Mecânica Quântica Avançada
Lista 1

Lucas Froguel
IFT

List of Exercises

Exercise 1 (4.4.1 - Dispersion and eigenvectors)**.** *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:

$$0 = \sqrt{\langle A^2\rangle - \langle A\rangle^2} \tag{4}$$
$$\Rightarrow \langle A^2\rangle = \langle A\rangle^2 \tag{5}$$

Ora, considere

$$\begin{aligned}
\langle\psi|A^2|\psi\rangle &= \langle\psi|A|\psi\rangle^2 \\
\langle\psi|A^2|\psi\rangle &= \langle\psi|A|\psi\rangle\langle\psi|A|\psi\rangle \\
A^2|\psi\rangle &= \langle\psi|A|\psi\rangle A|\psi\rangle \\
A|\psi\rangle &= \langle\psi|A|\psi\rangle|\psi\rangle
\end{aligned}$$

Logo, vemos que $|\psi\rangle$ é autovetor de A.

Exercise 2 (4.4.2 - The variational method)**.** ***Part 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 $E_M = \langle H\rangle_{\psi_M}$.

Part 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

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

Part 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:

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

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

Exercise 3 (4.4.3 - The Feynman-Hellmann theorem)**.** *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:

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

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:

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

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

Exercise 4 (4.4.4 - Time evolution of a two-level system). *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

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

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. Sabemos que

$$|\psi_t\rangle = \hat{U}\,|\psi_0\rangle \tag{30}$$

onde $\hat{U}$ é o operador de evolução temporal. Assim, usando a base dos autoestados de $\hat{H}$:

$$\begin{aligned} |\psi_t\rangle &= \hat{U}\,|\psi_0\rangle \\ &= e^{-i\hat{H}t/\hbar}\,(\lambda\,|\chi_+\rangle + \mu\,|\chi_-\rangle) \\ &= \lambda e^{-iE_+t/\hbar}\,|\chi_+\rangle + \mu e^{iE_-t/\hbar}\,|\chi_-\rangle \end{aligned}$$

Abrindo agora na base natural:

$$|\psi_t\rangle = \lambda e^{-iE_+t/\hbar}\left(\cos\frac{\theta}{2}|+\rangle + \sin\frac{\theta}{2}|-\rangle\right) + \mu e^{iE_-t/\hbar}\left(-\sin\frac{\theta}{2}|+\rangle + \cos\frac{\theta}{2}|-\rangle\right) \tag{31}$$

Por fim, calculamos $c_+(t) = \langle +|\psi_t\rangle$ e usamos $\Omega = 2E_\pm$:

$$c_+(t) = \lambda \mathrm{e}^{-\mathrm{i}\Omega t/2}\cos\frac{\theta}{2} - \mu \mathrm{e}^{\mathrm{i}\Omega t/2}\sin\frac{\theta}{2} \tag{32}$$

Part 3. *We assume that $c_+(0) = 0$. Find λ and μ up to a phase as well as $c_+(t)$. Show that the probability of finding the system in the state $|+\rangle$ at time t is*

$$\mathrm{p}_+(t) = \sin^2\theta \sin^2\left(\frac{\Omega t}{2}\right) = \frac{B^2}{A^2+B^2}\sin^2\left(\frac{\Omega t}{2}\right).$$

Answer. Se $c_+(0) = 0$, então precisa ser que

$$\lambda\cos(\theta/2) - \mu\sin(\theta/2) = 0 \tag{33}$$

Logo, é verdade que

$$\lambda = \mu\tan(\theta/2) \tag{34}$$

Mas, pela normalização:

$$\begin{aligned}
|\lambda|^2 + |\mu|^2 &= 1 \\
|\mu\tan(\theta/2)|^2 + |\mu|^2 &= 1 \\
|\mu|^2|\tan(\theta/2)|^2 + |\mu|^2 &= \\
|\mu|^2 &= \frac{1}{1+|\tan(\theta/2)|^2}
\end{aligned}$$

Logo, a menos de uma fase e^{ia},

$$\begin{aligned}
\mu = &= \frac{1}{\sqrt{1+|\tan(\theta/2)|^2}} \\
\lambda &= \frac{\tan(\theta/2)}{\sqrt{1+|\tan(\theta/2)|^2}}
\end{aligned}$$

