Theoretical Physics II B – Quantum Mechanics

Lecture 11

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Solutions to previous control questions

10.1 (a) Using $\left[\hat{S}_i,\,\hat{S}_j\right] = i\hbar\epsilon_{ijk}\hat{S}_k$ and $\hat{H} = \omega\hat{S}_z$, the E.o.M. are given by

$$\begin{aligned}
\frac{\mathrm{d}\hat{S}_x}{\mathrm{d}t} &= -\frac{i}{\hbar}\left[\hat{S}_x,\,\hat{H}\right] = -\frac{i\omega}{\hbar}\left[\hat{S}_x,\,\hat{S}_z\right] = -\omega\,\hat{S}_y\,,\\
\frac{\mathrm{d}\hat{S}_y}{\mathrm{d}t} &= -\frac{i}{\hbar}\left[\hat{S}_y,\,\hat{H}\right] = -\frac{i\omega}{\hbar}\left[\hat{S}_y,\,\hat{S}_z\right] = \omega\,\hat{S}_x\,,\\
\frac{\mathrm{d}\hat{S}_z}{\mathrm{d}t} &= -\frac{i}{\hbar}\left[\hat{S}_z,\,\hat{H}\right] = -\frac{i\omega}{\hbar}\left[\hat{S}_z,\,\hat{S}_z\right] = 0\,,
\end{aligned}$$

This yields as solutions:

$$\begin{aligned}
\hat{S}_x(t) &= \cos(\omega t)\hat{S}_x(0) - \sin(\omega t)\hat{S}_y(0)\\
\hat{S}_y(t) &= \cos(\omega t)\hat{S}_y(0) + \sin(\omega t)\hat{S}_x(0)\\
\hat{S}_z(t) &= \hat{S}_z(0)
\end{aligned}$$

(b) Time evolution of state kets through application of $\hat{U}(t) = \exp\left[-\frac{i}{\hbar}\hat{H}t\right]$:

$$
\begin{aligned}
|\psi_1(t)\rangle &= \exp\left[-\frac{i}{\hbar}\hat{H}t\right]|\uparrow\rangle = \exp\left[-\frac{i\omega t}{2}\right]|\uparrow\rangle \\
|\psi_\pm(t)\rangle &= \frac{1}{\sqrt{2}}\exp\left[-\frac{i}{\hbar}\hat{H}t\right]\left[|\uparrow\rangle \pm |\downarrow\rangle\right] \\
&= \frac{1}{\sqrt{2}}\left[\exp\left(-\frac{i\omega t}{2}\right)|\uparrow\rangle \pm \exp\left(\frac{i\omega t}{2}\right)|\downarrow\rangle\right]
\end{aligned}
$$

(c) Heisenberg picture:

$$
\begin{aligned}
\langle \mathcal{S}_z(t)\rangle_{|\psi_1\rangle} &= \left\langle \psi_1 \left| \hat{S}_z \right| \psi_1 \right\rangle = \frac{\hbar}{2}\,, \\
\langle \mathcal{S}_z(t)\rangle_{|\psi_\pm\rangle} &= \frac{1}{2}\left(\langle\uparrow| \pm \langle\downarrow|\right) \hat{S}_z \left(|\uparrow\rangle \pm |\downarrow\rangle\right) \\
&= \frac{\hbar}{4}\left(\left\langle \uparrow \left| \hat{S}_z \right| \uparrow \right\rangle + \left\langle \downarrow \left| \hat{S}_z \right| \downarrow \right\rangle\right) = 0\,; \\
\langle \mathcal{S}_x(t)\rangle_{|\psi_1\rangle} &= \cos(\omega t)\left\langle \psi_1 \left| \hat{S}_x \right| \psi_1 \right\rangle - \sin(\omega t)\left\langle \psi_1 \left| \hat{S}_y \right| \psi_1 \right\rangle = 0\,; \\
\langle \mathcal{S}_x(t)\rangle_{|\psi_\pm\rangle} &= \pm\frac{1}{2}\cos(\omega t)\left[\left\langle \uparrow \left| \hat{S}_x \right| \downarrow \right\rangle + \left\langle \downarrow \left| \hat{S}_x \right| \uparrow \right\rangle\right] \\
&\quad \mp\frac{1}{2}\sin(\omega t)\left[\left\langle \uparrow \left| \hat{S}_y \right| \downarrow \right\rangle + \left\langle \downarrow \left| \hat{S}_y \right| \uparrow \right\rangle\right] \\
&= \pm\frac{\hbar}{4}\cos(\omega t)\,(1+1) \mp \frac{\hbar}{4}\sin(\omega t)\,(-i+i) \\
&= \pm\frac{\hbar}{2}\cos(\omega t)\,.
\end{aligned}
$$

