Physics 143a – Workshop 1

On Vectors, Matrices, Eigenvalues, Eigenvectors, Spin Kets, and Hermitian Operators

Week Summary

- **Vectors and Basis Vectors:** A set of vectors $\{\hat{e}_j\}$ is said to *span* $\mathbb{R}^n$, if they satisfy

$$\hat{e}_i \cdot \hat{e}_j = \delta_{ij} \quad \text{[Orthonomality]}, \tag{1}$$

$$\sum_{i=1}^{n} \hat{e}_i^T \hat{e}_i = \mathbb{I} \quad \text{[Completeness]}. \tag{2}$$

  Only vectors which span $\mathbb{R}^n$ can act as the *basis vectors* for an arbitrary vector $\vec{v} \in \mathbb{R}^n$. The arbitrary vector $\vec{v}$ can then be written as a linear combination of the basis vectors: $\vec{v} = \sum_{j=1}^{n} c_j \vec{e}_j$

- **Square Matrices:** An $n \times n$ matrix $\hat{A}$ has four important mathematical quantities:
  - **Eigenvalues/vectors:** The *eigenvalue* λ_i and *eigenvector* $\vec{u}_i$ of $\hat{A}$ are the complex number and vector, respectively, that satisfy

$$\hat{A}\vec{v}_i = \lambda_i \vec{v}_i. \tag{3}$$

    The eigenvalues of $\hat{A}$ are found by solving the n^{th} order polynomial equation

$$\det(\hat{A} - \lambda \mathbb{I}) = 0, \tag{4}$$

    and the eigenvectors are found by solving for the vectors $\vec{v}_i$ for each $\lambda = \lambda_i$ solution to Eq.(4) satisfying

$$(A - \lambda_i)\vec{v}_i = 0. \tag{5}$$

  - **Trace:** sum of the diagonal elements of the matrix; sum of the eigenvalues: $\text{Tr}\, A = \sum_j A_{jj} = \sum_j \lambda_j$.
  - **Determinant:** has no simple qualitative definition; product of eigenvalues: $\det A = \prod_i \lambda_i$.

- **Spin Ket in Arbitrary Direction:** In the $(x,\ y,\ z)$ coordinate system with an azimuthal angle θ and an auxiliary angle ϕ, the state ket for an electron with spin pointing in the $\mathbf{n} = \sin\theta\cos\phi\mathbf{x} + \sin\theta\sin\phi\mathbf{y} + \cos\theta\mathbf{z}$ direction is

$$|+, \mathbf{n}(\theta,\phi)\rangle = \cos\frac{\theta}{2}|+,\mathbf{z}\rangle + \sin\frac{\theta}{2}e^{i\phi}|-,\mathbf{z}\rangle, \tag{6}$$

  which is written in the $\{|+,\mathbf{z}\rangle, |-,\mathbf{z}\rangle\}$ basis. The phase in this expression *is* physically important in determining the probability for $\hat{S}_x$ and $\hat{S}_y$ (but not $\hat{S}_z$) measurements.

- **Hermitian Observables:** An operator $\hat{A}$ is hermitian if it is equal to its hermitian conjugate:

$$\hat{A} = \hat{A}^\dagger. \tag{7}$$

  For matrix operators, the hermitian conjugate is the complex conjugate of the transpose. Hermitian operators (such as the Hamiltonian and Spin operator) have real eigenvalues, and all physical observables in quantum mechanics are represented by hermitian operators.

1 Problems

1. **Charge Conjugation**
   If $|\psi_q\rangle$ is any eigenstate of the electric charge operator Q corresponding to eigenvalue q, that is to say

$$Q|\psi_q\rangle = q|\psi_q\rangle, \tag{8}$$

   then the "charge conjugation" operator C applied to $|\psi_q\rangle$ leads to an eigenstate $|\psi_{-q}\rangle$ of Q corresponding to eigenvalue $-q$:

$$C|\psi_q\rangle = |\psi_{-q}\rangle. \tag{9}$$

   (a) Find the eigenvalues of the operator $CQ + QC$.
   (b) Can a state simultaneously be an eigenstate of C and of Q?

2. **Commutators and degenerate Eigenvalue**
   Let us take $N \times N$ matrices A, B, and C satisfying

$$[A, B] = 0, \quad [A, C] = 0, \quad [B, C] \neq 0. \tag{10}$$

   Show that at least one eigenvalue of A is degenerate. Why is $[B, C] \neq 0$ important in establishing this?

3. **NH_3 in an Electric Field**
   An ammonia molecule has an electric dipole moment d which points away from the plane of the hydrogen atoms and toward the lone nitrogen atom. The ammonia molecule can be approximated to exist be in one of two symmetric states:

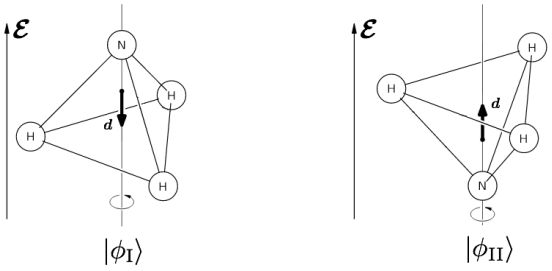

Figure 1: Feynman's depiction of two states of NH_3 molecule in an electric field.