Vamos supor, daqui em diante, $\theta \in [0,\pi]$ para tirarmos a tangente do módulo. Usando a solução geral de $c_+(t)$, basta usarmos os valores calculados de λ e μ:

$$\begin{aligned}
c_+(t) &= \left(\frac{\tan(\theta/2)}{\sqrt{1+\tan(\theta/2)^2}}\right)\mathrm{e}^{-\mathrm{i}\Omega t/2}\cos\frac{\theta}{2} - \left(\frac{1}{\sqrt{1+\tan(\theta/2)^2}}\right)\mathrm{e}^{\mathrm{i}\Omega t/2}\sin\frac{\theta}{2} \\
&= \frac{\sin(\theta/2)}{\sqrt{1+\tan^2(\theta/2)}}\left(e^{-i\Omega t/2} - e^{i\Omega t/2}\right) \\
&= \frac{-2i\sin(\theta/2)}{\sqrt{1+\tan^2(\theta/2)}}\sin\left(\frac{\Omega t}{2}\right)
\end{aligned}$$

Ora, tendo isso, a probabilidade é $p(t) = |c(t)|^2$. Portanto, considere:

$$\begin{aligned}
p(t) &= |c(t)|^2 \\
&= |c^2(t)| \\
&= \frac{2\sin^2(\theta/2)}{1+\tan^2(\theta/2)}\sin^2(\Omega t/2)
\end{aligned}$$

Aqui notamos que:

$$1+\tan^2(\theta/2) = 1 + \frac{\sin^2(\theta/2)}{\cos^2(\theta/2)} = \frac{\sin^2(\theta/2)+\cos^2(\theta/2)}{\cos^2(\theta/2)} = \frac{1}{\cos^2(\theta/2)} \tag{35}$$

Então, é fácil ver que

$$p(t) = \sin^2(\theta)\sin^2(\Omega t/2) \tag{36}$$

E ainda podemos escrever

$$c_+(t) = -i\sin(\theta)\sin(\Omega t/2) \tag{37}$$

Exercise 5 (4.4.5 - Unstable states)**.** *Let $|\varphi(0)\rangle$ represent the state vector at time $t = 0$ of an unstable particle, or more generally that of an unstable quantum state such as an atom in an excited state, and let* p(t) *be the probability (survival probability) that it has not decayed at time t. The particle is assumed to be isolated from external influences (but not from quantized fields), so that the Hamiltonian H that governs the decay is time-independent. Let $|\Psi(t)\rangle$ be the state vector at time t of the full quantum system*

$$|\Psi(t)\rangle = \exp\left(-\frac{iHt}{\hbar}\right)|\varphi(0)\rangle.$$

The probability amplitude for finding the state of the quantum system at time t in $|\varphi(0)\rangle$ is

$$c(t) = \langle\varphi(0) \mid \Psi(t)\rangle = \left\langle \varphi(0) \left| \exp\left(-\frac{\mathrm{i}Ht}{\hbar}\right) \right| \varphi(0) \right\rangle$$

and the survival probability is

$$\mathrm{p}(t) = |c(t)|^2 = |\langle\Psi(t) \mid \varphi(0)\rangle|^2 = \langle\Psi(t)|\mathcal{P}|\Psi(t)\rangle$$

where $\mathcal{P} = |\varphi(0)\rangle\langle\varphi(0)|$ is the projector on the initial state.

Part 1. *Let us first restrict ourselves to very short times. Show that for $t \to 0$*

$$\mathrm{p}(t) \simeq 1 - \frac{(\Delta H)^2}{\hbar^2}t^2$$

so that, for very short times, the decay law is certainly not exponential. The expectation values of H and H^2 are computed in the state $|\varphi(0)\rangle$. Note that ΔH must be finite, otherwise $|\varphi(0)\rangle$ would not belong to the domain of H^2, which would be difficult to imagine physically (see Chapter 7 for the definition of the domain of an operator).

