Theoretical Physics II B – Quantum Mechanics

Lecture 12

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Solutions to previous control questions

11.1 Properties of $\hat{T}(\mathrm{d}\underline{x}) = \hat{\mathbf{1}} - i\underline{\hat{K}} \cdot \mathrm{d}\underline{x}$, where the components of $\underline{\hat{K}}$ are Hermitean operators:

- Unitarity:

$$\begin{aligned}\hat{\mathbf{1}} &= \hat{T}^\dagger(\mathrm{d}\underline{x})\hat{T}(\mathrm{d}\underline{x}) = \left[\hat{\mathbf{1}} + i\underline{\hat{K}}^\dagger \cdot \mathrm{d}\underline{x}\right]\left[\hat{\mathbf{1}} - i\underline{\hat{K}} \cdot \mathrm{d}\underline{x}\right] \\ &= \hat{\mathbf{1}} - i\underbrace{\left[\underline{\hat{K}} - \underline{\hat{K}}^\dagger\right]}_{=0} \cdot \mathrm{d}\underline{x} + \mathcal{O}(\mathrm{d}\underline{x}^2) \approx \hat{\mathbf{1}}\,,\end{aligned}$$

  where terms of order $\mathrm{d}\underline{x}^2$ are ignored;
- Composition:

$$\begin{aligned}\hat{T}(\mathrm{d}\underline{x}_1)\hat{T}(\mathrm{d}\underline{x}_2) &= \left[\hat{\mathbf{1}} - i\underline{\hat{K}} \cdot \mathrm{d}\underline{x}_1\right]\left[\hat{\mathbf{1}} - i\underline{\hat{K}} \cdot \mathrm{d}\underline{x}_2\right] \\ &= \hat{\mathbf{1}} - i\underline{\hat{K}} \cdot [\mathrm{d}\underline{x}_1 + \mathrm{d}\underline{x}_2] + \mathcal{O}(\mathrm{d}\underline{x}^2) \approx \hat{T}(\mathrm{d}\underline{x}_1 + \mathrm{d}\underline{x}_2)\,;\end{aligned}$$

- Form of the inverse:

$$\begin{aligned}\hat{\mathbf{1}} &= \hat{T}^\dagger(\mathrm{d}\underline{x})\hat{T}(-\mathrm{d}\underline{x}) = \left[\hat{\mathbf{1}} - i\underline{\hat{K}}\cdot\mathrm{d}\underline{x}\right]\left[\hat{\mathbf{1}} - i\underline{\hat{K}}\cdot(-\mathrm{d}\underline{x})\right] \\ &= \hat{\mathbf{1}} - i\underline{\hat{K}}\cdot(\mathrm{d}\underline{x} - \mathrm{d}\underline{x}) + \mathcal{O}(\mathrm{d}\underline{x}^2) \approx \hat{\mathbf{1}}\,;\end{aligned}$$

- Limit

$$\lim_{\mathrm{d}\underline{x}\to 0}\hat{T}(\mathrm{d}\underline{x}) = \hat{\mathbf{1}} - i\lim_{\mathrm{d}\underline{x}\to 0}\underline{\hat{K}}\cdot\mathrm{d}\underline{x} = \hat{\mathbf{1}}\,.$$

11.2 Playing with the ket $\frac{\hat{\mathbf{1}}\pm\hat{\pi}}{2}|n\rangle$:

$$\pi_n\left[\frac{\hat{\mathbf{1}}\pm\hat{\pi}}{2}|n\rangle\right]=\hat{\pi}\left[\frac{\hat{\mathbf{1}}\pm\hat{\pi}}{2}|n\rangle\right] \quad = \quad \frac{\hat{\pi}\pm\hat{\pi}^2}{2}|n\rangle=\pm\frac{\hat{\mathbf{1}}\pm\hat{\pi}}{2}|n\rangle\ ,$$

i.e. the eigenvalue of the ket under parity indeed is $\pi_n=\pm 1$.

