FI-001 Mecânica Quântica I
Lista # 1

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1. **Notação de Dirac**

   Chamamos $\{|a_n >\}$ os autokets de um operador hermitiano A. Assumimos que os kets $\{|a_n >\}$ formam uma base ortonormalizada discreta do espaço vetorial. Definimos agora um operador $U(m, n)$ por:

   $$U(m, n) \equiv |a_m\rangle \cdot \langle a_n|$$

   i) Calcular o operador adjunto $U^\dagger(m, n)$ de $U(m, n)$;

   ii) Calcular o comutador $[A, U(m, n)]$;

   iii) Demonstrar a relação

   $$U(m, n) \cdot U^\dagger(p, q) = \delta_{nq}\, U(m, p)$$

   iv) Definimos o *Traço* de um operador por

   $$Tr\ \ (B) \equiv \sum_n \ \langle a_n |B| a_n\rangle \ \ .$$

   Calcule $Tr\{U(m, n)\}$;

   v) Seja B um outro operador com elementos de matriz $B_{mn} = \langle a_m |B| a_n\rangle$. Mostre a relação

   $$B = \sum_{m,n} \ B_{mn} \cdot U(m, n) \ ;$$

   vi) Mostre também a relação

   $$B_{pq} = Tr \left\{ BU^\dagger (p, q) \right\} \ \ .$$

   ■

2. **Desigualdades famosas**

   Sejam $|\alpha >$ e $|\beta >$ dois *kets* arbitrários, com $|\gamma >= |\alpha > + |\beta >$.

(a) Derive a desigualdade de Schwartz:

$$|\langle\alpha|\beta\rangle| \ \leq \ \sqrt{\langle\alpha|\alpha\rangle}\sqrt{\langle\beta|\beta\rangle}\ .$$

(b) Derive a desigualdade triangular:

$$\sqrt{\langle\gamma|\gamma\rangle} \ \leq \ \ \sqrt{\langle\alpha|\alpha\rangle}+\sqrt{\langle\beta|\beta\rangle}\ . \qquad \blacksquare$$

3. **Matrizes de Pauli**

Seja um espaço complexo de dimensão 2, com uma base normalizada $\{|1>,\ |2>\}$. Neste espaço temos operadores cujas representações matriciais são

$$\sigma_x=\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y=\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z=\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1}$$

Estas matrizes são chamadas de *Matrizes de Pauli*. Elas aparecem na nossa construcão dos operadores de spin 1/2 usando como base os autoestados de S_z.

a) Verifique que as matrizes acima são hermiteanas. Calcule os autovalores de todas as três e explique fisicamente o resultado. Calcule os autovetores em relação à base $\{|1>,\ |2>\}$.

b) Sempre usando a base $\{|1>,\ |2>\}$, encontre as matrizes que representam os projetores sobre os autovetores para as três matrizes de (1). Verifique que são satisfeitos os requerimentos para operadores de projeção. $\blacksquare$

4. **Método de Schmidt**

As funções potências

$$\{1, x, x^2, x^3, ..., x^n, ...\}, \tag{2}$$

são uma base para construir polinômios de grau arbitrário (aqui pensamos no caso de $n \to \infty$). Restringimos o domínio dessas funções para o intervalo real $[-1, 1]$, onde é definido um produto escalar por:

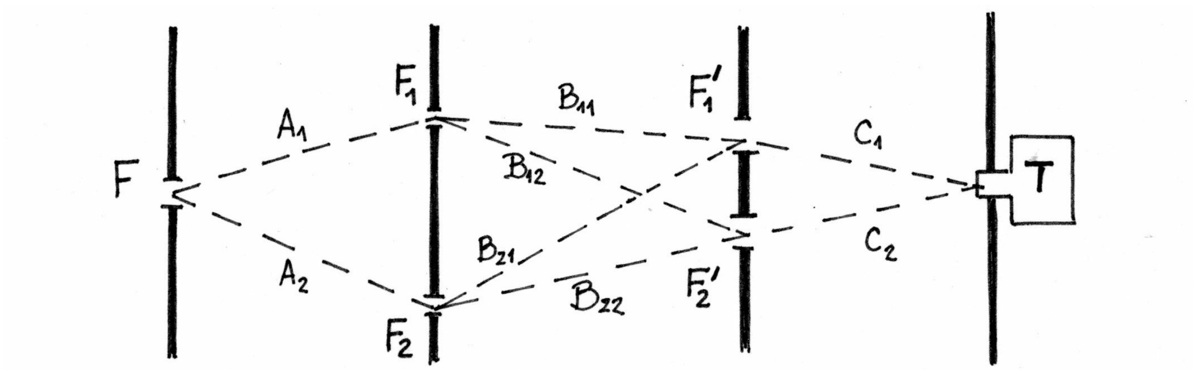
$$\langle f|g\rangle \ \equiv \ \int_{-1}^{1} \ dt\ f(t)g(t), \tag{3}$$

para duas funções f, g reais arbitrárias definidas no intervalo $[-1, 1]$. Certamente, com esse produto escalar, as funções de (2) não são ortogonais. Use o método de ortogonalização de Schmidt para construir polinômios ortogonais. Veja se pode reconher as funções obtidas.