Answer. Começamos lembrando que

$$(\Delta H)^2 = \langle H^2\rangle - \langle H\rangle^2 \tag{38}$$

Para $t \to 0$, podemos aproximar

$$e^{-iHt/\hbar} \approx 1 - \frac{iHt}{\hbar} - \frac{H^2t^2}{2\hbar^2} \tag{39}$$

Logo,

$$\begin{aligned} c(t) &= \langle\phi_0|1 - \frac{iHt}{\hbar} - \frac{H^2t^2}{2\hbar^2}|\phi_0\rangle \\ &= \langle\phi_0|\phi_0\rangle - \frac{it}{\hbar}\langle H\rangle - \frac{t^2\langle H^2\rangle}{2\hbar^2} \\ &= 1 - \frac{it\langle H\rangle}{\hbar} - \frac{t^2\langle H^2\rangle}{2\hbar^2} \end{aligned}$$

Portanto,

$$\begin{aligned} p(t) &= |c(t)|^2 \\ &= 1 - \frac{t^2 \langle H^2 \rangle}{\hbar^2} + \frac{t^2 \langle H \rangle^2}{\hbar^2} + \frac{t^4 \langle H^2 \rangle^2}{\hbar^4} \\ &= 1 - \frac{t^2}{\hbar^2} \left(\langle H^2 \rangle - \langle H \rangle^2 \right) + \mathcal{O}(t^4) \\ &= 1 - \frac{t^2 (\Delta H)^2}{\hbar^2} \end{aligned}$$

como queríamos mostrar.

Part 2. *A more general result is obtained as follows. Show first that*

$$\Delta \mathcal{P}^2 = \langle \mathcal{P} \rangle - \langle \mathcal{P} \rangle^2$$

and use (4.27) to deduce the inequality $\left(\Delta H = (\langle H^2 \rangle - \langle H \rangle^2)^{1/2} \right)$

$$\left| \frac{\mathrm{dp}(t)}{\mathrm{d}t} \right| \leq \frac{2\Delta H}{\hbar} \sqrt{\mathrm{p}(1-\mathrm{p})}$$

Integrating this differential equation, derive

$$\mathrm{p}(t) \geq \cos^2 \left(\frac{t \Delta H}{\hbar} \right) \quad 0 \leq t \leq \frac{\pi \hbar}{2 \Delta H}$$

Answer. Sabemos que $\mathcal{P} = |\psi_0\rangle \langle \psi_0|$. Assim, como $\mathcal{P}$ é um projetor, é trivial que seja idempotente:

$$\mathcal{P}^2 = (|\psi_0\rangle \langle \psi_0|) (|\psi_0\rangle \langle \psi_0|) = |\psi_0\rangle \langle \psi_0 | \psi_0 \rangle \langle \psi_0| = |\psi_0\rangle \langle \psi_0| = \mathcal{P} \tag{40}$$

À partir disso, decorre diretamente a propriedade de:

$$(\Delta \mathcal{P})^2 = \langle \mathcal{P} \rangle - \langle \mathcal{P} \rangle^2 \tag{41}$$

A Eq.(4.27) diz que

$$\Delta_\varphi H \Delta_\varphi A \geq \frac{1}{2} |\langle [A, H] \rangle_\varphi| = \frac{1}{2} \hbar \left| \frac{\mathrm{d}}{\mathrm{d}t} \langle A \rangle_\varphi (t) \right| \tag{42}$$

onde, no nosso caso, teremos $A = \mathcal{P}$. Usando $p(t) = \langle \mathcal{P} \rangle$ e aplicando para o nosso caso:

$$\left| \frac{dp}{dt} \right| \leq \frac{2\Delta H}{\hbar} \Delta \mathcal{P} \tag{43}$$

Então, basta escrever $\Delta \mathcal{P}$ na forma desejada. Ora, isso é fácil, pois

$$\begin{aligned} \Delta \mathcal{P} &= \sqrt{\langle \mathcal{P} \rangle - \langle \mathcal{P} \rangle^2} \\ &= \sqrt{p - p^2} \\ &= \sqrt{p(1-p)} \end{aligned}$$

Portanto,

$$\left|\frac{dp}{dt}\right| \leq \frac{2\Delta H}{\hbar}\sqrt{p(1-p)} \tag{44}$$

Vamos, agora, integrar essa inequação:

$$\begin{aligned}
\frac{dp}{\sqrt{p(1-p)}} &\leq \frac{2\Delta H}{\hbar}dt \\
\int \frac{dp}{\sqrt{p(1-p)}} &\leq \int \frac{2\Delta H}{\hbar}dt = \frac{2t\Delta H}{\hbar}
\end{aligned}$$

