Theoretical Physics II B – Quantum Mechanics

Lectures 7 & 8

Frank Krauss

February 11, 2014

1. The harmonic oscillator, once more

Solutions to previous control questions

6.1 Some properties of derivatives of operators:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\alpha_0}\left[\hat{A}(\alpha_0)\hat{B}(\alpha_0)\right] &= \left[\frac{\mathrm{d}}{\mathrm{d}\alpha_0}\hat{A}(\alpha_0)\right]\hat{B}(\alpha_0)+\hat{A}(\alpha_0)\left[\frac{\mathrm{d}}{\mathrm{d}\alpha_0}\hat{B}(\alpha_0)\right]\\ \frac{\mathrm{d}}{\mathrm{d}\alpha_0}e^{\alpha_0\hat{L}} &= \hat{L}e^{\alpha_0\hat{L}} = e^{\alpha_0\hat{L}}\hat{L}\,.\end{aligned}$$

Therefore:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\alpha_0}\hat{F}(\alpha_0) &= e^{\alpha_0\hat{L}}\hat{L}\hat{M}e^{-\alpha_0\hat{L}}-e^{\alpha_0\hat{L}}\hat{M}\hat{L}e^{-\alpha_0\hat{L}} = e^{\alpha_0\hat{L}}\left[\hat{L},\,\hat{M}\right]e^{-\alpha_0\hat{L}}\\ \frac{\mathrm{d}^2}{\mathrm{d}\alpha_0^2}\hat{F}(\alpha_0) &= \frac{\mathrm{d}}{\mathrm{d}\alpha_0}\left[e^{\alpha_0\hat{L}}\left[\hat{L},\,\hat{M}\right]e^{-\alpha_0\hat{L}}\right] = e^{\alpha_0\hat{L}}\left[\hat{L},\,\left[\hat{L},\,\hat{M}\right]\right]e^{-\alpha_0\hat{L}}\\ \frac{\mathrm{d}^n}{\mathrm{d}\alpha_0^n}\hat{F}(\alpha_0) &= \frac{\mathrm{d}}{\mathrm{d}\alpha_0}\left[e^{\alpha_0\hat{L}}\left[\hat{L},\,\hat{M}\right]_{(n-1)}e^{-\alpha_0\hat{L}}\right] = e^{\alpha_0\hat{L}}\left[\hat{L},\,\hat{M}\right]_{(n)}e^{-\alpha_0\hat{L}}\end{aligned}$$

Solutions to previous control questions

6.1 Continue by now choosing $\alpha = 1$ and $\alpha_0 = 0$ to write

$$\hat{F}(\alpha = 1) = \sum_{n=0}^{\infty} \frac{(1-\alpha_0)^n}{n!} \frac{\mathrm{d}^n}{\mathrm{d}\alpha_0^n} \hat{F}(\alpha_0)\Big|_{\alpha_0=0} = \sum_{n=0}^{\infty} \frac{1}{n!} \left[\hat{L},\, \hat{M}\right]_{(n)} .$$

Solutions to previous control questions

6.2 The commutators read $\left[\hat{S}_i,\, \hat{S}_j\right] = \frac{\hbar^2}{4}\left[\hat{\sigma}_i,\, \hat{\sigma}_j\right] = \frac{i\hbar^2\epsilon_{ijk}}{2}\hat{\sigma}_k = i\hbar\epsilon_{ijk}\hat{S}_k$.
Then

$$\exp\left[\frac{i\omega t}{\hbar}\hat{S}_z\right]\hat{S}_x\exp\left[-\frac{i\omega t}{\hbar}\hat{S}_z\right] = \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{i\omega t}{\hbar}\right)^n\left[\hat{S}_z,\, \hat{S}_x\right]_{(n)}$$

$$\begin{aligned} &= \hat{S}_x + \frac{i\omega t}{\hbar}(i\hbar)\hat{S}_y + \left(\frac{i\omega t}{\hbar}\right)^2\frac{\hbar^2}{2!}\hat{S}_x + \left(\frac{i\omega t}{\hbar}\right)^3\frac{i\hbar^3}{3!}\hat{S}_y + \dots \\ &= \cos(\omega t)\hat{S}_x - \sin(\omega t)\hat{S}_y\,; \end{aligned}$$

