Moderne Theoretische Physik I
Grundlagen der Quantenmechanik

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Exercise Sheet 8

Prof. Jörg Schmalian
Grgur Palle, Iksu Jang
Karlsruher Institut für Technologie (KIT)
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The problems whose solutions you need to upload are designated with stars.

⋆ Problem 1 ⋆ Operators as transformation generators

The exponential of an operator $\hat{A}$ is defined as

$$\exp(\hat{A}) = \mathrm{e}^{\hat{A}} \equiv \sum_{n=0}^{\infty} \frac{1}{n!} \hat{A}^n. \tag{1}$$

(Recall also the discussion of Problem 1 of Exercise Sheet 2.)

1. Consider a Hermitian operator $\hat{Q}$ and a state $|\psi\rangle$. If $|\psi'\rangle = \mathrm{e}^{-\mathrm{i}\hat{Q}} |\psi\rangle$, then find the formal expression for the $\hat{A}'$ entering
$$\left\langle \psi' \middle| \hat{A} \middle| \psi' \right\rangle = \left\langle \psi \middle| \hat{A}' \middle| \psi \right\rangle. \tag{2}$$
2. Now define the operator
$$\hat{A}_t = \mathrm{e}^{\mathrm{i}t\hat{Q}} \hat{A} \mathrm{e}^{-\mathrm{i}t\hat{Q}}, \tag{3}$$
where t is a real parameter. Find its n-th derivative at $t = 0$:
$$\left. \frac{\mathrm{d}^n}{\mathrm{d}t^n} \hat{A}_t \right|_{t=0} = ? \tag{4}$$
3. Prove the Baker-Campbell-Hausdorff lemma
$$\mathrm{e}^{\mathrm{i}t\hat{Q}} \hat{A} \mathrm{e}^{-\mathrm{i}t\hat{Q}} = \sum_{n=0}^{\infty} \frac{(\mathrm{i}t)^n}{n!} \operatorname{ad}_{\hat{Q}}^n \hat{A}. \tag{5}$$
Here $\operatorname{ad}_{\hat{Q}} \hat{A} \equiv [\hat{Q}, \hat{A}]$ so that $\operatorname{ad}_{\hat{Q}}^2 \hat{A} = [\hat{Q}, [\hat{Q}, \hat{A}]]$, $\operatorname{ad}_{\hat{Q}}^3 \hat{A} = [\hat{Q}, [\hat{Q}, [\hat{Q}, \hat{A}]]]$, etc.
4. Calculate
$$\mathrm{e}^{\mathrm{i}a\hat{p}/\hbar} \hat{x} \mathrm{e}^{-\mathrm{i}a\hat{p}/\hbar} = ? \tag{6}$$
$$\mathrm{e}^{-\mathrm{i}k\hat{x}/\hbar} \hat{p} \mathrm{e}^{\mathrm{i}k\hat{x}/\hbar} = ? \tag{7}$$
where $\hat{x}$ and $\hat{p}_x$ are the position and momentum operators and a, k are real numbers. Given a state $|\psi\rangle$, what does $\mathrm{e}^{-\mathrm{i}a\hat{p}/\hbar} |\psi\rangle$ and $\mathrm{e}^{\mathrm{i}k\hat{x}/\hbar} |\psi\rangle$ physically do to this state?

5. Now consider the angular momentum along z, $\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$. Calculate

$$\mathrm{e}^{\mathrm{i}\varphi \hat{L}_z/\hbar}\hat{x}\mathrm{e}^{-\mathrm{i}\varphi \hat{L}_z/\hbar} = ? \tag{8}$$

$$\mathrm{e}^{\mathrm{i}\varphi \hat{L}_z/\hbar}\hat{y}\mathrm{e}^{-\mathrm{i}\varphi \hat{L}_z/\hbar} = ? \tag{9}$$

What sort of transformation does this represent physically?