Vejamos o lado esquerdo com mais cuidado. Vamos usar a substituição $u = \sqrt{p}$, onde $2du = dp/\sqrt{p}$. Assim,

$$\int \frac{dp}{\sqrt{p(1-p)}} = \int \frac{2du}{\sqrt{1-u^2}} = 2\,\mathrm{acos}(u) \tag{45}$$

Agora, notamos que isso implica

$$0 \leq \frac{2t\Delta H}{\hbar} \leq \pi \tag{46}$$

Ou,

$$0 \leq t \leq \frac{\pi\hbar}{2\Delta H} \tag{47}$$

Voltando à inequação das integrais e usando que $u = \sqrt{p}$.

$$\begin{aligned}
\mathrm{acos}(u) &\leq \frac{t\Delta H}{\hbar} \\
\sqrt{p} &\geq \cos\left(\frac{t\Delta H}{\hbar}\right) \\
p(t) &\geq \cos^2\left(\frac{t\Delta H}{\hbar}\right)
\end{aligned}$$

o sinal da inegualdade muda, pois $\cos(x)$ decresce no intervalo $x \in [0, \pi]$.

Part 3. *Let $|n\rangle$ be a complete set of eigenstates of the Hamiltonian*

$$H|n\rangle = E_n|n\rangle$$

Show that $c(t)$ is given by the Fourier transform of a spectral function $w(E)$

$$w(E) = \sum_n |\langle n \mid \varphi(0)\rangle|^2 \delta\left(E - E_n\right)$$

Set $E_0 = \langle H\rangle$ and give the expression of $(\Delta H)^2$ in terms of $w(E)$ and E_0.
Answer. Por definição,

$$c(t) = \langle\varphi(0)|\Psi(t)\rangle \tag{48}$$

com

$$|\Psi(t)\rangle = \exp\left(-\frac{iHt}{\hbar}\right)|\varphi(0)\rangle \tag{49}$$

Vamos considerar $c(t)$ na base das autoenergias:

$$\begin{aligned} |\Psi(t)\rangle &= \exp\left(-\frac{iHt}{\hbar}\right)\sum_n \langle n|\psi_0\rangle |n\rangle \\ &= \sum_n \langle n|\psi_0\rangle e^{-iE_nt/\hbar}|n\rangle \end{aligned}$$

Logo, sendo

$$\langle\psi_0| = \sum_k \langle\psi_0|k\rangle \langle k| \tag{50}$$

Vale que

$$\begin{aligned} c(t) &= \langle\psi_0|\Psi_t\rangle \\ &= \left(\sum_k \langle\psi_0|k\rangle \langle k|\right)\left(\sum_n \langle n|\psi_0\rangle e^{-iE_nt/\hbar}|n\rangle\right) \\ &= \sum_{n,k} \langle\psi_0|k\rangle \langle n|\psi_0\rangle e^{-iE_nt/\hbar}\langle k|n\rangle \\ &= \sum_{n,k} \langle\psi_0|k\rangle \langle n|\psi_0\rangle e^{-iE_nt/\hbar}\delta(n-k) \\ &= \sum_n |\langle\psi_0|n\rangle|^2 e^{-iE_nt/\hbar} \end{aligned}$$

Aqui nós observamos que a transformada de fourier da delta de dirac é:

$$\int_{-\infty}^{\infty} \delta(E-E_n)e^{-2\pi itE}dE = e^{-2\pi itE_n} \tag{51}$$

da onde é óbvio a transformada inversa da exponencial que temos em mão. Portanto,

$$\begin{aligned} \omega(E) &= \mathcal{F}^{-1}\left(\sum_n |\langle\psi_0|n\rangle|^2 e^{-iE_nt/\hbar}\right) \\ &= \sum_n |\langle\psi_0|n\rangle|^2 \mathcal{F}^{-1}\left(e^{-iE_nt/\hbar}\right) \\ &= \sum_n |\langle\psi_0|n\rangle|^2 \delta(E-E_n) \end{aligned}$$

como queríamos mostrar.