$$\hat{H}\left[\frac{\hat{\mathbf{1}}\pm\hat{\pi}}{2}|n\rangle\right]=\frac{\hat{H}\pm\hat{H}\hat{\pi}}{2}|n\rangle=\frac{\hat{H}\pm\hat{\pi}\hat{H}}{2}|n\rangle=E_n\frac{\hat{\mathbf{1}}\pm\hat{\pi}}{2}|n\rangle$$

and because the energy eigenvalue is non-degenerate, there is only *one* eigenstate corresponding to it. This implies that

$$|n\rangle=\frac{\hat{\mathbf{1}}\pm\hat{\pi}}{2}|n\rangle \quad \text{and thus} \quad |n\rangle=\pm\hat{\pi}|n\rangle\ ,$$

where the sign signifies whether $|n\rangle$ is even or odd under parity transformations.

Rotation operators

- To play: Take a cuboid (like a book) and rotate by 90° around different axes. Check that such rotations do not commute.
- In general: represent rotations $\mathcal{R}$ in $\mathbf{R}^3$ by *orthogonal* 3×3 matrices $\hat{R}$ with real entries. (Orthogonal matrices satisfy $\hat{R}^T\hat{R} = \hat{R}\hat{R}^T = \hat{\mathbf{1}}$.)

$$\underline{V} \stackrel{\mathcal{R}}{\longrightarrow} \underline{V}' = \hat{R}\underline{V}$$

- They maintain the norm of any vector $\underline{V} = (V_x,\, V_y,\, V_Z)^T$:

$$||\underline{V}'|| = \sqrt{V_x'^2 + V_y'^2 + V_z'^2} = \sqrt{V_x^2 + V_y^2 + V_z^2} = ||\underline{V}||\,.$$

Representing rotations

- Rotations around different axes by an angle can be written as

$$\hat{R}_x(\phi_x) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\phi_x & -\sin\phi_x \\ 0 & \sin\phi_x & \cos\phi_x \end{pmatrix},$$

$$\hat{R}_y(\phi_y) = \begin{pmatrix} \cos\phi_y & 0 & \sin\phi_y \\ 0 & 1 & 0 \\ -\sin\phi_y & 0 & \cos\phi_y \end{pmatrix},$$

$$\hat{R}_z(\phi_z) = \begin{pmatrix} \cos\phi_z & -\sin\phi_z & 0 \\ \sin\phi_z & \cos\phi_z & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

- General rotations can be represented by a construction involving three *Euler angles* in consecutive rotations.
  Please check the literature if you want to know more.

Generating infinitesimal rotations

- The explicit form of the operators above refers to a notation, where the coordinate system has been fixed, and the vectors are rotated around. Had we, instead, rotated the axes in the coordinate system and kept the vectors fixed, we would have had to use the negative angles.
- Following our idea of last lecture, namely generating infinitesimally small spatial translations by applying the momentum operator, let us try to see which generators emerge when we generate infinitesimally small rotations.
- It will come as no surprise that these are related to angular momentum. However, because there are also internal degrees of freedom such as spin, related to rotations, it is a useful exercise to tackle this problem from a symmetry perspective.

Infinitesimal rotations

- Expanding up to terms of order ϵ^2, rotations around infinitesimal angles ϵ can be written as

$$\hat{R}_x(\epsilon) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1-\frac{\epsilon^2}{2} & -\epsilon \\ 0 & \epsilon & 1-\frac{\epsilon^2}{2} \end{pmatrix},$$

$$\hat{R}_y(\epsilon) = \begin{pmatrix} 1-\frac{\epsilon^2}{2} & 0 & \epsilon \\ 0 & 1 & 0 \\ -\epsilon & 0 & 1-\frac{\epsilon^2}{2} \end{pmatrix},$$

$$\hat{R}_z(\epsilon) = \begin{pmatrix} 1-\frac{\epsilon^2}{2} & -\epsilon & 0 \\ \epsilon & 1-\frac{\epsilon^2}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Commutation relations of infinitesimal rotation operators