Observação: A definição (3) satisfaz todos os requerimentos de um 'produto escalar'. $\blacksquare$

5. **Interferômetro multi-fendas**

Mostramos na figura o arranjo de um interferômetro, com um colimador em F e dois anteparos entre a fonte F e o detetor em T. Os anteparos possuem fendas que chamamos F_1, F_2, F_1' e F_2' , como mostrado na figura. As partículas são emitidas em F e coletadas no detetor T. Imaginamos que apenas uma partícula atravessa o interferômetro cada vez (intensidade do feixe baixa). As linhas tracejadas são apenas "guias para os olhos".



Figura

A figura também mostra todas as amplitudes de onda associadas. Por exemplo, A_1 é a amplitude da onda na fenda F_1 quando a amplitude no colimador F é igual a 1. B_{12} é a amplitude na fenda F_2' quando a amplitude na fenda F_1 é igual a 1 e nula na fenda F_2 (para determinar essa amplitude é necessário fechar a fenda F_2, para ter certeza que a partícula passou por F_1). C_1 é a amplitude no detetor T quando a amplitude na fenda F_1' é igual a 1 e nula na fenda F_2'. As outras amplitudes são definidas da mesma forma. Elas são chamadas *Amplitudes de Transferência* porque descreven a propagação da onda desde F até T. Em geral, as amplitudes são complexas. Em Mecânica Quântica, o Princípio de Superposição se aplica para as amplitudes e as probabilidades dos diversos eventos são obtidas tomando o módulo quadrado das correspondentes amplitudes. Exemplo, $P_{12} = |B_{12}|^2$ é a probabilidade da partícula passar pela fenda F_2' tendo passado pela fenda F_1 com probabilidade 1.

(a) Com todas as fendas abertas, qual é a probabilidade P de uma partícula que passou pela fenda F emergir na fenda do detetor T?

(b) A mesma pergunta, com a fenda F_1 fechada.

(c) A mesma pergunta de cima, com as fendas F_1 e F_1' fechadas.

Em todos os casos, indique os termos de interferência. ■

6. **Problemas de #1 a #16 do livro do Sakurai, Cap. 1 (ver anexo).**

   Para os problemas anexos, o símbolo

$$\vec{\boldsymbol{\sigma}} \cdot \vec{a}$$

   deve ser interpretado como

$$\vec{\boldsymbol{\sigma}} \cdot \vec{a} = \boldsymbol{\sigma}_x a_x + \boldsymbol{\sigma}_y a_y + \boldsymbol{\sigma}_z a_z,$$

   onde (a_x, a_y, a_z) são números, e as $(\boldsymbol{\sigma}_x, \boldsymbol{\sigma}_y, \boldsymbol{\sigma}_z)$ são as matrizes de Pauli definidas em (1). Portanto, o símbolo $(\vec{\boldsymbol{\sigma}} \cdot \vec{a})$ é uma matriz.

   O símbolos $[A, B]$ (*comutador*) e $\{A, B\}$ (*anticomutador*), para dois operadores A e B arbitrários, são definidos como:

$$[A, B] \equiv AB - BA \ ,$$

$$\{A, B\} \equiv AB + BA \ .$$

■

Problems

1. Prove

$$[AB, CD] = -AC\{D, B\} + A\{C, B\}D - C\{D, A\}B + \{C, A\}DB.$$

2. Suppose a 2×2 matrix X (not necessarily Hermitian, nor unitary) is written as

$$X = a_0 + \boldsymbol{\sigma} \cdot \mathbf{a},$$

where a_0 and $a_{1,2,3}$ are numbers.
a. How are a_0 and a_k $(k = 1, 2, 3)$ related to $\mathrm{tr}(X)$ and $\mathrm{tr}(\sigma_k X)$?
b. Obtain a_0 and a_k in terms of the matrix elements X_{ij}.