$$\exp\left[\frac{i\omega t}{\hbar}\hat{S}_z\right]\hat{S}_y\exp\left[-\frac{i\omega t}{\hbar}\hat{S}_z\right] = \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{i\omega t}{\hbar^n}\right)^n\left[\hat{S}_z,\, \hat{S}_y\right]_{(n)}$$

$$\begin{aligned} &= \hat{S}_y + \frac{i\omega t}{\hbar}(-i\hbar)\hat{S}_x + \left(\frac{i\omega t}{\hbar}\right)^2\frac{\hbar^2}{2!}\hat{S}_y + \left(\frac{i\omega t}{\hbar}\right)^3\frac{-i\hbar^3}{3!}\hat{S}_x + \dots \\ &= \cos(\omega t)\hat{S}_y + \sin(\omega t)\hat{S}_x\,. \end{aligned}$$

Solutions to previous control questions

6.3 The integrals to perform are

$$\langle \hat{p}_x \rangle_{|\psi\rangle} = \int\limits_{-\infty}^{\infty} \mathrm{d}x \psi^*(x)(-i\hbar)\frac{\partial}{\partial x}\psi(x)$$

$$= \frac{-i\hbar}{\sqrt{\pi}d}\int\limits_{-\infty}^{\infty} \mathrm{d}x \left(ip_x - \frac{x}{d^2}\right)\exp\left(-\frac{x^2}{d^2}\right) = \frac{\hbar p_x}{\sqrt{\pi}d}\sqrt{\pi}d = \hbar p_x\,,$$

where the symmetry of integrating an odd function over an even interval has been used to deal with the term $\propto x/d^2$.

Solutions to previous control questions

6.3 and

$$\langle \hat{p}_x^2\rangle_{|\psi\rangle} = \int\limits_{-\infty}^{\infty} \mathrm{d}x\psi^*(x)(-i\hbar)^2\frac{\partial^2}{\partial x^2}\psi(x)$$

$$= \frac{-\hbar^2}{\sqrt{\pi}d}\int\limits_{-\infty}^{\infty}\mathrm{d}x\left(-p_x^2 - \frac{1}{d^2} + \frac{x^2}{d^4}\right)\exp\left(-\frac{x^2}{d^2}\right)$$

$$= \frac{\hbar^2(p_x^2 - 1/d^2)}{\sqrt{\pi}d}\sqrt{\pi}d + \frac{\hbar^2}{\sqrt{\pi}d}\frac{\sqrt{\pi}d^3}{2d^4} = \hbar^2 p_x^2 + \frac{\hbar^2}{2d^2}\,.$$

Together this yields the dispersion in $\mathcal{P}_x$ as given in lecture 4.

Hamiltonian operator

- The Hamiltonian operator for the one-dimensional harmonic oscillator reads

$$\hat{H} = \frac{1}{2m}\hat{p}_x^2 + \frac{k}{2}\hat{x}^2 = \frac{1}{2m}\hat{p}_x^2 + \frac{m\omega^2}{2}\hat{x}^2\,, \quad \text{where } \omega^2 = \frac{k}{m}\,.$$

Creation and annihilation operators

- Introducing creation/lowering ($\hat{a}_+ = \hat{a}^\dagger$) and annihilation/raising ($\hat{a}_- = \hat{a}$) operators through

$$\hat{a}_\pm = \frac{1}{\sqrt{2\hbar m\omega}}\left[m\omega\,\hat{x} \mp i\,\hat{p}_x\right]$$

- Employing $[\hat{x},\, \hat{p_x}] = i\hbar$, they fulfil

$$\begin{aligned}
[\hat{a_\pm},\, \hat{a_\pm}] &= \hat{a}_\pm\hat{a}_\pm - \hat{a}_\pm\hat{a}_\pm = 0\\
[\hat{a_\pm},\, \hat{a_\mp}] &= \frac{1}{2\hbar m\omega}\left[m\omega\,\hat{x} \mp i\,\hat{p}_x,\, m\omega\,\hat{x} \pm i\,\hat{p}_x\right]\\
&= \frac{1}{2\hbar m\omega}\left(\left[m\omega\hat{x},\, \pm i\hat{p}_x\right] + \left[\mp i\hat{p}_x,\, m\omega\hat{x}\right]\right)\\
&= \pm\frac{i}{\hbar}\,[\hat{x},\, \hat{p_x}] = \mp 1\,.
\end{aligned}$$

