_j c_* \frac{\partial c_j}{\partial \alpha} \\
&= \sum E_j \partial_\alpha |c_j|^2 \\
&= \partial_\alpha \sum E_j |c_j|^2
\end{aligned}$$

É óbvio, então, que

$$E_m \partial_\alpha \sum |c_j|^2 \leq \partial_\alpha \sum E_j |c_j|^2 \leq E_M \partial_\alpha \sum |c_j|^2 \tag{18}$$

Portanto, concluímos que

$$E_m \leq \langle H \rangle_{\varphi(\alpha_0)} \leq E_M \tag{19}$$

Exercise 4 (4.4.2 - 3)**.** *If H acts in a two-dimensional space, its most general form is*

$$H = \begin{pmatrix} a+c & b \\ b & a-c \end{pmatrix},$$

where b can always be chosen to be real. Parametrizing $|\varphi(\alpha)\rangle$ as

$$|\varphi(\alpha)\rangle = \begin{pmatrix} \cos \alpha/2 \\ \sin \alpha/2 \end{pmatrix}$$

find the values of α_0 by seeking the extrema of $\langle \varphi(\alpha) | H | \varphi(\alpha) \rangle$. Rederive (2.35).

Answer. Começamos considerando a equação do valor médio explicitamente:

$$\begin{aligned}
\langle \psi | H | \psi \rangle &= \begin{bmatrix} \cos(\alpha/2) & \sin(\alpha/2) \end{bmatrix} \begin{bmatrix} a+c & b \\ b & a-c \end{bmatrix} \begin{bmatrix} \cos(\alpha/2) \\ \sin(\alpha/2) \end{bmatrix} \\
&= \begin{bmatrix} \cos(\alpha/2) & \sin(\alpha/2) \end{bmatrix} \begin{bmatrix} (a+c)\cos(\alpha/2) + b\sin(\alpha/2) \\ b\cos(\alpha/2) + (a-c)\sin(\alpha/2) \end{bmatrix} \\
&= (a+c)\cos^2(\alpha/2) + b\sin(\alpha/2)\cos(\alpha/2) + b\cos(\alpha/2)\sin(\alpha/2) + (a-c)\sin^2(\alpha/2) \\
&= a(\sin^2(\alpha/2) + \cos^2(\alpha/2)) + c(\cos^2(\alpha/2) - \sin^2(\alpha/2)) + b\sin(\alpha) \\
&= a + b\sin(\alpha) + c\cos(\alpha)
\end{aligned}$$

Vejamos os extremos dessa função:

$$\begin{aligned}
\partial_\alpha \langle \psi | H | \psi \rangle &= b\cos(\alpha) - c\sin(\alpha) = 0 \\
b\cos(\alpha) &= c\sin(\alpha) \\
\tan(\alpha) &= b/c \\
\alpha_0 &= \mathrm{atan}(b/c)
\end{aligned}$$

A Eq.(2.35) se refere aos autovetores e autovalores de H. Vejamos o caso do nosso ψ:

$$\begin{aligned} H\left|\psi\right\rangle &= \left(a\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix} + \sqrt{b^2+c^2}\begin{bmatrix}\cos\alpha & \sin\alpha\\ \sin\alpha & -\cos\alpha\end{bmatrix}\right)\begin{bmatrix}\cos(\alpha/2)\\ \sin(\alpha/2)\end{bmatrix} \\ &= a\begin{bmatrix}\cos(\alpha/2)\\ \sin(\alpha/2)\end{bmatrix} + \sqrt{b^2+c^2}\begin{bmatrix}\cos\alpha\cos(\alpha/2)+\sin\alpha\sin(\alpha/2)\\ \sin\alpha\cos(\alpha/2)-\cos\alpha\sin(\alpha/2)\end{bmatrix} \\ &= a+\sqrt{b^2+c^2}\begin{bmatrix}\cos(\alpha/2)\\ \sin(\alpha/2)\end{bmatrix}\end{aligned}$$

onde usamos a Eq.(2.34) e algumas identidades trigonométricas.

Exercise 5 (4.4.3)**.** *Let a Hamiltonian H depend on a parameter $\lambda : H = H(\lambda)$. Let $E(\lambda)$ be a nondegenerate eigenvalue and $|\varphi(\lambda)\rangle$ be the corresponding normalized eigenvector $(\|\varphi(\lambda)\|^2 = 1)$:*

$$H(\lambda)|\varphi(\lambda)\rangle = E(\lambda)|\varphi(\lambda)\rangle$$

Demonstrate the Feynman-Hellmann theorem:

$$\frac{\partial E}{\partial \lambda} = \left\langle \varphi(\lambda) \middle| \frac{\partial H}{\partial \lambda} \middle| \varphi(\lambda) \right\rangle.$$

Answer. Sabemos que podemos escrever

$$E(\lambda) = \langle\psi|H|\psi\rangle \tag{20}$$

Então considere:

$$\partial_\lambda E = \langle\partial_\lambda\psi|H|\psi\rangle + \langle\psi|\partial_\lambda|\psi\rangle + \langle\psi|H|\partial_\lambda\psi\rangle \tag{21}$$

Logo, é suficiente mostrar que

$$\langle\partial_\lambda\psi|H|\psi\rangle + \langle\psi|H|\partial_\lambda\psi\rangle = 0 \tag{22}$$

Considere:

$$\begin{aligned} \langle\partial_\lambda\psi|H|\psi\rangle + \langle\psi|H|\partial_\lambda\psi\rangle &= \langle\partial_\lambda\psi|E|\psi\rangle + \langle\psi|E^\dagger|\partial_\lambda\partial_\lambda\psi\rangle \\ &= E\left(\langle\partial_\lambda\psi|\psi\rangle + \langle\psi|\partial_\lambda\psi\rangle\right) \\ &= E(\partial_\lambda\left\langle\psi|\psi\right\rangle) \\ &= E\partial_\lambda 1 \\ &= 0 \end{aligned}$$

onde usamos o fato de H ser hermitiano e ter autovalores reais e de $|\psi\rangle$ ser normalizado. Portanto, fica demonstrado o teorema.