   When the molecule is placed in a non-uniform electric field $\mathcal{E}$, the dipole moment leads to an energy perturbation of the molecule. We can write the *Hamiltonian* (which we will learn represents the energy) of the ammonia molecule in a non-uniform field as

$$H = \begin{pmatrix} E_0 + d\mathcal{E} & -A \\ -A & E_0 - d\mathcal{E} \end{pmatrix} \tag{11}$$

   where E_0 and A have units of energy, the Hamiltonian is in the $\{|\varphi_1\rangle, |\varphi_2\rangle\}$ basis.

   (a) Compute the energy eigenvalues E_+ and E_- of this Hamiltonian matrix. (You do not need to compute the corresponding states $|\varphi_+\rangle$ and $|\varphi_-\rangle$.)
   (b) Taking $|d\mathcal{E}| \ll |A|$, compute the energy eigenvalues to lowest order in $\mathcal{E}$.
   (c) Let's interpret these energy eigenvalues as potential energies. We prepare a beam of NH_3 molecules in the state $|\psi\rangle = \frac{1}{\sqrt{2}}|\varphi_-\rangle + \frac{1}{\sqrt{2}}|\varphi_+\rangle$, and pass the beam through a monotonically increasing (in the z direction) electric field, $\mathcal{E}(z)$, which is perpendicular to the beam direction . (Assume the electric dipoles of the molecule are parallel to the field). What happens to the beam in the field region?

2 Solution

1. (a) We can find the eigenvalues of $CQ+QC$ by positing a guess for the eigenvector and determining its eigenvalues. Since the charge operator kets $|\psi_q\rangle$ are the only states we have in this problem, they are the natural choice. Operating on these kets with the given operator, we find

$$\begin{aligned}(CQ+QC)\,|\psi_q\rangle &= CQ|\psi_q\rangle + QC|\psi_q\rangle \\ &= qC|\psi_q\rangle + Q|\psi_{-q}\rangle \\ &= q|\psi_{-q}\rangle - q|\psi_q\rangle = 0. \end{aligned} \tag{12}$$

Thus, we find the degenerate eigenvalue of $CQ+QC$ is 0 with the eigenvector being any eigenket $|\psi_q\rangle$ of Q.

We can play around with this question a bit. What if we were asked for the eigenvalues of $C^2Q + QC^2$? In this case, since $C^2 = \mathbb{I}$, the eigenvalues of $C^2Q + QC^2$ are simply the eigenvalues of $2Q$, namely, 2q for an eiegenket $|\psi_{-q}\rangle$.

What if we were asked for the eigenvalues of $CQ^2 + Q^2C$? Applying this operator to the ket $|\psi_q\rangle$, we find

$$\begin{aligned}\left(CQ^2+Q^2C\right)|\psi_q\rangle &= CQ^2|\psi_q\rangle + Q^2C|\psi_q\rangle \\ &= q^2C|\psi_q\rangle + Q^2|\psi_{-q}\rangle \\ &= 2q^2|\psi_{-q}\rangle, \end{aligned} \tag{13}$$

which indicates that $|\psi_q\rangle$ is *not* an eigenket of $CQ^2 + Q^2C$. However, the two states

$$|\phi_\pm\rangle = \frac{1}{\sqrt{2}}\left(|\psi_q\rangle \pm |\psi_q\rangle\right), \tag{14}$$

are eigenkets of $CQ^2 + Q^2C$ and both have the eigenvalue $2q$.

(b) There is a state which is simultaneously an eigenket of Q and C if and only if we have $[Q, C] = 0$. Applying the ket $|\psi_q\rangle$ to this commutator we find

$$\begin{aligned}[Q,C]|\psi_{-q}\rangle &= QC|\psi_q\rangle - CQ|\psi_q\rangle \\ &= Q|\psi_{-q}\rangle - q|\psi_{-q}\rangle \\ &= -2q|\psi_{-q}\rangle. \end{aligned} \tag{15}$$

Eq.(15) implies $[Q, C] \neq 0$, and no state can simultaneously be an eigenket of Q and C.

