Today in Physics 237: operator and matrix algebra in Dirac notation

- Eigenvalues and eigenvectors of projection operators
- Rules of operator matrix-element algebra
    - Matrix elements of functions of operators
- An eigenvalue problem in a two-state system
- Changing bases in Dirac notation

$$\left(1+\hat{Q}\right)^p = \sum_{n=0}^{\infty} \frac{p!}{n!\left(p-n\right)!} = 1 + p\hat{Q} + \frac{p\left(p-1\right)}{2!}\hat{Q}^2 + \frac{p\left(p-1\right)\left(p-2\right)}{3!}\hat{Q}^3 + \ldots$$

$$\frac{1}{1-\hat{Q}} = \sum_{n=0}^{\infty} \hat{Q}^n = 1 + \hat{Q} + \hat{Q}^2 + \hat{Q}^3 + \hat{Q}^4 + \ldots$$

$$\ln\left(1+\hat{Q}\right) = \sum_{n=0}^{\infty} \left(-1\right)^n \frac{x^{n+1}}{n+1} = \hat{Q} - \frac{1}{2}\hat{Q}^2 + \frac{1}{3}\hat{Q}^3 - \frac{1}{4}\hat{Q}^4 + \ldots$$

$$\sin\hat{Q} = \sum_{n=0}^{\infty} \left(-1\right)^n \frac{x^{2n+1}}{\left(2n+1\right)!} = \hat{Q} - \frac{1}{6}\hat{Q}^3 + \frac{1}{120}\hat{Q}^5 - \ldots$$

Example: projection operators

G&S problem 3.23. Show that projection operators are **idempotent**: that $\hat{P}^2 = \hat{P}$. Determine the eigenvalues of $\hat{P}$, and characterize its eigenvectors.

- Suppose $|\beta\rangle$ and $|\alpha\rangle$ are normalized state vectors, and project $|\beta\rangle$ on $|\alpha\rangle$ twice:

$$\hat{P}^2|\beta\rangle = \hat{P}\left(\hat{P}|\beta\rangle\right) = \hat{P}\left(|\alpha\rangle\langle\alpha|\beta\rangle\right) = \langle\alpha|\beta\rangle\hat{P}|\alpha\rangle = \langle\alpha|\beta\rangle|\alpha\rangle\cancelto{1}{\langle\alpha|\alpha\rangle} = \langle\alpha|\beta\rangle|\alpha\rangle = \hat{P}|\beta\rangle \quad \boxed{\text{, q.e.d.}}$$

  Similarly one can show that $n > 1$ operations of a given projection operator gives the same result as just one.

- Eigenvalue: $\hat{P}|\gamma\rangle = \lambda|\gamma\rangle$ and $\hat{P}^2|\gamma\rangle = \lambda\hat{P}|\gamma\rangle = \lambda^2|\gamma\rangle$. So $\lambda^2 = \lambda$, for which the only solutions are $\boxed{\lambda = 1 \text{ and } \lambda = 0 \quad .}$

- Eigenvectors: here $\hat{P} = |\alpha\rangle\langle\alpha|$ is the operator for projection onto $|\alpha\rangle$; as one can see from above, $\boxed{\text{any multiple of } |\alpha\rangle}$ will do for $\lambda = 1$:

$$\hat{P}\left(c|\alpha\rangle\right) = c|\alpha\rangle\langle\alpha|\alpha\rangle = 1 \times c|\alpha\rangle \quad .$$

  And $\boxed{\text{any } |\beta\rangle \text{ orthogonal to } |\alpha\rangle}$ will do for $\lambda = 0$: $|\alpha\rangle\langle\alpha|\beta\rangle = 0 \times |\alpha\rangle$.