- For example, consider $\left[\hat{R}_x(\epsilon),\ \hat{R}_y(\epsilon)\right]$:

$$
\begin{aligned}
\left[\hat{R}_x(\epsilon),\ \hat{R}_y(\epsilon)\right] &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1-\frac{\epsilon^2}{2} & -\epsilon \\ 0 & \epsilon & 1-\frac{\epsilon^2}{2} \end{pmatrix} \begin{pmatrix} 1-\frac{\epsilon^2}{2} & 0 & \epsilon \\ 0 & 1 & 0 \\ -\epsilon & 0 & 1-\frac{\epsilon^2}{2} \end{pmatrix} \\
&\quad - \begin{pmatrix} 1-\frac{\epsilon^2}{2} & 0 & \epsilon \\ 0 & 1 & 0 \\ -\epsilon & 0 & 1-\frac{\epsilon^2}{2} \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1-\frac{\epsilon^2}{2} & -\epsilon \\ 0 & \epsilon & 1-\frac{\epsilon^2}{2} \end{pmatrix} \\
&= \begin{pmatrix} 0 & -\epsilon^2 & 0 \\ \epsilon^2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \hat{R}_z(\epsilon^2) - \hat{\mathbf{1}} = \hat{R}_z(\epsilon^2) - \hat{R}_{\rm any}(0)\,,
\end{aligned}
$$

where terms of order $\mathcal{O}(\epsilon^{\ni})$ and higher have been ignored.

Infinitesimal rotations in quantum mechanics

- Remember the general form of infinitesimal transformations:

$$\hat{U} = \hat{\mathbf{1}} - i\hat{G}\epsilon\,,$$

  where $\hat{G}$ was the generator of the transformation.

  By now we have seen $\hat{G} = \hat{H}/\hbar$ and $\epsilon = \mathrm{d}t$ for translations in time, and $\hat{G} = \underline{\hat{p}}/\hbar$ and $\epsilon = \mathrm{d}\underline{x}$ for spatial translations.

- Knowing, from classical mechanics, that angular momentum is the generator of rotations, it makes sense to *define* the angular momentum operators $\underline{\hat{J}}/\hbar$ to fill the role of $\hat{G}$.
- Note that we have carefully avoided to define the angular momentum operator to be the (*orbital*) angular momentum, given by $\underline{\hat{L}} = \underline{\hat{x}} \times \underline{\hat{p}}$, since the aim is to descibe external (orbital) and internal (spin) degrees of freedom on the same base.

- Defining a *vectorial* rotation angle by an angle ϕ and a (normalised) axis $\underline{n}$,

$$\underline{\phi} = \underline{n}\,\phi$$

an infinitesimal rotation operator looks like

$$\hat{R}(\mathrm{d}\underline{\phi}) = \hat{R}_{\underline{n}}(\mathrm{d}\phi) = \hat{\mathbf{1}} - \frac{i\hat{\underline{J}}\cdot\mathrm{d}\underline{\phi}}{\hbar} = \hat{\mathbf{1}} - \frac{i\hat{\underline{J}}\cdot\underline{n}}{\hbar}\mathrm{d}\phi\,.$$

- Finite rotations can thus be obtained by repeatedly applying infinitely many infinitesimal rotations, leading to

$$\hat{R}(\underline{\phi}) = \lim_{N\to\infty}\left[\hat{\mathbf{1}} - \frac{i\hat{\underline{J}}\cdot\underline{\phi}}{N\hbar}\right]^N = \exp\left[-\frac{i\hat{\underline{J}}\cdot\underline{\phi}}{\hbar}\right]\,.$$

- Note that the explicit form of the operators $\hat{J}_i$ depends on the kets, they're acting on. Acting on 2-component kets describing a pin-$\frac{1}{2}$ state, they are represented by 2×2 matrices, while acting on spatial vectors with three components they are represented by 3×3 matrices, like the ones encountered before.