Expressing the Hamiltonian through $\hat{a}_\pm$

- Invert the definition to express $\hat{x}$ and $\hat{p}_x$ through $\hat{a}_\pm$:

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left[\hat{a}_+ + \hat{a}_-\right] \quad \text{and} \quad \hat{p}_x = i\sqrt{\frac{\hbar m\omega}{2}}\left[\hat{a}_+ - \hat{a}_-\right]$$

- Insert into $\hat{H}$:

$$\begin{aligned}\hat{H} &= -\frac{1}{2m}\frac{\hbar m\omega}{2}\left[\hat{a}_+ - \hat{a}_-\right]^2 + \frac{m\omega^2}{2}\frac{\hbar}{2m\omega}\left[\hat{a}_+ + \hat{a}_-\right]^2 \\ &= \frac{\hbar\omega}{2}\left[\hat{a}_+\hat{a}_- + \hat{a}_-\hat{a}_+\right] = \hbar\omega\left[\hat{a}_+\hat{a}_- + \frac{1}{2}\right] \equiv \hbar\omega\left[\hat{N} + \frac{1}{2}\right],\end{aligned}$$

where $\hat{a}_-\hat{a}_+ = \hat{a}_+\hat{a}_- - [\hat{a_+}, \hat{a_-}]$ has been used, and where the *number operator* $\hat{N} = \hat{a}_+\hat{a}_-$ has been defined.

Commutators

- Calculate

$$\begin{aligned}\left[\hat{N},\,\hat{a_+}\right] &= \hat{a}_+\hat{a}_-\hat{a}_+ - \hat{a}_+\hat{a}_+\hat{a}_- = \hat{a}_+\left[\hat{a_-},\,\hat{a_+}\right] = \hat{a}_+\\ \left[\hat{N},\,\hat{a_-}\right] &= \hat{a}_+\hat{a}_-\hat{a}_- - \hat{a}_-\hat{a}_+\hat{a}_- = \left[\hat{a_+},\,\hat{a_-}\right]\hat{a}_- = -\hat{a}_-\,.\end{aligned}$$

and therefore $\boxed{\left[\hat{H},\,\hat{a_\pm}\right] = \hbar\omega\left[\hat{N},\,\hat{a_\pm}\right] = \pm\hbar\omega\hat{a}_\pm.}$

Energy eigenstates: ground state

- Denoting eigenstates $|E\rangle$ of the Hamiltonian as *energy eigenstates*

$$\begin{aligned}\hat{H}\,|E\rangle &= E\,|E\rangle \\ \longrightarrow &\quad \hat{H}\hat{a}_\pm\,|E\rangle = \left(\hat{a}_\pm\hat{H} \pm \hbar\omega\hat{a}_\pm\right)|E\rangle = (E \pm \hbar\omega)\,\hat{a}_\pm\,|E\rangle\end{aligned}$$

- Therefore, also state $\hat{a}_\pm\,|E\rangle$ are eigenstates of the Hamiltonian, with eigenvalues $E \pm \hbar\omega$, so these operators were rightly introduced as raising and lowering operators, since this is what they do.
- As the Hamiltonian only contains squares of Hermitean operators, the *energy eigenvalues must be non-negative*.
  This implies that if $|E_0\rangle$ is the lowest energy eigenstate,

$$\hat{a}_-\,|E_0\rangle \stackrel{!}{=} 0$$

  because otherwise $(E_0 - \hbar\omega)$ would be a lower energy.

Energy eigenstates: excited states

- Lowest energy E_0 given by multiplying $\hat{a}_- |E\rangle = 0$ from the left with $\hbar\omega\hat{a}_+$:

$$\begin{aligned}\hbar\omega\hat{a}_+\hat{a}_- |E_0\rangle &= \hbar\omega\hat{N}|E_0\rangle = \left(\hat{H} - \frac{\hbar\omega}{2}\right)|E_0\rangle = 0 \\ \longrightarrow & \quad \hat{H}|E_0\rangle = E_0|E_0\rangle = \frac{\hbar\omega}{2}|E_0\rangle \quad \longrightarrow \quad E_0 = \frac{\hbar\omega}{2}\,.\end{aligned}$$

