Mecânica Quântica Avançada
Lista 1

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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 1. *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 2. *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 3. *Vamos abrir a derivada:*

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

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

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