Theoretical Physics II B – Quantum Mechanics

Lecture 9

Frank Krauss

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1. The Schrödinger equation revisited

2. Two-body systems

Solutions to previous control questions

7.1 Inserting the expressions for $\hat{x}$ and $\hat{p}$ as functions of $\hat{a}_\pm$:

$$\begin{aligned}
\left\langle E_0 \left| \hat{x}^2 \right| E_0 \right\rangle &= \left\langle E_0 \left| \left[\frac{\hbar}{2m\omega} \left(\hat{a}_+^2 + \hat{a}_+\hat{a}_- + \hat{a}_-\hat{a}_+ + \hat{a}_-^2 \right) \right] \right| E_0 \right\rangle \\
&= \left\langle E_0 \left| \frac{\hbar}{2m\omega} \left(\hat{a}_-\hat{a}_+ \right) \right| E_0 \right\rangle = \frac{\hbar}{2m\omega} \\
\left\langle E_0 \left| \hat{p}^2 \right| E_0 \right\rangle &= \left\langle E_0 \left| \left[-\frac{\hbar m\omega}{2} \left(\hat{a}_+^2 - \hat{a}_+\hat{a}_- - \hat{a}_-\hat{a}_+ + \hat{a}_-^2 \right) \right] \right| E_0 \right\rangle \\
&= \frac{\hbar m\omega}{2} \left\langle E_0 \left| \frac{\hbar m\omega}{2} \left(\hat{a}_-\hat{a}_+ \right) \right| E_0 \right\rangle = \frac{\hbar m\omega}{2} \,,
\end{aligned}$$

where we have used that

$$\langle E_0 | \, \hat{a}_+ = \hat{a}_- \, | E_0 \rangle = 0 \quad \text{and} \quad \hat{a}_-\hat{a}_+ = -\left[\hat{a}_+, \, \hat{a}_-\right] + \hat{a}_+\hat{a}_- = \hat{1} + \hat{a}_+\hat{a}_- \,.$$

Solutions to previous control questions

7.1 Continued: The virial theorem states that, in average, kinetic and potential energy are equal, $\langle T\rangle = \langle V\rangle$. In the ground state, they are

$$\begin{aligned}\langle T\rangle &= \frac{1}{2m}\left\langle E_0\left|\hat{p}^2\right|E_0\right\rangle = \frac{\hbar\omega}{4}\\ \langle V\rangle &= \frac{m\omega^2}{2}\left\langle E_0\left|\hat{x}^2\right|E_0\right\rangle = \frac{\hbar\omega}{4}\end{aligned}$$

confirming its validity for the ground state of the one-dimensional harmonic oscillator in quantum mechanics:

$$\langle E\rangle = \frac{\hbar\omega}{2} = \langle T\rangle + \langle V\rangle = \frac{\langle T\rangle}{2} + \frac{\langle V\rangle}{2}\,.$$

Solutions to previous control questions

7.2 Completing the square yields

$$\frac{m\omega^2}{2}\hat{x}^2 + eE\hat{x} = \frac{m\omega^2}{2}\left(\hat{x} + \frac{eE}{m\omega^2}\right)^2 - \frac{(eE)^2}{2m\omega^2} = \frac{m\omega^2}{2}\hat{x}'^2 - x_0^2$$

and therefore the Hamiltonian can be rewritten as

$$\hat{H} = \frac{1}{2m}\hat{p}_x^2 + \frac{m\omega^2}{2}\hat{x}'^2 - x_0^2$$

As before, but with $\hat{x} \to \hat{x'}$, the raising and lowering operators are:

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

and they enjoy the same commutation relations as before.