(c) Schrödinger picture:

$$
\begin{aligned}
\langle \mathcal{S}_z\rangle_{|\psi_1\rangle(t)} &= \left\langle \uparrow \middle| \hat{S}_z \middle| \uparrow \right\rangle = \frac{\hbar}{2}\,, \\
\langle \mathcal{S}_z\rangle_{|\psi_\pm(t)\rangle} &= \frac{1}{2}\left(e^{i\omega t/2}\langle\uparrow| \pm e^{-i\omega t/2}\langle\downarrow|\right)\hat{S}_z\left(e^{-i\omega t/2}|\uparrow\rangle \pm e^{i\omega t/2}|\downarrow\rangle\right) \\
&= \frac{\hbar}{4}\left(\left\langle \uparrow \middle| \hat{S}_z \middle| \uparrow \right\rangle + \left\langle \downarrow \middle| \hat{S}_z \middle| \downarrow \right\rangle\right) = 0\,; \\
\langle \mathcal{S}_x\rangle_{|\psi_1\rangle(t)} &= \left\langle \uparrow \middle| \hat{S}_x \middle| \uparrow \right\rangle = 0\,; \\
\langle \mathcal{S}_x\rangle_{|\psi_\pm(t)\rangle} &= \frac{1}{2}\left(e^{i\omega t/2}\langle\uparrow| \pm e^{-i\omega t/2}\langle\downarrow|\right)\hat{S}_x\left(e^{-i\omega t/2}|\uparrow\rangle \pm e^{i\omega t/2}|\downarrow\rangle\right) \\
&= \pm\frac{\hbar}{4}\left(e^{i\omega t}\left\langle \uparrow \middle| \hat{S}_x \middle| \downarrow \right\rangle + e^{-i\omega t}\left\langle \downarrow \middle| \hat{S}_x \middle| \uparrow \right\rangle\right) \\
&= \pm\frac{\hbar}{4}\left(e^{i\omega t} + e^{-i\omega t}\right) = \pm\frac{\hbar}{2}\cos(\omega t)\,.
\end{aligned}
$$

Reminder: Infinitesimal time translations

- In lecture 6 we have seen that the time evolution operator for an infinitesimally small time step δt assumes the form

$$\begin{aligned}\hat{U}(t_0+\delta t,\, t_0) &= \hat{U}(t_0,\, t_0) - \frac{i}{\hbar}\hat{H}(t_0)\hat{U}(t_0,\, t_0)\delta t \\ &= \hat{\mathbf{1}} - \frac{i}{\hbar}\hat{H}(t_0)\delta t\end{aligned}$$

  allowing to interpret the Hamiltonian as the operator that *generates* such infinitesimal time steps.

- Phrased in other words:

  The Hamiltonian is the generator of translation in time

- We will see how this generalises to spatial translations.

Detour: Position eigenkets and position measurements

- Eigenkets of the position operator satisfy $\hat{\underline{x}}\,|\underline{x}\rangle = \underline{x}\,|\underline{x}\rangle$.
  The eigenket $|\underline{x}\rangle$ in fact is a simulataneous eigenket of $\hat{x}$, $\hat{y}$, and $\hat{z}$.
  Denoting them as $\hat{x}_i$ they satisfy $[\hat{x}_i, \hat{x}_j] = 0$.
- Since position is continous, one may only measure the particle to be in an interval of size $\Delta\underline{x}$ around some central position $\underline{X}$, and thus

$$|\psi\rangle = \int \mathrm{d}^3x\,|\underline{x}\rangle\,\langle\underline{x}|\psi\rangle \stackrel{\text{measurement}}{\longrightarrow} \int\limits_{\underline{X}-\Delta\underline{x}}^{\underline{X}+\Delta\underline{x}} \mathrm{d}^3x\,|\underline{x}\rangle\,\langle\underline{x}|\psi\rangle$$

Translation operator: Definition

- We define the operator $\hat{T}(\mathrm{d}\underline{x})$ that generates infinitesimal translations, i.e. shifts a state at $|\underline{x}\rangle$ to be at $|\underline{x}+\mathrm{d}\underline{x}\rangle$:

$$\hat{T}(\mathrm{d}\underline{x})\,|\underline{x}\rangle = |\underline{x}+\mathrm{d}\underline{x}\rangle\ .$$