Group structure of rotations

- The following properties of groups are respected by rotations $\mathcal{R}_i$ around different axes, with different angles. Of course, they are also respected by their corresponding operators $\hat{R}$:
  - Identity: $\exists 1\ \text{(unique)}:\ \ \mathcal{R}\cdot 1 = 1\cdot\mathcal{R} = \mathcal{R}\ \ \forall\mathcal{R}$;
  - Closure: $\mathcal{R}_1\cdot\mathcal{R}_2 = \mathcal{R}_3\ \ \forall\mathcal{R}_{1,2}$;
  - Inverse element: $\forall\mathcal{R}:\ \ \exists\mathcal{R}^{-1}\ \text{(unique)},\ \ \mathcal{R}\cdot\mathcal{R}^{-1} = \mathcal{R}^{-1}\cdot\mathcal{R} = 1$, the identity element;
  - Associativity: $(\mathcal{R}_1\cdot\mathcal{R}_2)\cdot\mathcal{R}_3 = \mathcal{R}_1\cdot(\mathcal{R}_2\cdot\mathcal{R}_3)\ \ \forall\mathcal{R}_{1,2,3}$

Commutators, reloaded

- Calculating, once more, the commutators of two rotation operators and using the result obtained before,

$$\left[\exp(-\frac{i\hat{J}_x\epsilon}{\hbar}),\,\exp(-\frac{i\hat{J}_y\epsilon}{\hbar})\right]$$

$$\begin{aligned}
&= \left(1-\frac{i\hat{J}_x\epsilon}{\hbar}-\frac{\hat{J}_x^2\epsilon^2}{2\hbar^2}\dots\right)\left(1-\frac{i\hat{J}_y\epsilon}{\hbar}-\frac{\hat{J}_y^2\epsilon^2}{2\hbar^2}\dots\right)-\left(1-\frac{i\hat{J}_y\epsilon}{\hbar}-\frac{\hat{J}_y^2\epsilon^2}{2\hbar^2}\dots\right)\left(1-\frac{i\hat{J}_x\epsilon}{\hbar}-\frac{\hat{J}_x^2\epsilon^2}{2\hbar^2}\dots\right)\\
&= \left[1-\frac{i(\hat{J}_x+\hat{J}_y)\epsilon}{\hbar}-\frac{(2\hat{J}_x\hat{J}_y+\hat{J}_x^2+\hat{J}_y^2)\epsilon^2}{2\hbar^2}\dots\right]-\left[1-\frac{i(\hat{J}_x+\hat{J}_y)\epsilon}{\hbar}-\frac{(2\hat{J}_y\hat{J}_x+\hat{J}_x^2+\hat{J}_y^2)\epsilon^2}{2\hbar^2}\dots\right]\\
&= -\frac{\epsilon^2}{\hbar^2}\left[\hat{J}_x,\,\hat{J}_y\right]+\mathcal{O}(\epsilon^3)\stackrel{!}{=}1-\frac{i\hat{J}_z\epsilon^2}{\hbar}-1
\end{aligned}$$

or, repeating the exercise for other pairs of rotation operators

$$\boxed{\left[\hat{J}_i,\,\hat{J}_j\right]=i\hbar\epsilon_{ijk}\hat{J}_k}$$

Learning outcomes

- Rotations and rotation matrices in 3 dimensions
- Infinitesimal rotations in 3 dimensions
- Angular momentum as generator of rotations
- Commutator relations for angular momentum

Control questions

12.1 Consider operators $\hat{G}_i$ which, in components, are given by $(\hat{G}_i)_{jk} = -i\hbar\epsilon_{ijk}$.

(a) Write down the representation as explicit 3×3 matrices of the three operators $\hat{G}_1$, $\hat{G}_2$, and $\hat{G}_3$.

(b) Calculate the commutator $\left[\hat{G}_i,\, \hat{G}_j\right]$ of all three non-vanishing pairs.

12.2 Consider *orbital angular momentum*, given by $\underline{\hat{L}} = \underline{\hat{x}} \times \underline{\hat{p}}$. Check, by explicit calculation, that its components also satisfy the commutator relation $\left[\hat{L}_i,\, \hat{L}_j\right] = i\hbar\epsilon_{ijk}\hat{L}_k$.