Solutions to previous control questions

7.2 Continued: This allows to introduce, as before, the number operator $\hat{N}' = \hat{a}'_+\hat{a}'_- + \hat{a}'_-\hat{a}'_+$. Therefore the Hamiltonian reads

$$\hat{H} = \hat{N}' + \frac{1}{2} - x_0^2\,.$$

This implies a shift of the ground state and all other energies, lowering them by x_0^2:

$$E'_n = \left(n + \frac{1}{2}\right)\hbar\omega - x_0^2 = \left(n + \frac{1}{2}\right)\hbar\omega - \frac{(eE)^2}{2m\omega^2}\,.$$

Solutions to previous control questions

7.3 A little bit of care has to be taken due to the anticommutators.

(a) Hermiticity:

$$\hat{N}^\dagger = \left[\hat{b}^\dagger\hat{b}\right]^\dagger = \hat{b}^\dagger\left(\hat{b}^\dagger\right)^\dagger = \hat{b}^\dagger\hat{b}.$$

Direct calculation:

$$\hat{N}^2 = \hat{b}^\dagger\hat{b}\hat{b}^\dagger\hat{b} = \hat{b}^\dagger\left[1-\hat{b}^\dagger\hat{b}\right]\hat{b} = \hat{b}^\dagger\hat{b} = \hat{N}\,.$$

(b) Because of that, the eigenvalues λ must satisfy $\lambda^2 = \lambda$, therefore $\lambda = 0,\,1$. As a consequence there are two eigenstates, $|0\rangle$ and $|1\rangle$.

(c) Again, brute force:

$$\left[\hat{N},\,\hat{b}^{(\dagger)}\right] = \hat{b}^\dagger\hat{b}\hat{b}^{(\dagger)} - \hat{b}^{(\dagger)}\hat{b}^\dagger\hat{b} = \left\{\begin{array}{lcl} 0-\left(1-\hat{b}^\dagger\hat{b}\right)\hat{b} & = & -\hat{b} \\ \hat{b}^\dagger\left(1-\hat{b}^\dagger\hat{b}\right)-0 & = & \hat{b}^\dagger \end{array}\right.$$

Solutions to previous control questions

7.3 Continued:

(c) Now check the effect of $\hat{b}^{(\dagger)}$ on the state $|0\rangle$:

$$\begin{aligned}\hat{N}\left(\hat{b}^\dagger|0\rangle\right) &= \left(\left[\hat{N},\,\hat{b}^\dagger\right]+\hat{b}^\dagger\hat{N}\right)|0\rangle = (n_0+1)\left(\hat{b}^\dagger|0\rangle\right) = \left(\hat{b}^\dagger|0\rangle\right)\\ \hat{N}\left(\hat{b}|0\rangle\right) &= \hat{b}^\dagger\hat{b}\hat{b}|0\rangle = 0\,.\end{aligned}$$

Therefore $\hat{b}$ annihilates the ground state, and $\hat{b}^\dagger|0\rangle = |1\rangle$. Obviously, now,

$$\hat{b}^\dagger|1\rangle = \hat{b}^\dagger\hat{b}^\dagger|0\rangle = 0\,,$$

indicating that $|1\rangle$ is the only state other than the ground state.

Time evolution of a system

- Describing a system by the time-dependent state vector $|\psi(t)\rangle$, its time-evolution is governed by

Postulate 7: The time evolution of a system is determined by the time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \ ,$$

where $\hat{H}$ is the Hamiltonian operator of the system, also called the total energy operator.

Some example Hamiltonians

- N-particle system with potential V:

$$\hat{H} = \sum_{i=1}^{N} \left(\frac{\underline{\hat{p}}_i^2}{2m_i}\right) + \hat{V}(\underline{\hat{r}}_1, \underline{\hat{r}}_2, \ldots, \underline{\hat{r}}_N, t)\,;$$

- Particle with mass m and charge q moving in a vector potential $\underline{A}$ and scalar potential ϕ:

$$\begin{aligned} \hat{H} &= \frac{1}{2m}\left[\underline{\hat{p}} - q\underline{\hat{A}}(\underline{\hat{r}}, t)\right]^2 + q\hat{\phi}(\underline{\hat{r}}, t) \\ &= \frac{\underline{\hat{p}}^2}{2m} + \frac{q}{2m}\left(\underline{\hat{A}}\cdot\underline{\hat{p}} + \underline{\hat{p}}\cdot\underline{\hat{A}}\right) + \frac{q^2}{2m}\underline{\hat{A}}^2 + q\hat{\phi}\,, \end{aligned}$$

where operator products have been symmetrised to guarantee Hermiticity of the Hamiltonian.