Exercise 6 (4.4.4)**.** *We consider a two-level system with Hamiltonian H represented by the matrix*

$$H = \hbar\begin{pmatrix} A & B\\ B & -A\end{pmatrix}$$

in the basis

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

According to (2.35), the eigenvalues and eigenvectors of H are

$$\begin{aligned} E_+ &= \hbar\sqrt{A^2+B^2}, \quad |\chi_+\rangle = \cos\tfrac{\theta}{2}|+\rangle + \sin\tfrac{\theta}{2}|-\rangle \\ E_- &= -\hbar\sqrt{A^2+B^2}, \quad |\chi_-\rangle = -\sin\tfrac{\theta}{2}|+\rangle + \cos\tfrac{\theta}{2}|-\rangle \end{aligned}$$

with

$$A = \sqrt{A^2+B^2}\cos\theta, \quad B = \sqrt{A^2+B^2}\sin\theta, \quad \tan\theta = \frac{B}{A}$$

Part 1. *The state vector $|\varphi(t)\rangle$ at time t can be decomposed on the $\{|+\rangle, |-\rangle\}$ basis:*

$$|\varphi(t)\rangle = c_+(t)|+\rangle + c_-(t)|-\rangle$$

Write down the system of coupled differential equations which the components $c_+(t)$ and $c_-(t)$ satisfy.

Answer. Começamos escrevendo:

$$|\varphi(t)\rangle = \begin{pmatrix} c_+(t) \\ c_-(t) \end{pmatrix} \tag{23}$$

Agora montamos a equação de Schrödinger:

$$\begin{aligned} H\,|\varphi(t)\rangle &= -i\hbar\partial_t\,|\varphi(t)\rangle \\ \hbar\begin{pmatrix} A & B \\ B & -A \end{pmatrix}\begin{pmatrix} c_+(t) \\ c_-(t) \end{pmatrix} &= -i\hbar\begin{pmatrix} \partial_t c_+(t) \\ \partial_t c_-(t) \end{pmatrix} \\ \begin{pmatrix} Ac_+ + Bc_- \\ Bc_+ - Ac_- \end{pmatrix} &= -i\begin{pmatrix} \dot{c}_+(t) \\ \dot{c}_-(t) \end{pmatrix} \end{aligned}$$

Ou seja, temos as equações diferenciais:

$$i\dot{c}_+ = Ac_+ + Bc_- \tag{24}$$

$$i\dot{c}_- = Bc_+ - Ac_- \tag{25}$$

Part 2. *Let $|\varphi(t=0)\rangle$ be decomposed on the $\{|\chi_+\rangle, |\chi_-\rangle\}$basis:*

$$|\varphi(t=0)\rangle = |\varphi(0)\rangle = \lambda\,|\chi_+\rangle + \mu\,|\chi_-\rangle, \quad |\lambda|^2 + |\mu|^2 = 1$$

Show that $c_+(t) = \langle + \mid \varphi(t)\rangle$ is written as

$$c_+(t) = \lambda \mathrm{e}^{-\mathrm{i}\Omega t/2}\cos\frac{\theta}{2} - \mu\mathrm{e}^{\mathrm{i}\Omega t/2}\sin\frac{\theta}{2}$$

with $\Omega = 2\sqrt{A^2+B^2}$. Here $\hbar\Omega$ is the energy difference of the two levels. Show that $c_+(t)$ (as well as $c_-(t)$) satisfies the differential equation

$$\ddot{c}_+(t) + \left(\frac{\Omega}{2}\right)^2 c_+(t) = 0.$$

Answer. Vamos começar pela segunda parte, mostrando a validez da equação diferencial. Considere as EDOs que obtemos e vamos deriva-las mais uma vez (faremos as contas para c_+, pois são análogas para c_-.):

$$i\ddot{c}_+ = A\dot{c}_+ + B\dot{c}_- \tag{26}$$

Mas note, também, que:

$$\begin{aligned} A\dot{c}_+ &= -iA^2c_+ - iABc_- \\ B\dot{c}_- &= -iB^2c_+ + iABc_- \end{aligned}$$

Logo,

$$A\dot{c}_+ + B\dot{c}_- = -i(A^2 + B^2)c_+ \tag{27}$$

Portanto,

$$i\ddot{c}_+ = -i(A^2 + B^2)c_+ \tag{28}$$

que, simplificando, implica na expressão desejada

$$\ddot{c}_+ + \left(\frac{\Omega}{2}\right)^2 c_+ = 0 \tag{29}$$

Vamos considerar agora a outra parte. Ela nos dá condições iniciais:

$$|\varphi_0\rangle = \begin{pmatrix} \lambda\cos(\theta/2) - \mu\sin(\theta/2) \\ \lambda\sin(\theta/2) + \mu\cos(\theta/2) \end{pmatrix} \tag{30}$$

Ou seja,

$$\begin{aligned} c_+(0) &= \lambda\cos(\theta/2) - \mu\sin(\theta/2) \\ c_-(0) &= \lambda\sin(\theta/2) + \mu\cos(\theta/2) \end{aligned}$$

Usando a equação diferencial que deduzimos, é fácil ver que (novamente, apenas para c_+):

$$c_+(t) = Ae^{i\Omega t/2} + Be^{-i\Omega t/2} \tag{31}$$