- Note that while $|\underline{x}\rangle$ and $|\underline{x}+\mathrm{d}\underline{x}\rangle$ are eigenvectors of $\hat{\underline{x}}$, they are not eigenkets of $\hat{T}$. Therefore, shifting an arbitrary state $|\psi\rangle$ yields

$$\begin{aligned}|\psi\rangle \xrightarrow{\mathcal{T}} |\psi'\rangle &= \hat{T}(\mathrm{d}\underline{x})\,|\psi\rangle = \hat{T}(\mathrm{d}\underline{x})\int \mathrm{d}^3\underline{x}\,|\underline{x}\rangle\,\langle\underline{x}|\psi\rangle \\ &= \int \mathrm{d}^3\underline{x}\,|\underline{x}+\mathrm{d}\underline{x}\rangle\,\langle\underline{x}|\psi\rangle \\ &= \int \mathrm{d}^3\underline{x}\,|\underline{x}\rangle\,\langle\underline{x}-\mathrm{d}\underline{x}|\psi\rangle\ .\end{aligned}$$

The last line holds true because the integration is over all space.

Translation operator: Definition

- Unitarity: Demanding that an infinitesimal translation does not change the norm of the ket yields

$$\langle\psi|\psi\rangle = \left\langle\psi\left|\hat{T}^\dagger(\mathrm{d}\underline{x})\hat{T}(\mathrm{d}\underline{x})\right|\psi\right\rangle \quad\longleftrightarrow\quad \hat{T}^\dagger(\mathrm{d}\underline{x})\hat{T}(\mathrm{d}\underline{x}) = \hat{\mathbf{1}}\,,$$

  and therefore the translation operator must be unitary.
- Composition: $\hat{T}(\mathrm{d}\underline{x}_1)\hat{T}(\mathrm{d}\underline{x}_2) = \hat{T}(\mathrm{d}\underline{x}_1 + \mathrm{d}\underline{x}_2)$.
- Inverse given by reverse translation: $\hat{T}(-\mathrm{d}\underline{x}) = \hat{T}^{-1}(\mathrm{d}\underline{x}) = \hat{T}^\dagger(\mathrm{d}\underline{x})$.
- Identity as limit: $\lim\limits_{\mathrm{d}\underline{x}\to 0}\hat{T}(\mathrm{d}\underline{x}) = \hat{\mathbf{1}}$.
- Represent translation operator through *Hermitean operators* $\underline{\hat{K}}$ as

$$\hat{T}(\mathrm{d}\underline{x}) = \hat{\mathbf{1}} - i\underline{\hat{K}}\cdot\mathrm{d}\underline{x}\,.$$

Commutators

- Consider

$$\left[\underline{\hat{x}},\ \hat{T}(\mathrm{d}\underline{x})\right]|\underline{x}\rangle = \hat{x}\,|\underline{x}+\mathrm{d}\underline{x}\rangle - \hat{T}(\mathrm{d}\underline{x})\cdot\underline{x}\,|\underline{x}\rangle = \mathrm{d}\underline{x}\,|\underline{x}+\mathrm{d}\underline{x}\rangle$$

  indicating that

$$\left[\underline{\hat{x}},\ \hat{T}(\mathrm{d}\underline{x})\right] = -i\left[\underline{\hat{x}},\ \underline{\hat{K}}\right]\cdot\mathrm{d}\underline{x} = \mathrm{d}\underline{x} \quad\longleftrightarrow\quad \left[\hat{x}_i,\ \hat{K}_j\right] = i\delta_{ij}\hat{\mathbf{1}}\,.$$

- At the same time, it is simple to see that

$$\left[\hat{T}(\mathrm{d}\underline{x}_1),\ \hat{T}(\mathrm{d}\underline{x}_2)\right]|\underline{x}\rangle = 0 \quad\longleftrightarrow\quad \left[\hat{K}_i,\ \hat{K}_j\right] = 0\,.$$

- This motivates to identify the Hermitean operators $\underline{\hat{K}}$ with the momentum operators $\underline{\hat{p}}$ (the *generators* of spatial translation)

$$\boxed{\underline{\hat{K}} = \frac{\underline{\hat{p}}}{\hbar} = -i\underline{\hat{\nabla}}}$$