Solution 1

1. One finds that

$$\begin{aligned}\left\langle \psi' \middle| \hat{A} \middle| \psi' \right\rangle &= \left\langle \mathrm{e}^{-\mathrm{i}\hat{Q}}\psi \middle| \hat{A}\mathrm{e}^{-\mathrm{i}\hat{Q}}\psi \right\rangle = \left\langle \psi \middle| \left(\mathrm{e}^{-\mathrm{i}\hat{Q}}\right)^\dagger \hat{A}\mathrm{e}^{-\mathrm{i}\hat{Q}}\psi \right\rangle \\ &= \left\langle \psi \middle| \mathrm{e}^{+\mathrm{i}\hat{Q}^\dagger} \hat{A}\mathrm{e}^{-\mathrm{i}\hat{Q}} \middle| \psi \right\rangle = \left\langle \psi \middle| \mathrm{e}^{\mathrm{i}\hat{Q}} \hat{A}\mathrm{e}^{-\mathrm{i}\hat{Q}} \middle| \psi \right\rangle, \\ &\implies \hat{A}' = \mathrm{e}^{\mathrm{i}\hat{Q}}\hat{A}\mathrm{e}^{-\mathrm{i}\hat{Q}}.\end{aligned}$$

This motivates the study of $\hat{A}_t$.

2. Using the product rule

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\hat{A}_t &= \frac{\mathrm{d}\mathrm{e}^{\mathrm{i}t\hat{Q}}}{\mathrm{d}t}\hat{A}\mathrm{e}^{-\mathrm{i}t\hat{Q}} + \mathrm{e}^{\mathrm{i}t\hat{Q}}\frac{\mathrm{d}\hat{A}}{\mathrm{d}t}\mathrm{e}^{-\mathrm{i}t\hat{Q}} + \mathrm{e}^{\mathrm{i}t\hat{Q}}\hat{A}\frac{\mathrm{d}\mathrm{e}^{-\mathrm{i}t\hat{Q}}}{\mathrm{d}t} \\ &= \mathrm{i}\hat{Q}\mathrm{e}^{\mathrm{i}t\hat{Q}}\hat{A}\mathrm{e}^{-\mathrm{i}t\hat{Q}} + \mathrm{e}^{\mathrm{i}t\hat{Q}}\hat{A}(-\mathrm{i}t\hat{Q})\mathrm{e}^{-\mathrm{i}t\hat{Q}} \\ &= \mathrm{i}\hat{Q}\left(\mathrm{e}^{\mathrm{i}t\hat{Q}}\hat{A}\mathrm{e}^{-\mathrm{i}t\hat{Q}}\right) - \left(\mathrm{e}^{\mathrm{i}t\hat{Q}}\hat{A}\mathrm{e}^{-\mathrm{i}t\hat{Q}}\right)\mathrm{i}\hat{Q} = \mathrm{i}[\hat{Q}, \hat{A}_t]\end{aligned}$$

Here the key thing to notice is that $\hat{Q}$ commutes with itself so its exponential has similar formal properties as in the case of scalars. Similarly

$$\begin{aligned}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\hat{A}_t &= \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{i}[\hat{Q}, \hat{A}_t] = \mathrm{i}[\frac{\mathrm{d}\hat{Q}}{\mathrm{d}t}, \hat{A}_t] + \mathrm{i}[\hat{Q}, \frac{\mathrm{d}}{\mathrm{d}t}\hat{A}_t] \\ &= \mathrm{i}[\hat{Q}, \mathrm{i}[\hat{Q}, \hat{A}_t]] = \mathrm{i}^2[\hat{Q}, [\hat{Q}, \hat{A}_t]] = \mathrm{i}^2 \operatorname{ad}_{\hat{Q}}^2 \hat{A}_t,\end{aligned}$$

and by induction

$$\frac{\mathrm{d}^n}{\mathrm{d}t^n}\hat{A}_t = \mathrm{i}^n \operatorname{ad}_{\hat{Q}}^n \hat{A}_t.$$

At $t = 0$, $\hat{A}_t = \hat{A}$.

3. The Baker-Campbell-Hausdorff lemma directly follows from Taylor's theorem applied to $\hat{A}_t$:

$$\mathrm{e}^{\mathrm{i}t\hat{Q}}\hat{A}\mathrm{e}^{-\mathrm{i}t\hat{Q}} = \hat{A}_t = \sum_{n=0}^{\infty} \frac{t^n}{n!}\frac{\mathrm{d}^n}{\mathrm{d}t^n}\hat{A}_t\bigg|_{t=0} = \sum_{n=0}^{\infty}\frac{t^n}{n!}\mathrm{i}^n \operatorname{ad}_{\hat{Q}}^n \hat{A}_t,$$

which we wanted to prove.