Rules of operator matrix-element algebra

- Operators act on state vectors as the matrices act on vectors:

$$\left|\beta\right\rangle = \sum_n b_n \left|e_n\right\rangle \quad , \quad \left|\alpha\right\rangle = \sum_n a_n \left|e_n\right\rangle \quad \left|\beta\right\rangle = \hat{Q}\left|\alpha\right\rangle = \sum_n a_n \hat{Q}\left|e_n\right\rangle \quad ;$$

$$\Rightarrow \quad b_m = \left\langle e_m\right| \sum_n a_n \hat{Q}\left|e_n\right\rangle = \sum_n a_n \left\langle e_m\right|\hat{Q}\left|e_n\right\rangle = \sum_n Q_{mn} a_n \leftrightarrow \boldsymbol{\beta} = \overleftrightarrow{\boldsymbol{Q}} \cdot \boldsymbol{\alpha} \quad .$$

- So do products of operators, e.g. $\left|\gamma\right\rangle = \hat{P}\hat{Q}\left|\alpha\right\rangle = \sum_n a_n \hat{P}\hat{Q}\left|e_n\right\rangle$:

$$c_m = \left\langle e_m\right| \sum_n a_n \hat{P}\hat{Q}\left|e_n\right\rangle = \sum_n \sum_p a_n \left\langle e_m\right|\hat{P}\left|e_p\right\rangle\left\langle e_p\right|\hat{Q}\left|e_n\right\rangle = \sum_n \sum_p P_{mp} Q_{pn} a_n \leftrightarrow \boldsymbol{\gamma} = \overleftrightarrow{\boldsymbol{P}} \cdot \overleftrightarrow{\boldsymbol{Q}} \cdot \boldsymbol{\alpha} \quad .$$

- Algebra with functions of operators are just like that with products of operators, as long as we can expand the function in a power series. Frequently appearing, for example:

$$e^{\hat{Q}} = \sum_{n=0}^{\infty} \frac{\hat{Q}^n}{n!} = 1 + \hat{Q} + \frac{1}{2!}\hat{Q}^2 + \frac{1}{3!}\hat{Q}^3 + \ldots$$

Rules of operator matrix-element algebra (continued)

- A few others you will probably run into:

$$\left(1+\hat{Q}\right)^p = \sum_{n=0}^{\infty} \frac{p!\hat{Q}^n}{n!\left(p-n\right)!} = 1 + p\hat{Q} + \frac{p\left(p-1\right)}{2!}\hat{Q}^2 + \frac{p\left(p-1\right)\left(p-2\right)}{3!}\hat{Q}^3 + \ldots$$

$$\frac{1}{1-\hat{Q}} = \sum_{n=0}^{\infty} \hat{Q}^n = 1 + \hat{Q} + \hat{Q}^2 + \hat{Q}^3 + \hat{Q}^4 + \ldots$$

(which may not converge)

$$\ln\left(1+\hat{Q}\right) = \sum_{n=0}^{\infty} (-1)^n \frac{x^{n+1}}{n+1} = \hat{Q} - \frac{1}{2}\hat{Q}^2 + \frac{1}{3}\hat{Q}^3 - \frac{1}{4}\hat{Q}^4 + \ldots$$

$$\sin\hat{Q} = \sum_{n=0}^{\infty} (-1)^n \frac{x^{2n+1}}{(2n+1)!} = \hat{Q} - \frac{1}{6}\hat{Q}^3 + \frac{1}{120}\hat{Q}^5 - \ldots$$

Rules of operator matrix-element algebra (continued)

Example: Expand $e^{i\hat{A}}\hat{B}e^{-i\hat{A}}$ into products of $\hat{A}$ and $\hat{B}$, and simplify.

$$e^{iA}\hat{B}e^{-iA}=\left(\sum_n\frac{(i\hat{A})^n}{n!}\right)\left(\sum_m\frac{(-1)^m\hat{B}(i\hat{A})^m}{m!}\right)=\left(1+(i\hat{A})+\frac{1}{2!}(i\hat{A})^2+\ldots\right)\left(\hat{B}-\hat{B}(i\hat{A})+\frac{1}{2!}\hat{B}(i\hat{A})^2-\ldots\right)$$