Eigenkets of the translation operator

- Since the generators of infinitesimal translations, the momentum operators, commute, the corresponding group is called *Abelian*.
- Using the fact that $\underline{\hat{p}}\left|\underline{p}\right\rangle = \underline{p}\left|\underline{p}\right\rangle$ allows to write

$$\hat{T}(\mathrm{d}\underline{x})\left|\underline{p}\right\rangle = \left[\hat{\mathbf{1}} - \frac{i\mathrm{d}\underline{x}\cdot\underline{\hat{p}}}{\hbar}\right]\left|\underline{p}\right\rangle = \left[1\frac{i\mathrm{d}\underline{x}\cdot\underline{p}}{\hbar}\right]\left|\underline{p}\right\rangle ,$$

  and we see that the eigenkets of $\hat{T}$ are the momnetum eigenkets. The eigenvalues, though, are complex; acting with an infinitesimal translation on a momentum eigenket generates a phase.

Symmetries and conservation laws

- Consider now a general continuous symmetry operation $\mathcal{S}$.
- Following the example of spatial translations below, it does not seem to far fetched, to construct a corresponding operator $\hat{S}$, which represents an infinitesimal version of $\mathcal{S}$, parametrised by ε:

  $$\hat{S}(\varepsilon) = \hat{\mathbf{1}} - \frac{i\varepsilon}{\hbar}\hat{G}\,.$$

  Here $\hat{G}$ is the *generator* related to the symmetry.
- Demanding invariance of the Hamiltonian under this operation, i.e. $\hat{S}^\dagger\hat{H}\hat{S} = \hat{H}$ yields $\left[\hat{G},\,\hat{H}\right] = 0$.
- Using Heisenberg's equation of motion we find that

  $$\frac{\mathrm{d}\hat{G}^{(H)}}{\mathrm{d}t} = \frac{1}{i\hbar}\left[G^{(H)},\,\hat{H}\right]\,.$$

$$\boxed{\hat{G} \text{ represents a conserved quantity, if it generates an invariance of } \hat{H}.}$$

Example: Momentum conservation

- As an example consider the case of spatial translations.
- Assume invariance of the Hamiltonian under spatial translations, realised by the operator $\hat{T}(\mathrm{d}\underline{x}) = 1 - \frac{i\mathrm{d}\underline{x}\cdot\hat{\underline{p}}}{\hbar}$,

$$\hat{H} \xrightarrow{\mathcal{T}} \hat{H}' = \hat{T}^\dagger(\mathrm{d}\underline{x})\hat{H}\hat{T}(\mathrm{d}\underline{x}) \stackrel{!}{=} \hat{H}\,,$$

Expanding this up to first order in $\mathrm{d}\underline{x}$ yields

$$\left[1 + \frac{i\mathrm{d}\underline{x}\cdot\hat{\underline{p}}}{\hbar}\right]\hat{H}\left[1 - \frac{i\mathrm{d}\underline{x}\cdot\hat{\underline{p}}}{\hbar}\right] = \frac{i\mathrm{d}\underline{x}}{\hbar}\cdot\left[\hat{p},\,\hat{H}\right] + \mathcal{O}(\mathrm{d}^2\underline{x}) = 0$$

and therefore momentum is conserved:

$$\frac{\mathrm{d}\hat{\underline{p}}^{(H)}}{\mathrm{d}t} = \frac{1}{i\hbar}\left[\underline{p}^{(\hat{H})},\,\hat{H}\right]$$

Discrete symmetries: Space inversion (parity)

- Consider the operation of space inversion $\mathcal{P}$, which transforms left- to right-handed coordinate system, and vice versa, by reflecting all spatial coordinates.
- To see how this works, take an arbitrary state $|\psi\rangle$ and apply the *unitary parity operator* $\hat{\pi}$:
$$|\psi\rangle \xrightarrow{\mathcal{P}} |\psi'\rangle = \hat{\pi}\,|\psi\rangle.$$
The expectation value of the position operator with respect to this ket is required to change sign:
$$\langle\psi'\,|\hat{x}|\,\psi'\rangle = \left\langle\psi\left|\hat{\pi}^\dagger\hat{x}\hat{\pi}\right|\psi\right\rangle \stackrel{!}{=} -\langle\psi\,|\hat{x}|\,\psi\rangle.$$
- This is realised if $\hat{\pi}^\dagger\hat{x}\hat{\pi} = -\hat{x}$, or $\hat{x}\hat{\pi} = -\hat{\pi}\hat{x}$, or $\{\hat{\pi},\,\hat{x}\} = 0$.

