Theoretical Physics II B – Quantum Mechanics

Lecture 10

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Solutions to previous control questions

9.1 (a) The Hamiltonian already is diagonal,

$$\hat{H} = \frac{\hbar\omega}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and therefore

$$E_\pm = \pm\frac{\hbar\omega}{2} \text{ for } |E_+\rangle = |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } |E_-\rangle = |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

(b) The time evolution operator is given by

$$\begin{aligned} \hat{U}(t,\, t_0) &= \exp\left[-\frac{i}{\hbar}\hat{H}(t-t_0)\right] \\ &= \begin{pmatrix} \exp\left[-\frac{i\omega(t-t_0)}{2}\right] & 0 \\ 0 & \exp\left[\frac{i\omega(t-t_0)}{2}\right] \end{pmatrix} \end{aligned}$$

9.1 (b) Continued: Applying it to a general linear combination $|\psi\rangle = c_\uparrow |\uparrow\rangle + c_\downarrow |\downarrow\rangle$ will result in time-dependent prefactors

$$\begin{aligned} c_\uparrow(t) &= \exp\left[-\frac{i\omega(t-t_0)}{2}\right] c_\uparrow(t_0) \\ c_\downarrow(t) &= \exp\left[\frac{i\omega(t-t_0)}{2}\right] c_\downarrow(t_0) \end{aligned}$$

(c) Since the Hamiltonian and the spin-operator in z direction do not depend explicitly on time, and because they also commute we find that

$$\frac{\mathrm{d}\langle\mathcal{E}\rangle}{\mathrm{d}t} = 0 = \frac{\mathrm{d}\langle\mathcal{S}_z\rangle}{\mathrm{d}t}\,.$$

Calculating the expectation value directly, we find

$$\begin{aligned} \langle\mathcal{S}_z\rangle &= \left\langle\psi\left|\hat{S}_z\right|\psi\right\rangle = \frac{\hbar}{2}(|c_\uparrow(t_0)|^2 - |c_\downarrow(t_0)|^2) \\ \langle\mathcal{E}\rangle &= \left\langle\psi\left|\hat{H}\right|\psi\right\rangle = \frac{\hbar\omega}{2}(|c_\uparrow(t_0)|^2 - |c_\downarrow(t_0)|^2) = \omega\langle\mathcal{S}_z\rangle\,. \end{aligned}$$

9.1 (d) The time evolution of the expectation value can in this case be written as

$$\begin{aligned}\langle \mathcal{S}_x \rangle &= \left\langle \psi \left| \hat{S}_x \right| \psi \right\rangle \\ &= \frac{\hbar}{2} \left\{ c_\uparrow^* c_\downarrow \exp\left[i\omega t\right] + c_\downarrow^* c_\uparrow \exp\left[-i\omega t\right] \right\} = \frac{\hbar}{2} \cos\left(\omega t\right) ,\end{aligned}$$

and similarly

$$\begin{aligned}\langle \mathcal{S}_y \rangle &= \left\langle \psi \left| \hat{S}_y \right| \psi \right\rangle \\ &= \frac{\hbar}{2} \left\{ -i c_\uparrow^* c_\downarrow \exp\left[i\omega t\right] + i c_\downarrow^* c_\uparrow \exp\left[-i\omega t\right] \right\} = \frac{\hbar}{2} \sin\left(\omega t\right) ,\end{aligned}$$

i.e. the spin experiences a precession movement around the z-axis. To obtain the results above, we have used that $c_\downarrow = c_\uparrow = \frac{1}{\sqrt{2}}$.