Part 4. *If $w(E)$ has a Lorentzian shape*

$$w(E) = \frac{\Gamma\hbar}{2\pi}\frac{1}{(E-E_0)^2+\hbar^2\Gamma^2/4}$$

show that

$$c(t) = \mathrm{e}^{-\mathrm{i}E_0t/\hbar}\mathrm{e}^{-\Gamma t/2}$$

and that the decay law is an exponential. The width of $w(E)$ is $\hbar\Gamma$, but ΔH is infinite, Thus ΔH is a rather poor measure of energy spread, and the width $\hbar\Gamma = \Delta E$ is the physically relevant quantity.
Answer. Iremos realizar a transformada de Fourier dessa função:

$$\begin{aligned} c(t) &= \mathcal{F}(\omega(E)) \\ &= \int_{-\infty}^{\infty} \frac{\Gamma\hbar}{2\pi} \frac{e^{-2i\pi tE}}{(E-E_0)^2 + \hbar^2\Gamma^2/4} dE \end{aligned}$$

*

Exercise 6 (4.4.6 - The solar neutrino puzzle). *The nuclear reactions occurring in the interior of the Sun produce an abundance of electron neutrinos ν_e; 95% of these are produced in the reaction*

$$\mathrm{p} + \mathrm{p} \rightarrow {}^2\mathrm{H} + \mathrm{e}^+ + \nu_\mathrm{e}$$

The Earth receives 6.5×10^{14} neutrinos per second and per square metre from the Sun. For about thirty years several experiments sought to detect these neutrinos, but all of them concluded that the measured neutrino flux is only about half the flux calculated using the standard solar model. Now this model is considered to be quite reliable, in particular owing to recent results from helioseismology. In any case, the uncertainties in the solar model cannot explain this "solar neutrino deficit."The combined results of three experiments (see Footnote 4, Chapter 1) have now shown with no possible doubt that this neutrino deficit is due to the transformation of ν_e neutrinos into other types of neutrino during the passage from the Sun to the Earth. These experiments show that the total neutrino flux predicted by the solar model is correct, but that the measured electron neutrino flux is too small. We shall construct a simplified theory which gives the essential physics. We assume that

- *there exist only two types of neutrino, the electron neutrino ν_e and the muon neutrino v_μ (in fact, there is also a third type, the τ neutrino ν_τ);*
- *the entire phenomenon takes place in a vacuum during the propagation from the Sun to the Earth (the propagation inside the Sun actually plays an important role).*

It has long been thought that neutrinos have zero mass. If, on the contrary, they are massive, we can place them in their rest frame and write down the Hamiltonian in the $\{|\nu_\mathrm{e}\rangle, |\nu_\mu\rangle\}$ basis:

$$|v_\mathrm{e}\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |v_\mu\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad H = c^2 \begin{pmatrix} m_\mathrm{e} & m \\ m & m_\mu \end{pmatrix}.$$

Part 1. *Show that the states of definite mass are $|v_1\rangle$ and $|v_2\rangle$:*

$$\begin{aligned} |v_1\rangle &= \cos\frac{\theta}{2}|v_\mathrm{e}\rangle + \sin\frac{\theta}{2}|v_\mu\rangle, \\ |v_2\rangle &= -\sin\frac{\theta}{2}|v_\mathrm{e}\rangle + \cos\frac{\theta}{2}|v_\mu\rangle, \end{aligned}$$

with

$$\tan\theta = \frac{2m}{m_\mathrm{e} - m_\mu}$$

and that the masses m_1 and m_2 are

$$m_1 = \frac{m_\mathrm{e} + m_\mu}{2} + \sqrt{m^2 + \left(\frac{m_\mathrm{e} - m_\mu}{2}\right)^2},$$
$$m_2 = \frac{m_\mathrm{e} + m_\mu}{2} - \sqrt{m^2 + \left(\frac{m_\mathrm{e} - m_\mu}{2}\right)^2}.$$

Answer. Esse problema é resolvido pela diagonalização da matriz. Como a matriz é 2×2, esse é um processo fácil. Vejamos os autovalores

$$\begin{aligned} (m_e - \lambda)(m_\mu - \lambda) - m^2 &= 0 \\ m_e m_\mu - \lambda(m_e + m_\mu) + \lambda^2 - m^2 &= 0 \end{aligned}$$