$$=\hat{B}+(i\hat{A})\hat{B}+\frac{1}{2!}(i\hat{A})^2\hat{B}-\hat{B}(i\hat{A})-(i\hat{A})\hat{B}(i\hat{A})-\frac{1}{2!}(i\hat{A})^2\hat{B}(i\hat{A})+\frac{1}{2!}\hat{B}(i\hat{A})^2+\frac{1}{2!}(i\hat{A})\hat{B}(i\hat{A})^2+\frac{1}{2!^2}(i\hat{A})^2\hat{B}(i\hat{A})^2+\ldots$$

$$=\hat{B}+i(\hat{A}\hat{B}-\hat{B}\hat{A})+\frac{i^2}{2!}\left(\hat{A}^2\hat{B}-2!\hat{A}\hat{B}\hat{A}+\hat{B}\hat{A}^2\right)+\ldots$$

keeping terms through third order
in the products of $\hat{A}$ and $\hat{B}$

$$=\hat{B}+i[\hat{A},\hat{B}]+\frac{i^2}{2!}\left(\hat{A}^2\hat{B}-\hat{A}\hat{B}\hat{A}-\hat{A}\hat{B}\hat{A}+\hat{B}\hat{A}^2\right)+\ldots=\hat{B}+i[\hat{A},\hat{B}]+\frac{i^2}{2!}[\hat{A},(\hat{A}\hat{B}-\hat{B}\hat{A})]+\ldots$$

$$\boxed{=\hat{B}+i[\hat{A},\hat{B}]+\frac{i^2}{2!}[\hat{A},[\hat{A},\hat{B}]]+\ldots+\frac{i^n}{n!}\overbrace{\left[\hat{A},\left[\hat{A},\ldots\left[\hat{A},[\hat{A},\hat{B}]\right]\ldots\right]\right]}^{n\text{ brackets}}+\ldots}$$

Example of a two-state system and its Hamiltonian

G&S example 3.8. Imagine a system in which there are two discrete, linearly independent states, and Hamiltonian $\overleftrightarrow{\boldsymbol{H}}$:

$$|1\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad , \quad |2\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad , \quad \overleftrightarrow{\boldsymbol{H}} = \begin{bmatrix} h & g \\ g & h \end{bmatrix} \quad ,$$

where g and h are real constants. The most general state is (of course) a normalized linear combination of $|1\rangle$ and $|2\rangle$:

$$|S(t)\rangle = a|1\rangle + b|2\rangle \quad , \quad |a|^2 + |b|^2 = 1 \quad .$$

The system is in state $|1\rangle$ at t = 0. What is $|S(t)\rangle$?

- We will suppose that we can approach this with a separation solution to the Schrödinger equation, and start by finding the eigenvalues and eigenvectors of the time-independent part:

$$-i\hbar\frac{\partial}{\partial t}S(t) = \hat{H}S(t) \quad , \quad S(t) = se^{-iEt/\hbar} \quad , \quad \hat{H}s = Es \quad .$$

Example of a two-state system and its Hamiltonian (continued)

- As you learned in MATH 165 or 173, the eigenvalues *E* of the matrix $\overleftrightarrow{\boldsymbol{H}}$ are determined by

$$\begin{vmatrix} h-E & g \\ g & h-E \end{vmatrix} = (h-E)^2 - g^2 = E^2 - 2hE + \left(h^2 - g^2\right) = 0 \quad \Rightarrow \quad E = \frac{1}{2}\left(2h \pm \sqrt{4h^2 - 4\left(h^2 - g^2\right)}\right) = \boxed{h \pm g} \ ,$$

and the corresponding eigenvectors by

$$\begin{bmatrix} h & g \\ g & h \end{bmatrix}\begin{bmatrix} \alpha \\ \beta \end{bmatrix} = E\begin{bmatrix} \alpha \\ \beta \end{bmatrix} = (h \pm g)\begin{bmatrix} \alpha \\ \beta \end{bmatrix} \quad \Rightarrow \quad \begin{bmatrix} h\alpha + g\beta \\ g\alpha + h\beta \end{bmatrix} = \begin{bmatrix} h\alpha \pm g\alpha \\ h\beta \pm g\beta \end{bmatrix} \quad \Rightarrow \quad \begin{matrix} \beta = \pm\alpha \\ \alpha = \pm\beta \end{matrix} \ ,$$

which both say that $\beta = \pm\alpha$: $\quad s_\pm = \alpha\begin{bmatrix} 1 \\ \pm 1 \end{bmatrix}$, and normalization gives $\quad 1 = |\alpha|^2 \begin{bmatrix} 1 & \pm 1 \end{bmatrix}\begin{bmatrix} 1 \\ \pm 1 \end{bmatrix} = 2|\alpha|^2 \quad \Rightarrow \quad \alpha = \frac{1}{\sqrt{2}}$.