Time evolution operator: Definition

- The structure of the Schrødinger equation indicates that $\psi(t)$ is determined for all times t, once it is defined at some time t_0. This allows to introduce a *time evolution operator* $\hat{U}(t,\, t_0)$ such that

$$|\psi(t)\rangle = \hat{U}(t,\, t_0)\,|\psi(t_0)\rangle \quad \text{with} \quad \hat{U}(t_0, t_0) = \hat{\mathbf{1}}\,.$$

- In addition the time evolution operator fulfils

$$\begin{array}{rcl} \hat{U}(t,\, t_0) & = & \hat{U}(t,\, t')\hat{U}(t',\, t_0) \\ \hat{U}^{-1}(t,\, t_0) & = & \hat{U}(t_0,\, t)\,, \end{array}$$

indicating the non-Abelian group property of time evolution.

Time evolution operator: Construction

- Substituting the definition $|\psi(t)\rangle = \hat{U}(t,\, t_0)\,|\psi(t_0)\rangle$ into the Schrödinger equation yields a differential equation for the time evolution operator:

$$i\hbar\frac{\partial}{\partial t}\hat{U}(t,\, t_0) = \hat{H}\hat{U}(t,\, t_0)$$

- A general solution is given by:

$$\hat{U}(t,\, t_0) = \exp\left[-\frac{i}{\hbar}\int\limits_{t_0}^{t}\mathrm{d}t'\,\hat{H}(t')\right] \stackrel{\text{time-indep.}}{\longrightarrow} \exp\left[-\frac{i}{\hbar}\hat{H}(t-t_0)\right]\,,$$

where the right expression relates to *time-independent* Hamiltonians.

Unitarity of the time evolution operator

- Conservation of probability (a.k.a. "unitarity") demands

$$\begin{aligned}\langle\psi(t_0)|\psi(t_0)\rangle &= \langle\psi(t)|\psi(t)\rangle = \left\langle \hat{U}(t,\,t_0)\psi(t_0)\middle|\hat{U}(t,\,t_0)\psi(t_0)\right\rangle\\ &= \left\langle\psi(t_0)\middle|\hat{U}^\dagger(t,\,t_0)\hat{U}(t,\,t_0)\middle|\psi(t_0)\right\rangle \longrightarrow \hat{U}^\dagger(t,\,t_0)\hat{U}(t,\,t_0) = \hat{\mathbf{1}}\,,\end{aligned}$$

and therefore $\hat{U}$ must be unitary.

Infinitesimal time translations

- This property is related to the Hermiticity of the Hamiltonian, made explicit by considering infinitesimal time evolution:

$$i\hbar\left[\hat{U}(t_0+\delta t,\, t_0) - \hat{U}(t_0,\, t_0)\right] = \hat{H}(t_0)\delta t$$

and therefore

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

allowing to interpret the Hamiltonian as generator of infinitesimal time translations.

Expectation values

- Clearly, expectation values of observables $\mathcal{A}$ with respect to states $|\psi(t)\rangle$ will vary, with a rate of change given by

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\langle\mathcal{A}\rangle_{|\psi(t)\rangle} = \frac{\mathrm{d}}{\mathrm{d}t}\left\langle\psi(t)\left|\hat{A}\right|\psi(t)\right\rangle \\
&= \left\langle\frac{\mathrm{d}}{\mathrm{d}t}\psi(t)\left|\hat{A}\right|\psi(t)\right\rangle + \left\langle\psi(t)\left|\frac{\partial}{\partial t}\hat{A}\right|\psi(t)\right\rangle + \left\langle\psi(t)\left|\hat{A}\right|\frac{\mathrm{d}}{\mathrm{d}t}\psi(t)\right\rangle \\
&= \frac{i}{\hbar}\left[\left\langle\hat{H}\psi(t)\left|\hat{A}\right|\psi(t)\right\rangle - \left\langle\psi(t)\left|\hat{A}\right|\hat{H}\psi(t)\right\rangle\right] + \left\langle\psi(t)\left|\frac{\partial\hat{A}}{\partial t}\right|\psi(t)\right\rangle \\
&= \frac{i}{\hbar}\left\langle\psi(t)\left|\left[\hat{H},\,\hat{A}\right]\right|\psi(t)\right\rangle + \left\langle\psi(t)\left|\frac{\partial\hat{A}}{\partial t}\right|\psi(t)\right\rangle
\end{aligned}
$$