3. Show that the determinant of a 2×2 matrix $\boldsymbol{\sigma} \cdot \mathbf{a}$ is invariant under

$$\boldsymbol{\sigma} \cdot \mathbf{a} \to \boldsymbol{\sigma} \cdot \mathbf{a}' \equiv \exp\left(\frac{i\boldsymbol{\sigma} \cdot \hat{\mathbf{n}}\phi}{2}\right) \boldsymbol{\sigma} \cdot \mathbf{a} \exp\left(\frac{-i\boldsymbol{\sigma} \cdot \hat{\mathbf{n}}\phi}{2}\right).$$

Find a'_k in terms of a_k when $\hat{\mathbf{n}}$ is in the positive z-direction and interpret your result.

4. Using the rules of bra-ket algebra, prove or evaluate the following:
a. $\mathrm{tr}(XY) = \mathrm{tr}(YX)$, where X and Y are operators;
b. $(XY)^\dagger = Y^\dagger X^\dagger$, where X and Y are operators;
c. $\exp[if(A)] = ?$ in ket-bra form, where A is a Hermitian operator whose eigenvalues are known;
d. $\sum_{a'} \psi^*_{a'}(\mathbf{x}') \psi_{a'}(\mathbf{x}'')$, where $\psi_{a'}(\mathbf{x}') = \langle \mathbf{x}' | a' \rangle$.

5. a. Consider two kets $|\alpha\rangle$ and $|\beta\rangle$. Suppose $\langle a'|\alpha\rangle$, $\langle a''|\alpha\rangle, \dots$ and $\langle a'|\beta\rangle$, $\langle a''|\beta\rangle, \dots$ are all known, where $|a'\rangle$, $|a''\rangle, \dots$ form a complete set of base kets. Find the matrix representation of the operator $|\alpha\rangle\langle\beta|$ in that basis.
   b. We now consider a spin $\frac{1}{2}$ system and let $|\alpha\rangle$ and $|\beta\rangle$ be $|s_z = \hbar/2\rangle$ and $|s_x = \hbar/2\rangle$, respectively. Write down explicitly the square matrix that corresponds to $|\alpha\rangle\langle\beta|$ in the usual (s_z diagonal) basis.
6. Suppose $|i\rangle$ and $|j\rangle$ are eigenkets of some Hermitian operator A. Under what condition can we conclude that $|i\rangle + |j\rangle$ is also an eigenket of A? Justify your answer.
7. Consider a ket space spanned by the eigenkets $\{|a'\rangle\}$ of a Hermitian operator A. There is no degeneracy.
   a. Prove that

$$\prod_{a'} (A - a')$$

   is the null operator.
   b. What is the significance of

$$\prod_{a'' \neq a'} \frac{(A - a'')}{(a' - a'')}?$$

   c. Illustrate (a) and (b) using A set equal to S_z of a spin $\frac{1}{2}$ system.
8. Using the orthonormality of $|+\rangle$ and $|-\rangle$, prove

$$[S_i, S_j] = i\varepsilon_{ijk}\hbar S_k, \qquad \{S_i, S_j\} = \left(\frac{\hbar^2}{2}\right)\delta_{ij},$$

   where

$$S_x = \frac{\hbar}{2}(|+\rangle\langle-| + |-\rangle\langle+|), \qquad S_y = \frac{i\hbar}{2}(-|+\rangle\langle-| + |-\rangle\langle+|),$$

$$S_z = \frac{\hbar}{2}(|+\rangle\langle+| - |-\rangle\langle-|).$$

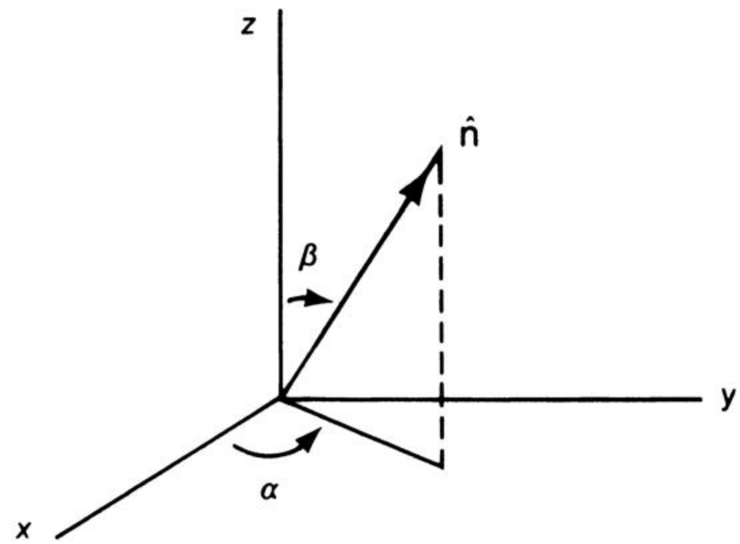
9. Construct $|\mathbf{S}\cdot\hat{\mathbf{n}}; +\rangle$ such that

$$\mathbf{S}\cdot\hat{\mathbf{n}}|\mathbf{S}\cdot\hat{\mathbf{n}}; +\rangle = \left(\frac{\hbar}{2}\right)|\mathbf{S}\cdot\hat{\mathbf{n}}; +\rangle$$

   where $\hat{\mathbf{n}}$ is characterized by the angles shown in the figure. Express your answer as a linear combination of $|+\rangle$ and $|-\rangle$. [*Note*: The answer is

$$\cos\left(\frac{\beta}{2}\right)|+\rangle + \sin\left(\frac{\beta}{2}\right)e^{i\alpha}|-\rangle.$$