Properties of the parity operator

- Claiming that eigenkets of the position operator behave like
$$\hat{\pi}\,|\underline{x}\rangle = e^{i\delta}\,|-\underline{x}\rangle \text{ with } \delta \in \mathbf{R}$$
results in
$$\hat{\underline{x}}\hat{\pi}\,|\underline{x}\rangle = -\hat{\pi}\hat{\underline{x}}\,|\underline{x}\rangle = -\underline{x}\hat{\pi}\,|\underline{x}\rangle,$$
indicating that $\hat{\pi}\,|x\rangle$ is an eigenket of $\hat{x}$ with eigenvalue $-\underline{x}$, which must be the same as a position eigenket $|-\underline{x}\rangle$ up to a phase factor.
- By convention, this phase factor is chosen as $e^{i\delta} = 1$, or $\delta = 0$.
- Substituting this back yields $\hat{\pi}^2 = \hat{\mathbf{1}}$ or $\hat{\pi}^{-1} = \hat{\pi}^\dagger = \hat{\pi}$.
- In addition, the eigenvalues of $\hat{\pi}$ can only be ± 1.
- To see how the momentum operator behaves under parity, one could argue that momentum is like $m\mathrm{d}\underline{x}/\mathrm{d}t$, and thus must also be odd (have a negative eigenvalue) under parity.
A better way to see this, though, is by taking momentum as the generator of translation and compare translation followed by reflection with reflection followed by translation.

Wave functions under parity

- Consider the wave function of a spin-less particle, $\psi(\underline{x}) = \langle \underline{x}|\psi\rangle$ and the wave function of the space-inverted state, $\psi(\underline{x}) = \langle \underline{x}\,|\hat{\pi}|\,\psi\rangle$.
- If $|\psi\rangle$ is an eigenket of the parity operator, $\hat{\pi}\,|\psi\rangle = \pm\,|\psi\rangle$, then
$$\psi(-\underline{x}) = \langle \underline{x}\,|\hat{\pi}|\,\psi\rangle = \pm\psi(\underline{x}),$$
where the $+$ (-) sign refers to even (odd) parity.
- If $\left[\hat{\pi},\, \hat{H}\right] = 0$ and $|n\rangle$ is a non-degenerate eigenvector of $\hat{H}$ with (energy-)eigenvalue E_n, then $|n\rangle$ is also a parity eigenket.
As an example consider the harmonic oscillator. The ground state, $|0\rangle$, having a Gaussian wave function, has even parity, and the first excited state, $|1\rangle = \hat{a}_+\,|0\rangle$, has odd parity, since $\hat{a}_+$ is linear in $\hat{x}$ and $\hat{p}$. Conversely, the second excited state is even, and so on.
However, it is important to stress that this works only, because the states are non-degenerate. For example, for the hydrogen atom, it is well-known that the states are degenerate, and energy eigenkets are not parity eigenkets.

Learning outcomes

- Intimate connection of continuous symmetries and their generators. (Example: space translation and momentum, later: rotation and angular momentum)
- Continuous symmetries enforce conserved quantities, give by their generators.
- Special role of discrete symmetries: parity as example.

Control questions

11.1 Check that indeed the representation $\hat{T}(\mathrm{d}\underline{x}) = \hat{\mathbf{1}} - i\underline{\hat{K}} \cdot \mathrm{d}\underline{x}$ of the infinitesimal translation operator satisfies the demands of unitarity, the composition property, the form of the inverse and the recovery of the identity as the limit. You may ignore terms of order $\mathrm{d}\underline{x}^2$ throughout.

11.2 Prove that $|n\rangle$ is a parity eigenket if $\left[\hat{\pi},\, \hat{H}\right] = 0$ and $|n\rangle$ is a non-degenerate eigenvector of $\hat{H}$ with (energy-)eigenvalue E_n. To this end, first use $\hat{\pi}^2 = \hat{\mathbf{1}}$ to show that $\frac{\hat{\mathbf{1}}\pm\hat{\pi}}{2}\,|n\rangle$ is a parity eigenket with eigenvalues ± 1. Show that this state is also an energy eigenket and determine its energy eigenvalue. What does this imply, taking into account that $|n\rangle$ is non-degenerate?