- So $\boxed{\left|s_+\right\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad \text{and} \quad \left|s_-\right\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix} \quad .}$

Example of a two-state system and its Hamiltonian (continued)

- Now express the initial state, $\begin{bmatrix}1\\0\end{bmatrix}$, as a linear combination of our new eigenvectors, which can be done simply:

$$\left|S(0)\right\rangle=\begin{bmatrix}1\\0\end{bmatrix}=\frac{1}{2}\left(\begin{bmatrix}1\\1\end{bmatrix}+\begin{bmatrix}1\\-1\end{bmatrix}\right)=\frac{1}{\sqrt{2}}\left(\left|s_+\right\rangle+\left|s_-\right\rangle\right)\quad .$$

- Finally, restore the time dependence, multiplying by $e^{-iEt/\hbar}$:

$$\left|S(t)\right\rangle=\frac{1}{\sqrt{2}}\left(e^{-i(h+g)t/\hbar}\left|s_+\right\rangle+e^{-i(h-g)t/\hbar}\left|s_-\right\rangle\right)=\frac{1}{2}\left(e^{-i(h+g)t/\hbar}\begin{bmatrix}1\\1\end{bmatrix}+e^{-i(h-g)t/\hbar}\begin{bmatrix}1\\-1\end{bmatrix}\right)$$

$$=\frac{e^{-iht/\hbar}}{2}\begin{bmatrix}e^{-igt/\hbar}+e^{igt/\hbar}\\e^{-igt/\hbar}-e^{igt/\hbar}\end{bmatrix}=\boxed{e^{-iht/\hbar}\begin{bmatrix}\cos(gt/\hbar)\\-i\sin(gt/\hbar)\end{bmatrix}}\ .$$

Changing bases in Dirac notation

- Projection operators can implement changes of basis sets. For example, the properties of projection operators we noted in Lecture 11:

$$\sum_n |n\rangle\langle n| = 1 \quad , \quad \int dx\, |x\rangle\langle x| = 1 \quad , \quad \int dp\, |p\rangle\langle p| = 1$$

  turn smoothly into

$$|S(t)\rangle = \sum_n |n\rangle\langle n|S(t)\rangle = \sum_n c_n |n\rangle \quad ,$$

$$= \int dx\, |x\rangle\langle x|S(t)\rangle = \int dx\, \Psi(x,t)|x\rangle \quad ,$$

$$= \int dp\, |p\rangle\langle p|S(t)\rangle = \int dp\, \Phi(p,t)|p\rangle \quad .$$

Changing bases in Dirac notation (continued)

G&S example 3.10. Obtain the position operator in the momentum basis by use of projections.

$$\langle p|\hat{x}|S(t)\rangle = \langle p|\hat{x}\int dx\,|x\rangle\langle x|S(t)\rangle$$

$$= \int \langle p|\hat{x}|x\rangle\langle x|S(t)\rangle dx = \int x\langle p|x\rangle\Psi(x,t)\,dx$$

$|x\rangle$ is an eigenstate of $\hat{x}$ with eigenvalue x

$$= \int x\frac{e^{-ipx/\hbar}}{\sqrt{2\pi\hbar}}\Psi(x,t)\,dx = i\hbar\frac{\partial}{\partial p}\int\frac{e^{-ipx/\hbar}}{\sqrt{2\pi\hbar}}\Psi(x,t)\,dx$$

see Lecture 10, p. 7

$$= \boxed{i\hbar\frac{\partial}{\partial p}}\Phi(p,t) \quad .$$

see Lecture 10, p. 9