   But do not just verify that this answer satisfies the above eigenvalue equation. Rather, treat the problem as a straightforward eigenvalue



problem. Also do not use rotation operators, which we will introduce later in this book.]

10. The Hamiltonian operator for a two-state system is given by

$$H = a\left(|1\rangle\langle 1| - |2\rangle\langle 2| + |1\rangle\langle 2| + |2\rangle\langle 1|\right),$$

where a is a number with the dimension of energy. Find the energy eigenvalues and the corresponding energy eigenkets (as linear combinations of $|1\rangle$ and $|2\rangle$).

11. A two-state system is characterized by the Hamiltonian

$$H = H_{11}|1\rangle\langle 1| + H_{22}|2\rangle\langle 2| + H_{12}\left[|1\rangle\langle 2| + |2\rangle\langle 1|\right]$$

where H_{11}, H_{22}, and H_{12} are real numbers with the dimension of energy, and $|1\rangle$ and $|2\rangle$ are eigenkets of some observable ($\neq H$). Find the energy eigenkets and corresponding energy eigenvalues. Make sure that your answer makes good sense for $H_{12} = 0$. (You need not solve this problem from scratch. The following fact may be used without proof:

$$(\mathbf{S}\cdot\hat{\mathbf{n}})|\hat{\mathbf{n}};+\rangle = \frac{\hbar}{2}|\hat{\mathbf{n}};+\rangle,$$

with $|\hat{\mathbf{n}};+\rangle$ given by

$$|\hat{\mathbf{n}};+\rangle = \cos\frac{\beta}{2}|+\rangle + e^{i\alpha}\sin\frac{\beta}{2}|-\rangle,$$

where β and α are the polar and azimuthal angles, respectively, that characterize $\hat{\mathbf{n}}$.)

12. A spin $\frac{1}{2}$ system is known to be in an eigenstate of $\mathbf{S}\cdot\hat{\mathbf{n}}$ with eigenvalue $\hbar/2$, where $\hat{\mathbf{n}}$ is a unit vector lying in the xz-plane that makes an angle γ with the positive z-axis.

a. Suppose S_x is measured. What is the probability of getting $+\hbar/2$?
b. Evaluate the dispersion in S_x, that is,

$$\langle (S_x - \langle S_x \rangle)^2 \rangle.$$

(For your own peace of mind check your answers for the special cases $\gamma = 0$, $\pi/2$, and π.)

13. A beam of spin $\frac{1}{2}$ atoms goes through a series of Stern-Gerlach-type measurements as follows:
    a. The first measurement accepts $s_z = \hbar/2$ atoms and rejects $s_z = -\hbar/2$ atoms.
    b. The second measurement accepts $s_n = \hbar/2$ atoms and rejects $s_n = -\hbar/2$ atoms, where s_n is the eigenvalue of the operator $\mathbf{S}\cdot\hat{\mathbf{n}}$, with $\hat{\mathbf{n}}$ making an angle β in the xz-plane with respect to the z-axis.
    c. The third measurement accepts $s_z = -\hbar/2$ atoms and rejects $s_z = \hbar/2$ atoms.

    What is the intensity of the final $s_z = -\hbar/2$ beam when the $s_z = \hbar/2$ beam surviving the first measurement is normalized to unity? How must we orient the second measuring apparatus if we are to maximize the intensity of the final $s_z = -\hbar/2$ beam?

14. A certain observable in quantum mechanics has a 3×3 matrix representation as follows:

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

    a. Find the normalized eigenvectors of this observable and the corresponding eigenvalues. Is there any degeneracy?
    b. Give a physical example where all this is relevant.

15. Let A and B be observables. Suppose the simultaneous eigenkets of A and B $\{|a', b'\rangle\}$ form a *complete* orthonormal set of base kets. Can we always conclude that

$$[A, B] = 0?$$

    If your answer is yes, prove the assertion. If your answer is no, give a counterexample.

16. Two Hermitian operators anticommute:

$$\{A, B\} = AB + BA = 0.$$

    Is it possible to have a simultaneous (that is, common) eigenket of A and B? Prove or illustrate your assertion.