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2. We can demonstrate this by contradiction. First we will assume that A has N distinct eigenvalues λ_i and corresponding eigenvectors $\vec{v}_i$ defined via

$$\hat{A}\vec{v}_i = \lambda_i\vec{v}_i. \tag{16}$$

By the commutation relations $[\hat{A}, \hat{B}] = 0$ and $[\hat{A}, \hat{C}] = 0$, we find

$$\hat{A}\left(\hat{B}\vec{v}_i\right) = \lambda_i\left(\hat{B}\vec{v}_i\right) \tag{17}$$

$$\hat{A}\left(\hat{C}\vec{v}_i\right) = \lambda_i\left(\hat{C}\vec{v}_i\right), \tag{18}$$

which are two eigenvalue equations for eigenvectors $\hat{B}\vec{v}_i$ and $\hat{C}\vec{v}_i$. But, if we are to assume that $\hat{A}$ has distinct (i.e., non-degenerate) eigenvalues then the vectors $\hat{B}\vec{v}_i$ and $\hat{C}\vec{v}_i$ cannot represent eigenvectors different from $\vec{v}_i$. Therefore, both vectors must be proportional to $\vec{v}_i$. Defining the proportionality constants as γ_i and δ_i for $\hat{B}\vec{v}_i$ and $\hat{C}\vec{v}_i$, respectively, we find

$$\hat{B}\vec{v}_i = \gamma_i\vec{v}_i \tag{19}$$

$$\hat{C}\vec{v}_i = \delta_i\vec{v}_i, \tag{20}$$

which are eigenvalue equations for $\hat{B}$ and $\hat{C}$ in terms of their mutual set of eigenvectors $\{\vec{v}_i\}$. However, if $\hat{B}$ and $\hat{C}$ share an eigenspace, then their commutator must be zero as can be seen from

$$\begin{aligned}[\hat{B},\hat{C}]\vec{v}_i &= \hat{B}\hat{C}\vec{v}_i - \hat{C}\hat{B}\vec{v}_i \\ &= (\delta_i\gamma_i - \gamma_i\delta_i)\vec{v}_i = 0\end{aligned} \tag{21}$$

Thus we cannot both have $\hat{A}$ with non-degenerate eigenvalues and the three conditions $[\hat{A},\hat{B}] = 0$, $[\hat{A},\hat{C}] = 0$, and $[\hat{B},\hat{C}] \neq 0$.

To complete the demonstration, we engineer this argument in reverse: If $[\hat{B},\hat{C}] \neq 0$, then $\hat{B}$ and $\hat{C}$ do not share a set of eigenvectors and thus $\hat{B}\vec{v}_i$ and $\hat{C}\vec{v}_i$ must represent distinct eigenvectors from each other. Thus Eq.(17) and Eq.(18) represent two eigenvector-eigenvalue equations of $\hat{A}$ defined by two eigenvectors but only a single eigenvalue λ_i. Thus, at least one eigenvalue, λ_i, of $\hat{A}$ is degenerate[1].

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3. (a) To compute the energy eigenvalues of the Hamiltonian, we employ the eigenvalue formula for a 2×2 matrix:

$$\begin{aligned}E_\pm &= \frac{\mathrm{Tr}\, H \pm \sqrt{(\mathrm{Tr}\, H)^2 - 4\det H}}{2} \\ &= \frac{2E_0 \pm \sqrt{4E_0^2 - 4(E_0^2 - d^2\mathcal{E}^2 - A^2)}}{2} \\ &= E_0 \pm A\sqrt{1 + \frac{d^2\mathcal{E}^2}{A^2}}\end{aligned} \tag{22}$$

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(b) If we take $|d\mathcal{E}| \ll A$, then we can expand Eq.(22) to obtain

$$\begin{aligned}E_\pm &= E_0 \pm A\sqrt{1 + \frac{d^2\mathcal{E}^2}{A^2}} \\ &= E_0 \pm A\left(1 + \frac{d^2\mathcal{E}^2}{2A^2}\right).\end{aligned} \tag{23}$$

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(c) If we, were to interpret the above computed energies as *potential energies*, then the potential energy for particles in the state $|\varphi_\pm\rangle$ in a non electric field $\mathcal{E}(z)$ would be

$$U_\pm(z) = \pm\frac{d^2\mathcal{E}^2(z)}{2A} \tag{24}$$

[1] An interesting question is why does this result only apply to "at least one eigenvalue"? In this derivation we did not select out any particular eigenvalue for the analysis, so shouldn't the result imply that all eigenvalues are degenerate?

where we ignored the z independent terms which don't affect dynamics. By the definition of force as $F_z(z) = -U'(z)$, we thus find that the force on the particles in the $|\varphi_+\rangle$ state is

$$F_z^-(z) = -\frac{d^2}{2A}\frac{d}{dz}\mathcal{E}^2(z) < 0, \tag{25}$$

and the force on the particles in the $|\varphi_-\rangle$ state is

$$F_z^-(z) = +\frac{d^2}{2A}\frac{d}{dz}\mathcal{E}^2(z) > 0, \tag{26}$$

that is the particles in the $|\varphi_+\rangle$ and $|\varphi_-\rangle$ states feel equal and opposite forces which push them away from the collimated beam. Thus if we have a beam of $N \gg 1$ NH_3 molecules, each of which is prepared in the state $|\psi\rangle = \frac{1}{\sqrt{2}}|\varphi_-\rangle + \frac{1}{\sqrt{2}}|\varphi_+\rangle$, then as this beam passes through an electric field pointing in a direction perpendicular to the beam (and increasing in that direction) then about $N/2$ of the molecules will be deflected upwards and $N/2$ of the molecules will be deflected downwards.

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