Logo,

$$\begin{aligned} \lambda_\pm &= \frac{m_e + m_\mu}{2} \pm \frac{1}{2}\sqrt{(m_e + m_\mu)^2 - 4(m_e m_\mu - m^2)} \\ &= \frac{m_e + m_\mu}{2} \pm \sqrt{\frac{m_e^2 + m_\mu^2}{4} + \frac{m_e m_\mu}{2} - m_e m_\mu + m^2} \\ &= \frac{m_e + m_\mu}{2} \pm \sqrt{m^2 + \left(\frac{m_e - m_\mu}{2}\right)^2} \end{aligned}$$

aonde identificamos $m_1 = \lambda_+$ e $m_2 = \lambda_-$. Agora iremos achar os autovetores. Considere $|v_1\rangle$ primeiramente:

$$\begin{aligned} H v_1 &= m_1 v_1 \\ \begin{pmatrix} m_\mathrm{e} & m \\ m & m_\mu \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} &= \begin{pmatrix} a m_1 \\ b m_1 \end{pmatrix} \\ m_e a + m b &= a m_1 \end{aligned}$$

Então podemos escrever

$$\begin{aligned} b &= \frac{a(m_1 - m_e)}{m} \\ &= a \left(\frac{m_\mu - m_e}{2m} + \sqrt{1 + \left(\frac{m_\mu - m_e}{2m}\right)^2} \right) \end{aligned}$$

Seja, pois, $\tan\theta = 2m/(m_e - m_\mu)$. Temos aqui:

$$\begin{aligned} b &= a\left(-\cot\theta + \sqrt{1 + \cot^2\theta}\right) \\ &= a\left(-\cot\theta + \csc\theta\right) \\ &= a\left(-\frac{\cos\theta}{\sin\theta} + \frac{1}{\sin\theta}\right) \\ &= a\left(\frac{1 - \cos\theta}{\sin\theta}\right) \\ &= a\left(\frac{\sin\theta/2}{\cos\theta/2}\right) \end{aligned}$$

Então fazemos a escolha $a = \cos\theta/2$, o que resulta em $b = \sin\theta/2$. Portanto,

$$|v_1\rangle = \cos\frac{\theta}{2}|v_e\rangle + \sin\frac{\theta}{2}|v_\mu\rangle \tag{52}$$

Fazendo contas análogas para $|v_2\rangle$, chegamos na expressão

$$\begin{aligned} b &= -a\left(\frac{1+\cos\theta}{\sin\theta}\right) \\ &= -a\left(\frac{\cos\theta/2}{\sin\theta/2}\right) \end{aligned}$$

Aqui fazemos a escolha $a = -\sin\theta/2$, que resulta em $b = \cos\theta/2$. Portanto, concluímos que

$$|v_2\rangle = -\sin\frac{\theta}{2}|v_\mathrm{e}\rangle + \cos\frac{\theta}{2}|v_\mu\rangle \tag{53}$$

Part 2. *Neutrinos propagate with a speed close to that of light; their energy is very high compared with $\langle m\rangle c^2$, where $\langle m\rangle$ is the typical mass in H. Show that if an electron neutrino is produced inside the Sun at time $t=0$ with state vector*

$$|\varphi(t=0)\rangle = |v_\mathrm{e}\rangle = \cos\frac{\theta}{2}|v_1\rangle - \sin\frac{\theta}{2}|v_2\rangle$$

the state vector at time t has component on $|v_\mathrm{e}\rangle$ given by

$$\langle\nu_\mathrm{e} \mid \varphi(t)\rangle = \mathrm{e}^{-\mathrm{i}E_1 t/\hbar}\left(\cos^2\frac{\theta}{2} + \sin^2\frac{\theta}{2}\mathrm{e}^{-\mathrm{i}\Delta E t/\hbar}\right),$$

where $\Delta E = E_2 - E_1$. Show that the probability of finding a neutrino ν_e at time t is

$$\mathrm{p_e}(t) = 1 - \sin^2\theta\sin^2\left(\frac{\Delta E t}{2\hbar}\right)$$