Unitary transformations, again

- Remember that the time evolution operator $\hat{U}(t,\,t_0)$ is unitary. This implies *probability conservation*:

$$\langle\psi(t)|\psi(t)\rangle = \left\langle\psi(t_0)\left|\hat{U}^\dagger(t,\,t_0)\hat{U}(t,\,t_0)\right|\psi(t_0)\right\rangle = \langle\psi(t_0)|\psi(t_0)\rangle\ ,$$

  i.e. the norm of a state ket does not change during time evolution.
- Instead, time evolution merely acts like a phase factor on the state ket, rotating it in Hilbert space.
- Even more, phase differences between *different* kets are invariant:

$$\langle\chi(t)|\psi(t)\rangle = \left\langle\chi(t_0)\left|\hat{U}^\dagger(t,\,t_0)\hat{U}(t,\,t_0)\right|\psi(t_0)\right\rangle = \langle\chi(t_0)|\psi(t_0)\rangle\ ,$$

Interpreting time evolution

- Consider now an aribtrary operator sandwich with an explicitly time-independent operator $\hat{O}$ and keep in mind that for measurements we're mainly interested in the case where we sandwich with identical states, i.e. where $\langle\chi| \to \langle\psi|$. Under time evolution,

$$\left\langle \chi(t_0) \left| \hat{O} \right| \psi(t_0) \right\rangle \longrightarrow$$
$$\left\langle \chi(t) \left| \hat{O} \right| \psi(t) \right\rangle = \left\langle \chi(t_0) \left| \hat{U}^\dagger(t,\, t_0) \hat{O} \hat{U}(t,\, t_0) \right| \psi(t_0) \right\rangle .$$

- There's two extreme ways to interpret this:
    1. Schrödinger picture:
    Time evolution for state kets, $|\psi(t)\rangle \longrightarrow \hat{U}(t,\, t_0)\,|\psi(t_0)\rangle$,
    with *operators unchanged*, $\hat{O} \longrightarrow \hat{O}$.
    2. Heisenberg picture:
    Time evolution for operators, $\hat{O}(t) \longrightarrow \hat{U}^\dagger(t,\, t_0)\hat{O}(t_0)\hat{U}(t,\, t_0)$,
    with *state kets unchanged*, $|\psi\rangle \longrightarrow |\psi\rangle$.

Kets and operators in both pictures

- For the sake of a compact notation, assume $t_0 = 0$.
- Assume kets and operators to coincide for $t = t_0$: operators in the Schrödinger and Heisenberg picture are equal, $\hat{O}^{(S)} = \hat{O}^{(H)}(0)$ and the state kets are equal, $\left|\psi^{(S)}(0)\right\rangle = \left|\psi^{(H)}\right\rangle$.
- Then:

$$
\begin{aligned}
\hat{O}^{(H)}(t) &= \hat{U}^{\dagger}(t)\hat{O}^{(S)}\hat{U}(t) \\
\left|\psi^{(S)}(t)\right\rangle &= \hat{U}(t)\left|\psi^{(H)}\right\rangle .
\end{aligned}
$$

But the expecation values are equal:

$$
\left\langle\psi^{(H)}\left|\hat{O}^{(H)}(t)\right|\psi^{(H)}\right\rangle = \left\langle\psi^{(S)}(t)\left|\hat{O}^{(S)}\right|\psi^{(S)}(t)\right\rangle .
$$

Heisenberg equation of motion

- Assuming the operator $\hat{O}$ in the Schrödinger picture and the Hamiltonian to be explicitly time-independent,

$$\begin{aligned}\frac{\mathrm{d}\hat{O}^{(H)}(t)}{\mathrm{d}t} &= \frac{\partial\hat{U}^\dagger(t)}{\partial t}\hat{O}^{(S)}\hat{U}(t) + \hat{U}^\dagger(t)\hat{O}^{(S)}\frac{\partial\hat{U}(t)}{\partial t}\\ &= +\frac{i}{\hbar}\hat{U}^\dagger(t)\hat{H}\hat{O}^{(S)}\hat{U}(t) - \frac{i}{\hbar}\hat{U}^\dagger(t)\hat{O}^{(S)}\hat{H}\hat{U}(t)\\ &= +\frac{i}{\hbar}\hat{U}^\dagger(t)\hat{H}\hat{U}(t)\hat{U}^\dagger(t)\hat{O}^{(S)}\hat{U}(t) - \frac{i}{\hbar}\hat{U}^\dagger(t)\hat{O}^{(S)}\hat{U}(t)\hat{U}^\dagger(t)\hat{H}\hat{U}(t)\\ &= -\frac{i}{\hbar}\left[\hat{O}^{(H)}(t),\,\hat{U}^\dagger(t)\hat{H}\hat{U}(t)\right] = -\frac{i}{\hbar}\left[\hat{O}^{(H)}(t),\,\hat{H}\right]\,,\end{aligned}$$