- Therefore

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle \hat{A}\right\rangle = \frac{i}{h}\left\langle \left[\hat{H},\,\hat{A}\right]\right\rangle + \left\langle \frac{\partial\hat{A}}{\partial t}\right\rangle$$

- If $\hat{A}$ is not explicitly time-dependent, then $\partial\hat{A}/\partial t = 0$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle \hat{A}\right\rangle = \frac{i}{h}\left\langle \left[\hat{H},\,\hat{A}\right]\right\rangle$$

- If, in addition, $\hat{A}$ commutes with the Hamilton operator, its expectation value (and, of course, that of the observable $\mathcal{A}$) do not vary with time, and $\mathcal{A}$ *is a constant of motion*.

Energy conservation

- As an example, consider a time-independent Hamiltonian, related to the total energy $\mathcal{E}$ of the system as observable:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\langle\mathcal{E}\right\rangle = \frac{\mathrm{d}}{\mathrm{d}t}\left\langle\hat{H}\right\rangle = \frac{i}{h}\left\langle\left[\hat{H},\,\hat{H}\right]\right\rangle = 0\,,$$

which thus becomes a constant.

- For time-independent Hamiltonians, the energy eigenkets $|\psi_E(t)\rangle$ have a time evolution which is just a rotation in complex space:

$$|\psi_E(t)\rangle = \exp\left[-\frac{iEt}{\hbar}\right]|\psi_E\rangle$$

The virial theorem

- Consider a particle in a potential V, with Hamiltonian

$$\hat{H} = \frac{\underline{\hat{p}}^2}{2m} + \hat{V}(\underline{r})$$

and consider the observable $\hat{A} = \underline{\hat{r}} \cdot \underline{\hat{p}}$. Its time evolution is given by the expectation value of the commutator with the Hamiltonian:

$$\begin{aligned}\left[\underline{\hat{r}} \cdot \underline{\hat{p}},\, \hat{H}\right] &= \left[(\hat{x}\hat{p}_x + \hat{y}\hat{p}_y + \hat{z}\hat{p}_z),\, \frac{1}{2m}\left(\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2\right) + \hat{V}(\hat{x},\, \hat{y},\, \hat{z})\right] \\ &= \frac{i\hbar}{m}\left(\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2\right) - i\hbar\left(\frac{\hat{x}\partial\hat{V}}{\partial\hat{x}} + \frac{\hat{y}\partial\hat{V}}{\partial\hat{y}} + \frac{\hat{z}\partial\hat{V}}{\partial\hat{z}}\right) \\ &= 2i\hbar\hat{T} - i\hbar\left(\underline{\hat{r}} \cdot \underline{\nabla}\hat{V}\right),\end{aligned}$$

where T is the kinetic energy of the particle.

- Therefore, if $\mathrm{d}\langle\hat{\underline{r}}\cdot\hat{\underline{p}}\rangle/\mathrm{d}t = 0$,

$$2\left\langle\hat{T}\right\rangle = \left\langle\hat{\underline{r}}\cdot\underline{\nabla}\hat{V}\right\rangle$$

and for central potentials of the form $V(r) = r^n$

$$2\left\langle\mathcal{T}\right\rangle = n\left\langle\mathcal{V}\right\rangle\,.$$