- Applying the raising operator $\hat{a}_+$ n-times on $|E_0\rangle$ thus yields

$$\hat{a}_+^n |E_0\rangle = |E_n\rangle \quad \text{and} \quad \hat{H}|E_n\rangle = E_n|E_n\rangle = \left(n + \frac{1}{2}\right)\hbar\omega|E_n\rangle$$

Energy eigenstates: normalisation

- Demanding that $\langle E_n|E_n\rangle = 1$ yields normalisation constant C_n:

$$|E_{n+1}\rangle = C_{n+1}\hat{a}_+\,|E_n\rangle \quad \longleftrightarrow \quad 1 = \langle E_{n+1}|E_{n+1}\rangle = |C_{n+1}|^2 \langle E_n\,|\hat{a}_-\hat{a}_+|\,E_n\rangle$$

- Use $\hat{a}_-\hat{a}_+ = \hat{H}/(\hbar\omega) + 1/2$ and remember that $\langle E_n|E_n\rangle = 1$:

$$\begin{aligned} 1 &= |C_{n+1}|^2 \langle E_n\,|\hat{a}_-\hat{a}_+|\,E_n\rangle = |C_{n+1}|^2 \left(n + \frac{1}{2} + \frac{1}{2}\right) \langle E_n|E_n\rangle \\ &= |C_{n+1}|^2 (n+1) \quad \longleftrightarrow \quad C_{n+1} = \frac{1}{\sqrt{n+1}}\,. \end{aligned}$$

- Therefore $\hat{a}_+\,|E_n\rangle = \sqrt{n+1}\,|E_{n+1}\rangle$ and

$$|E_n\rangle = \frac{1}{\sqrt{n!}}\hat{a}_+^n\,|E_0\rangle$$

Calculating expectation values

- By expressing $\hat{x}$ and $\hat{p}_x$ in terms of the creation and annihilation operators, it is possible to calculate expectation values of various operators with respect to the energy eigenstates. For example

$$\begin{aligned}\left\langle E_0 \left| \hat{x^4} \right| E_0 \right\rangle &= \frac{\hbar^2}{4m^2\omega^2} \left\langle E_0 \left| \hat{a}_+^4 + \hat{a}_+^3\hat{a}_- + \ldots \right| E_0 \right\rangle \\ \xrightarrow{\hat{a}_-|E_0\rangle=0,\ \langle E_0|\hat{a}_+=0} & \frac{\hbar^2}{4m^2\omega^2} \left\langle E_0 \left| \left(\hat{a}_-^2\hat{a}_+^2 + \hat{a}_-\hat{a}_+\hat{a}_-\hat{a}_+\right) \right| E_0 \right\rangle \\ = & \frac{\hbar^2}{4m^2\omega^2} \left\langle E_0 \left| (2+1) \right| E_0 \right\rangle = \frac{3\hbar^2}{4m^2\omega^2}\,,\end{aligned}$$

where it has been used that, ultimately, in order to allow a non-vanishing sandwich between the ground states, there must be equal numbers of raising and lowering operators.

Representing operators in the $|E_n\rangle$-base

- Since the $|E_n\rangle$ are the eigenkets of both the Hamiltonian and the number operator, both being Hermitean, they form an orthonormal base with

$$\langle E_k|E_n\rangle = \delta_{kn}\,.$$

The two operators are diagonal when expressed in this base:

$$\hat{H} = \frac{\hbar\omega}{2}\begin{pmatrix} 1 & 0 & 0 & \dots \\ 0 & 3 & 0 & \dots \\ 0 & 0 & 5 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \quad \text{and} \quad \hat{N} = \begin{pmatrix} 0 & 0 & 0 & \dots \\ 0 & 1 & 0 & \dots \\ 0 & 0 & 2 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

- In contrast the matrix elements of the ladder operators read

$$(\hat{a}_+)_{kn} = \sqrt{n+1}\,\delta_{k(n+1)} \quad \text{and} \quad (\hat{a}_-)_{kn} = \sqrt{k+1}\,\delta_{(k+1)n}$$

or, explicitly,

$$\hat{a}_+ = \begin{pmatrix} 0 & 0 & 0 & \dots \\ \sqrt{1} & 0 & 0 & \dots \\ 0 & \sqrt{2} & 0 & \dots \\ 0 & 0 & \sqrt{3} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \quad \hat{a}_- = \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \dots \\ 0 & 0 & \sqrt{2} & 0 & \dots \\ 0 & 0 & 0 & \sqrt{3} & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

- This also allows to reconstruct the matrix representation of $\hat{x}$ and $\hat{p}_x$ by summing the two operators above and multiplying with appropriate factors.