where in going to the last expression use has been made from the fact that if $\hat{H}$ does not depend explicitly on time, $\hat{U} = \exp\left[-i\hat{H}t/\hbar\right]$ and $\left[\hat{U},\,\hat{H}\right] = 0$.

Connection to classical physics

- The Heisenberg equation of motion

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

  is strikingly similar to the *classical equations of motion* in the same setup (explicitly time-independent Hamiltonians), which, using Poisson brackets, can be written as

$$\frac{\mathrm{d}O}{\mathrm{d}t} = [O,\, H]_{\mathrm{classical}}$$

  leading to the assumption

$$[\,,\,]_{\mathrm{classical}} \longleftrightarrow \frac{[\,,\,]_{\mathrm{quantum}}}{i\hbar}$$

- It is worth noting, though, that this stretches to observables, such as spin, which do not have any classical analogue.
- However, analogue above indicates that in many aspects the dynamics in the Heisenberg picture and their interpretation are closer in spirit to classical physics. There is also no notion of a state ket of any dynamical consequence.

Base kets in the Heisenberg picture

- Common *misconception* of the Heisenberg picture: all kets are stationary. This is *not true*, only **state kets stationary**, the **base kets move!**
- Base kets are usually the eigenkets of an operator $\hat{L}$; multiplying the eigenvalue equation from the left with $\hat{U}^\dagger$ yields

$$\begin{aligned}\hat{U}^\dagger(t)\hat{L}^{(S)}\left|\lambda_i\right\rangle &= \hat{U}^\dagger(t)\hat{L}^{(S)}\hat{U}(t)\hat{U}^\dagger(t)\left|\lambda_i\right\rangle \\ &= \hat{L}^{(H)}(t)\left(\hat{U}^\dagger(t)\left|\lambda_i\right\rangle\right) = \hat{U}^\dagger(t)\lambda_i\left|\lambda_i\right\rangle .\end{aligned}$$

- This indicates that the base kets in the Heisenberg picture indeed move with time, but *opposite* to the way the state kets evolve in the Schrödinger picture.
- However, the component representation of state kets behaves the same way in both the Schrödinger and the Heisenberg picture:

$$\psi_k(t) = \left\langle \lambda_k^{(H)}(t)|\psi^{(H)}\right\rangle = \left\langle \lambda_k^{(S)}|\psi^{(S)}(t)\right\rangle = \left\langle \lambda_k\left|\hat{U(t)}\right|\psi\right\rangle .$$

Reminder: Hamiltonian

- From classical Hamiltonian to ladder operators:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 = \hbar\omega\left(\hat{N} + \frac{1}{2}\right) = \hbar\omega\left(\hat{a}_+\hat{a}_- + \frac{1}{2}\right) .$$

- Commutators of creation and annihilation operators:

$$[\hat{a_+}, \hat{a_-}] = -1 , \quad \left[\hat{N}, \hat{a_\pm}\right] = \pm\hat{a}_\pm , \quad \left[\hat{H}, \hat{a_\pm}\right] = \pm\hbar\omega\hat{a}_\pm .$$