Classical Hamiltonian

- As you know, the classical two-particle Hamiltonian

$$H = \frac{\underline{p}_1^2}{2m_1} + \frac{\underline{p}_2^2}{2m_2} + V(\underline{r}_1 - \underline{r}_2)$$

can effectively be cast into a one-particle Hamiltonian

$$H = \frac{\underline{P}^2}{2M} + \frac{\underline{p}^2}{2\mu} + V(\underline{r})$$

by introducing total and relative coordinates

$$\begin{aligned} \underline{r} &= \underline{r}_1 - \underline{r}_2 & \underline{R} &= \frac{m_1\underline{r}_1 + m_2\underline{r}_2}{m_1 + m_2} \\ \underline{p} &= \frac{m_1\underline{p}_1 - m_2\underline{p}_2}{m_1 + m_2} & \underline{P} &= \underline{p}_1 + \underline{p}_2 \\ M &= m_1 + m_2 & \mu &= \frac{m_1 m_2}{m_1 + m_2} \end{aligned}$$

Structure of the solution

- When analysing the equations of motion it becomes quickly apparent that the total system moves with constant momentum, while the relative motion of the two particles w.r.t each other and to the centre-of-mass system decouples.

Structure of the solution

- The same procedure can be applied in quantum mechanics - there just all dynamical quantities – positions and momenta – become operators. Expressed in energy eigenvalues this allows to write a state ket, which separates total and relative momenta and positions:

$$|\Psi\rangle = |\Phi\rangle\,|\psi\rangle\ ,$$

where

$$\frac{\hat{\underline{P}}^2}{2M}\,|\Phi\rangle = E_{\rm cm}\,|\Phi\rangle \quad \text{and} \quad \left[\frac{\hat{\underline{p}}^2}{2\mu} - V(\hat{\underline{r}})\right]|\psi\rangle = E_{\rm rel}\,|\psi\rangle\ .$$

Expressed through position space wave functions this becomes

$$\Psi(\underline{R},\,\underline{r},\,t) = \Phi(\underline{R})\psi(\underline{r})\,\exp\left[-\frac{i(E_{\rm cm}+E_{\rm rel})t}{\hbar}\right]$$

with

$$\left[\frac{\hbar^2}{2M}\hat{\underline{\nabla}}_R^2 + E_{\rm cm}\right]\Phi(\underline{R}) = 0 \quad \text{and} \quad \left[\frac{\hbar^2}{2\mu}\hat{\underline{\nabla}}_r^2 + E_{\rm rel} - V(\underline{r})\right]\psi(\underline{r}) = 0$$

Learning outcomes

- Schrödinger equation for kets
- Formal solution through unitary time evolution operator and its explicit form as given by the Hamiltonian
- Hamiltonian as generator of infinitesimal time translations

Control questions

9.1 Consider a spin-$\frac{1}{2}$ particle with magnetic moment $\mu = e\hbar/(2mc)$ in a magnetic field $\underline{B} = B\underline{e}_z$ oriented along the z-axis. The Hamiltonian is given by

$$\hat{H} = -\mu\underline{\hat{\sigma}} \cdot \underline{B} = -\frac{eB}{mc}\hat{S}_z = \omega\hat{S}_z\,.$$

Here $\hat{S}_i = \frac{\hbar}{2}\sigma_i$, with $\hat{\sigma}_i$ the Pauli matrices satisfying $\hat{\sigma}_i^2 = \hat{\mathbf{1}}$, $[\hat{\sigma}_i,\,\hat{\sigma}_j] = 2i\epsilon_{ijk}\hat{\sigma}_k$, and in explicit representation

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\,,\quad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\,,\quad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\,.$$

For this system:

(a) Determine eigenvalues and normalised eigenkets of this Hamiltonian.

(b) Construct the time evolution operator $\hat{U}(t,\, t_0)$ of the system and apply it to a state ket $|\psi\rangle$ expressed as linear combination of the two eigenkets.

(c) Calculate the time evolution of the expectation value of the energy (through the Hamilton operator), and of the spin in z-direction (through the operator $\hat{S}_z$).

(d) What is the time evolution of the spin in x- and in y-direction for a system given by a ket $|\psi_0\rangle$ that at some inital time $t_0 = 0$ is defined as linear combination of the two energy eigenkets

$$|\psi_0\rangle = \frac{1}{\sqrt{2}}\left[|e_+\rangle + |e_-\rangle\right]?$$