Going to position space

- Identifying and using $x \longrightarrow \zeta = \sqrt{m\omega/\hbar}\,x$:

$$0 = \langle x\,|\hat{a_-}|\,E_0\rangle = \frac{1}{\sqrt{2\hbar m\omega}}\left\langle x\left|\left(m\omega\hat{x}+i\hat{p}_x\right)\right|E_0\right\rangle$$
$$= \frac{1}{\sqrt{2\hbar m\omega}}\left(m\omega x+\hbar\frac{\mathrm{d}}{\mathrm{d}x}\right)\psi_0(x) = \frac{1}{\sqrt{2}}\left(\zeta+\frac{\mathrm{d}}{\mathrm{d}\zeta}\right)\psi_0(\zeta)\,,$$

- The solution is given by

$$\psi_0(x) = N_0\exp\left(-\frac{m^2\omega^2x^2}{2\hbar}\right) = \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}}\exp\left(-\frac{m^2\omega^2x^2}{2\hbar}\right)\,.$$

- The wave functions of higher excitation states are obtained by repeatedly applying $\hat{a}_+$ in position space:

$$\begin{aligned}\psi_n(\zeta) &= \frac{1}{\sqrt{n!}}\left[\frac{1}{\sqrt{2}}\left(\zeta - \frac{\mathrm{d}}{\mathrm{d}\zeta}\right)\right]^n \psi_0(\zeta) \\ &= \left(\frac{m\omega}{\hbar\pi(2^n n!)^2}\right)^{\frac{1}{4}} \exp\left(-\frac{\zeta^2}{2}\right) H_n(\zeta)\,,\end{aligned}$$

where the H_n are Hermite's polynomials of order n encountered in last term's lecture in the Foundations of Physics module. In fact, returning from ζ to x, the result obtained there is found again here.

Learning outcomes

- Hamiltonian operator of an 1-dimensional harmonic oscillator expressed by position and momentum operators and by raising and lowering operators.
- Raising and lowering operators and their algebra: their commutators among themselves and with the Hamiltonian and the number operator.
- Energy eigenstates as obtained through multiple application of raising and lowering operators, and their normalisation.
- Operators represented in the energy base.
- Calculating expectation values of operators.
- Position space wave functions.

Control questions

7.1 Consider a one-dimensional harmonic oscillator and calculate the following expectation values:

$$\left\langle E_0 \left| \hat{x^2} \right| E_0 \right\rangle, \left\langle E_0 \left| \hat{p^2} \right| E_0 \right\rangle$$

and check that the virial theorem holds true for the ground state of the system (kinetic and potential energy identical).

7.2 Add a homogeneous electrical field E to the harmonic oscillator such that its Hamiltonian reads

$$\hat{H} = \frac{1}{2m}\hat{p}_x^2 + \frac{m\omega^2}{2}\hat{x}^2 + eE\hat{x}\,,$$

where e is the charge of the particle.
By completing the square, bring this Hamiltonian to a form quadratic in generalised position and momentum operators plus some constant terms. Transform to raising and lowering operators and calculate the energy eigenvalues.

7.3 The Hamiltonian of the fermionic harmonic oscillator is given by

$$\hat{H} = \epsilon \hat{N} = \epsilon \hat{b}^\dagger \hat{b}\,,$$

with ϵ a positive number with units of energy and the creation and annihilation operators satisfying

$$\left\{\hat{b}^\dagger,\, \hat{b}\right\} \;=\; 1 \quad \text{and} \quad \hat{b}^2 = \left(\hat{b}^\dagger\right)^2 = 0\,.$$

(a) Show that $\hat{N}$ is Hermitian and $\hat{N}^2 = \hat{N}$.
(b) What are therefore the eigenvalues of $\hat{N}$ and $\hat{H}$ and the eigenstates?
(c) Construct the spectrum of $\hat{H}$ by calculating suitable commutators of $\hat{N}$, $\hat{b}$ and $\hat{b}^\dagger$, starting from a ground state $|0\rangle$.