- Connection to position and momentum operators:

$$\hat{a}_\pm = \frac{m\omega\hat{x} \mp i\hat{p}}{\sqrt{2\hbar m\omega}} , \quad \hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left[\hat{a}_+ + \hat{a}_-\right] , \quad \hat{p} = i\sqrt{\frac{\hbar m\omega}{2}}\left[\hat{a}_+ - \hat{a}_-\right] .$$

Time development in the Heisenberg picture

- Heisenberg E.o.M. yields two coupled differential equations for $\hat{x}$ & $\hat{p}$

$$\frac{\mathrm{d}\hat{p}}{\mathrm{d}t} = -\frac{i}{\hbar}\left[\hat{p},\,\hat{H}\right] = -m\omega^2\hat{x} \quad \text{and} \quad \frac{\mathrm{d}\hat{x}}{\mathrm{d}t} = -\frac{i}{\hbar}\left[\hat{x},\,\hat{H}\right] = \frac{\hat{p}}{m}$$

- Decouple nicely when going to ladder operators:

$$\frac{\mathrm{d}\hat{a}_\pm}{\mathrm{d}t} = -\frac{i}{\hbar}\left[\hat{a_\pm},\,\hat{H}\right] = \pm i\omega\hat{a}_\pm \quad \longrightarrow \quad \hat{a}_\pm(t) = \exp\left(\pm i\omega t\right)\,\hat{a}_\pm(0)$$

- Therefore:

$$\begin{aligned}\hat{x}(t) = \sqrt{\frac{\hbar}{2m\omega}}\left[\exp\left(i\omega t\right)\,\hat{a}_{+}(0) + \exp\left(-i\omega t\right)\,\hat{a}_{-}(0)\right] \\ = \sqrt{\frac{\hbar}{2m\omega}}\left[\cos(\omega t)(\hat{a}_{+} + \hat{a}_{-}) + i\sin(\omega t)(\hat{a}_{+} - \hat{a}_{-})\right] \\ = \cos(\omega t)\,\hat{x}(0) + \frac{\sin(\omega t)}{m\omega}\,\hat{p}(0)\,.\end{aligned}$$

  and similarly

$$\hat{p}(t) = \cos(\omega t)\,\hat{p}(0) - m\omega\sin(\omega t)\,\hat{x}(0)\,.$$

- They look like their classical analogue: the position and momentum operators $\hat{x}$ and $\hat{p}$ "oscillate" with frequency ω.

Alternative derivation

- Alternatively, can also apply time-evolution operator directly:

$$\hat{x}(t) = \hat{U}^\dagger(t)\hat{x}(0)\hat{U}(t) = \exp\left[\frac{i\hat{H}t}{\hbar}\right]\hat{x}(0)\exp\left[-\frac{i\hat{H}t}{\hbar}\right]$$

- Using the Baker-Hausdorff formula

$$\exp(i\hat{G}\lambda)\hat{A}\exp(-i\hat{G}\lambda) = \hat{A} + i\lambda\left[\hat{G},\,\hat{A}\right] + \left[\hat{G},\,\left[\hat{G},\,\hat{A}\right]\right] + \dots$$

and by repeatedly identifying

$$\left[\hat{H},\,x(\hat{0})\right] = -\frac{i\hbar\hat{p}(0)}{m} \quad \text{and} \quad \left[\hat{H},\,p(\hat{0})\right] = i\hbar m\omega\hat{x}(0)$$

the result of the previous slide can be confirmed.

Expectation values $\langle\mathcal{X}\rangle$ and $\langle\mathcal{P}\rangle$

- Since the operators $\hat{x}(t)$ and $\hat{p}(t)$ oscillate like

$$\begin{aligned}\hat{x}(t) &= \cos(\omega t)\,\hat{x}(0) + \frac{\sin(\omega t)}{m\omega}\,\hat{p}(0)\\ \hat{p}(t) &= \cos(\omega t)\,\hat{p}(0) - m\omega\sin(\omega t)\,\hat{x}(0)\,,\end{aligned}$$

  one would maybe naively expect that also the expectation values of the corresponding observables oscillate in a similar fashion.
- This however is not true: Consider the expectation value with respect to the nth eigenstate, $|\phi_n\rangle$:

$$\langle\psi_n\,|\hat{x}|\,\psi_n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\,\langle\psi_n\,|[\hat{a}_+ + \hat{a}_-]|\,\psi_n\rangle = 0\,,$$

  because the creation and annihilation operators and thus the position and momentum operators have only non-diagonal entries in this base.