This transformation phenomenon is called neutrino oscillation.
Answer. Sabemos que

$$\begin{aligned} |\psi_t\rangle &= e^{-iHt/\hbar}|\psi_0\rangle \\ &= e^{-iHt/\hbar}\left(\cos(\theta/2)|v_1\rangle - \sin(\theta/2)|v_2\rangle\right) \\ &= e^{-iE_1 t/\hbar}\cos(\theta/2)|v_1\rangle - e^{-iE_2 t/\hbar}\sin(\theta/2)|v_2\rangle \end{aligned}$$

Logo, projetando em $|v_e\rangle$, temos:

$$\begin{aligned} \langle v_e|\psi_t\rangle &= e^{-iE_1 t/\hbar}\cos(\theta/2)\langle v_e|v_1\rangle - e^{-iE_2 t/\hbar}\sin(\theta/2)\langle v_e|v_2\rangle \\ &= e^{-iE_1 t/\hbar}\cos^2(\theta/2) + e^{-iE_2 t/\hbar}\sin^2(\theta/2) \end{aligned}$$

onde usamos as expressões calculadas no item anterior para expressar $|v_1\rangle, |v_2\rangle$ em termos de $|v_e\rangle, |v_\mu\rangle$. Podemos escrever a expressão acima como:

$$\langle v_e|\psi_t\rangle = e^{-iE_1 t/\hbar}\left(\cos^2(\theta/2) + \sin^2(\theta/2)e^{-i\Delta E t/\hbar}\right) \tag{54}$$

Ora, a probabilidade é apenas o módulo quadrado dessa expressão:

$$\begin{aligned} p_e(t) &= |\langle v_e|\psi_t\rangle|^2 \\ &= \left|\cos^4(\theta/2) + 2\sin^2(\theta/2)\cos^2(\theta/2)e^{-i\Delta Et/\hbar} + \sin^4(\theta/2)e^{-2i\Delta Et/\hbar}\right| \\ &= \left|\frac{e^{-i\Delta Et/\hbar}}{2i}\left(\cos\left(\frac{\Delta Et}{\hbar}\right)\left(\cos^4(\theta/2)+\sin^4(\theta/2)\right) + i\sin\left(\frac{\Delta Et}{\hbar}\right)\left(\cos^4(\theta/2)-\sin^4(\theta/2)\right)\right) + \sin^2\theta e^{-\cdots}\right. \\ &= \left|\cos\left(\frac{\Delta Et}{\hbar}\right)\frac{\cos^2(\theta)+1}{4i} + \frac{1}{4}\sin\left(\frac{\Delta Et}{\hbar}\right)\cos(\theta) + \sin^2\theta\right| \end{aligned}$$

*

Part 3. *If $p \gg \langle m\rangle c$ is the neutrino momentum, show that ΔE, as measured in the Sun rest frame, is*

$$\Delta E = \frac{(m_2^2 - m_1^2)\,c^3}{2p} = \frac{\Delta m^2 c^3}{2p}$$

with $\Delta m^2 = m_2^2 - m_1^2$. Then t must also be measured in the Sun rest frame, and not in the neutrino rest frame!
Answer. *

Exercise 7 (5.5.1 - An orthonormal basis of eigenvectors)**.** *Show by explicit calculation that the vectors $|\chi_s\rangle$ (5.12) form an orthonormal basis: $\langle\chi_{s'} \mid \chi_s\rangle = \delta_{s's}$*

Answer. Foi mostrado que

$$|\chi_s\rangle = \frac{1}{\sqrt{N}}\sum_{n=0}^{N-1} e^{in\delta_s}|\phi_n\rangle \tag{55}$$

com

$$\delta_s = \frac{2\pi s}{N} \tag{56}$$

Então, considere:

$$\begin{aligned} \langle\chi_{s'}|\chi_s\rangle &= \frac{1}{N}\sum_{n=0}^{N-1}\sum_{p=0}^{N-1} e^{in\delta s}e^{-ip\delta_{s'}}\langle\phi_p|\phi_n\rangle \\ &= \frac{1}{N}\sum_{n=0}^{N-1} e^{in(\delta_s-\delta_{s'})} \\ &= \frac{1}{N}\sum_{n=0}^{N-1} e^{2\pi in(s-s')/N} \end{aligned}$$