- Therefore, to observe oscillations that look anything like a classical oscillator, the states must be *superpositions* of different energy eigenstates.
- For example, consider, in obvious notation, a state
$$|\psi\rangle = c_0\,|0\rangle + c_1\,|1\rangle.$$
- Taking the expectation value with respect to such a state

$$\langle\psi\,|\hat{x}|\,\psi\rangle \;=\; \sqrt{\frac{\hbar}{2m\omega}}\left[c_0^* c_1 \left\langle 0\left|\hat{a}_-(t)\right|1\right\rangle + c_1^* c_0 \left\langle 1\left|\hat{a}_+(t)\right|0\right\rangle\right] \neq 0$$

is non-vanishing and will indeed lead to some oscillatory movement.

Coherent states

- Following the logic above, a state b$|\lambda\rangle$ could be constructed as a superposition of energy eigenstates, such that it most closely imitates the classical oscillator.
- Such a *coherent state* is defined by the eigenvalue equation for the non-Hermitian annihilation operator $\hat{a}_-$:

$$\hat{a}_- \,|\lambda\rangle = \lambda \,|\lambda\rangle \;,$$

which clearly must be a superposition of all energy eigenstates:

$$|\lambda\rangle = \sum_{n=0}^{\infty} f(n)\,|n\rangle \;, \quad \text{where} \;\; |f(n)|^2 = \frac{\bar{n}^n}{n!}\exp(-\bar{n})\,,$$

the distribution of the energy eigenkets n follows a Poisson distribution around a mean $\bar{n}$.

- Such a state can be obtained by translating the gound state energy of the oscialltor by some finite amount, and it satisfies the minimal uncertainty product at all times.

Learning outcomes

- Heisenberg vs. Schrödinger picture:

	Heisenberg picture	Schrödinger picture
State kets	Stationary	Moving ($\|\psi(t)\rangle = \hat{U}\|\psi\rangle$)
Observables	Moving ($\hat{O}(t) = \hat{U}^\dagger\hat{O}\hat{U}$)	Stationary
Base kets	Moving oppositely ($\|b_k(t)\rangle = \hat{U}^\dagger\|b_k\rangle$)	Stationary

- In all cases, time evolution operator given by

$$\hat{U}(t) = \exp\left[-\frac{i}{\hbar}\int\limits_0^t \mathrm{d}t'\hat{H}(t')\right] \overset{\hat{H}\text{ is }t'-\text{indep.}}{\longrightarrow} \exp\left[-\frac{i}{\hbar}\hat{H}t\right]\,.$$

Control questions

10.1 Consider, once again, the Hamiltonian

$$\hat{H} = -\frac{eB}{mc}\,\hat{S}_z = \omega\hat{S}_z\,.$$

already encountered in the control questions to the last lecture.

(a) Write the Heisenberg E.o.M. for the three time-dependent spin operators $\hat{S}_{x,\,y,\,z}(t)$ and solve them.

(b) For the states $|\psi_1\rangle = |\uparrow\rangle$ and $|\psi_\pm\rangle = \frac{1}{\sqrt{2}}\left[|\uparrow\rangle \pm |\downarrow\rangle\right]$ write down the Schrödinger equation and solve it explicitly, i.e. give expressions for these three states as functions of time in the Schrödinger picture.

(c) Compare the time evolution of the expectation values of $\mathcal{S}_{x,z}$ with respect to those three states in both pictures and check that they coincide.