Agora, notamos que caso $s = s'$, então a exponencial vira $e^0 = 1$ e o somatório resulta em N, de modo que $\langle\chi_s|\chi_s\rangle = 1$. Vamos, então, considerar o caso estrito $s \neq s'$. Nesse caso, escreveremos $s - s' = k$, onde k é um número inteiro. Então, teremos

$$\langle\chi_{s'}|\chi_s\rangle = \frac{1}{N}\sum_{n=0}^{N-1} e^{2\pi inp/N} \tag{57}$$

Geometricamente, esse somatório significa dar N passos de tamanho $2\pi p/N$ no círculo unitário, que resulta em p voltas, a partir do ponto $(1, 0)$. Então, em termos físicos, podemos interpretar essa equação como calculando a posição média de uma partícula dando a volta em uma circunferência de raio 1 (em passos de tamanho $2\pi p/N$). Evidentemente, se dermos uma quantidade inteira de voltas completas, a média da posição será 0. Como nosso somatório equivale a exatamente p voltas, temos diretamente que:

$$\langle \chi_{s'} | \chi_s \rangle = 0 \tag{58}$$

se $s' \neq 0s$. Portanto, no geral,

$$\langle \chi_{s'} | \chi_s \rangle = \delta_{s's} \tag{59}$$

Exercise 8 (5.5.2 - The electric dipole moment of formaldehyde)***. Part 1.*** *We wish to model the behavior of the two π electrons of the double bond in the formaldehyde molecule* $\mathrm{H_2 - C = O}$*. Using the fact that oxygen is more electronegative than carbon, show that the Hamiltonian of an electron takes the form*

$$\begin{pmatrix} E_\mathrm{C} & -A \\ -A & E_\mathrm{O} \end{pmatrix}$$

with $E_\mathrm{O} < E_\mathrm{C}$, where $E_\mathrm{C}\,(E_\mathrm{O})$ is the energy of an electron localized at a carbon (oxygen) atom.
Answer. Um elétron pode estar ligado tanto ao carbono com energia E_c ou ao oxigênio com energia E_o. Os autoestados da hamiltoniana pura, então, são

$$\begin{aligned} H\,|\phi_e\rangle &= E_c\,|\phi_c\rangle \\ H\,|\phi_o\rangle &= E_o\,|\phi_o\rangle \end{aligned}$$

Para ter a hamiltoniana completa precisamos introduzir uma perturbação na anti-diagonal simétrica. Logo,

$$H = \begin{pmatrix} E_c & -A \\ -A & E_o \end{pmatrix} \tag{60}$$

Part 2. *We define*

$$B = \frac{1}{2}\left(E_\mathrm{C} - E_\mathrm{O}\right) > 0$$

and the angle θ by

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

Calculate as a function of θ the probability of finding a π electron localized at a carbon or oxygen atom.
Answer. As probabilidades são dadas por $p_c = |\,\langle \phi_c | \phi_c \rangle\,|^2$ e $p_o = |\,\langle \phi_o | \phi_o \rangle\,|^2$. Vamos diagonalizar a matriz e calcular os autovetores, num processo análogo ao do Ex.(6). Usando os resultados de lá como base:

$$E_\pm = \frac{E_c + E_o}{2} \pm \sqrt{A^2 + \left(\frac{E_c - E_o}{2}\right)^2} \tag{61}$$

Sendo $\phi_\pm = (a_\pm, b_\pm)$, os autovetores são dados pelas equações (novamente, invocando resultados do outro exercício):

$$\begin{aligned}
b_\pm &= a_\pm \left(\frac{E_c - E_o}{2A} \pm \sqrt{1 + \left(\frac{E_c - E_o}{2A} \right)^2} \right) \\
&= a_\pm \left(\frac{B}{A} \pm \sqrt{1 + \left(\frac{B}{A} \right)^2} \right) \\
&= a_\pm \left(\frac{B}{A} \pm \frac{B}{A \cos\theta} \right) \\
&= a_\pm \frac{B}{A} (1 \pm \sec\theta) \\
&= a_\pm \frac{B}{A} \left(\frac{\cos\theta \pm 1}{\cos\theta} \right)
\end{aligned}$$

Então, escolhemos $a_\pm = A\cos\theta$ e temos $b_\pm = B(\cos\theta \pm 1)$. Isso gera os autoestados:

$$|\phi_\pm\rangle = A\cos\theta \, |\phi_e\rangle + B(\cos\theta \pm 1) \, |\phi_o\rangle \tag{62}$$