4. Since

$$\begin{aligned}\mathrm{i}a/\hbar \operatorname{ad}_{\hat{p}} \hat{x} &= \mathrm{i}a[\hat{p}, \hat{x}]/\hbar = a, \\ -\mathrm{i}k/\hbar \operatorname{ad}_{\hat{x}} \hat{p} &= -\mathrm{i}k[\hat{x}, \hat{p}]/\hbar = k\end{aligned}$$

are both scalars, it follows that the higher order commutators in the Baker-Campbell-Hausdorff lemma all vanish. Thus only the $n = 0, 1$ terms survive:

$$\begin{aligned}\mathrm{e}^{\mathrm{i}a\hat{p}/\hbar}\hat{x}\mathrm{e}^{-\mathrm{i}a\hat{p}/\hbar} &= \hat{x} + a, \\ \mathrm{e}^{-\mathrm{i}k\hat{x}/\hbar}\hat{p}\mathrm{e}^{\mathrm{i}k\hat{x}/\hbar} &= \hat{p} + k.\end{aligned}$$

From the above we see that $\mathrm{e}^{-\mathrm{i}a\hat{p}/\hbar}|\psi\rangle$ is translated in real space by a relative to $|\psi\rangle$, whereas $\mathrm{e}^{\mathrm{i}k\hat{x}/\hbar}|\psi\rangle$ is translated in momentum space (boosted, velocity increased) by k relative to $|\psi\rangle$.

5. We start by noticing that

$$\mathrm{i}\varphi[\hat{L}_z, \hat{x}]/\hbar = -\varphi\hat{y},$$
$$\mathrm{i}\varphi[\hat{L}_z, \hat{y}]/\hbar = \varphi\hat{x}$$

map into each under commutation by $\hat{L}_z$. Hence

$$\begin{aligned}
\mathrm{e}^{\mathrm{i}\varphi\hat{L}_z/\hbar}\hat{x}\mathrm{e}^{-\mathrm{i}\varphi\hat{L}_z/\hbar} &= \sum_{n=0}^{\infty}\frac{(\mathrm{i}\varphi)^n}{\hbar^n n!}\,\mathrm{ad}^n_{\hat{L}_z}\,\hat{x} = \hat{x} - \frac{\varphi}{1!}\hat{y} - \frac{\varphi^2}{2!}\hat{x}^2 + \frac{\varphi^3}{3!}\hat{y} + \cdots \\
&= \sum_{n=0}^{\infty}\frac{(-1)^n\varphi^{2n}}{(2n)!}\hat{x} - \sum_{n=0}^{\infty}\frac{(-1)^n\varphi^{2n+1}}{(2n+1)!}\hat{y} \\
&= \cos(\varphi)\hat{x} - \sin(\varphi)\hat{y}.
\end{aligned}$$

Analogously one finds

$$\mathrm{e}^{\mathrm{i}\varphi\hat{L}_z/\hbar}\hat{y}\mathrm{e}^{-\mathrm{i}\varphi\hat{L}_z/\hbar} = \cos(\varphi)\hat{y} + \sin(\varphi)\hat{x}.$$

This mapping between $\hat{x}$ and $\hat{y}$ is a rotation around the z axis by φ.

⋆ Problem 2 ⋆ Particle in a central potential in two dimensions

Consider a particle subject to a radially symmetric potential $V(r)$, $r = \sqrt{x^2 + y^2}$, in two dimensions.

1. Formulate the Schrödinger equation in polar coordinates. Using separation of variables, derive the radial Schrödinger equation for a state of fixed energy E.
2. Now use a substitution $R(r) = r^{-\alpha}u(r)$ and choose α so that one of the terms vanishes. Find the effective potential $V_{\text{eff}}(r)$ from the resulting radial Schrödinger equation.
3. Next, find the energies when $V(r) = -e^2/r$. You may invoke the results from the analysis of the 3D hydrogen atom from the lectures, if relevant.

Solution 2

1. Since in polar coordinates

$$\nabla^2 = \partial_r^2 + \frac{1}{r}\partial_r + \frac{1}{r^2}\partial_\phi^2,$$

the stationary Schrödinger equation has the form:

$$\left[\frac{-\hbar^2}{2m}\left(\partial_r^2 + \frac{1}{r}\partial_r\right) - \frac{\hbar^2}{2mr^2}\partial_\phi^2 + V(r)\right]\psi(r,\phi) = E\,\psi(r,\phi).$$

Assuming $\psi(r,\phi) = R(r)Y(\phi)$, we find that

$$\frac{2mr^2}{\hbar^2}\cdot\frac{1}{R}\left[\frac{-\hbar^2}{2m}\left(\partial_r^2 + \frac{1}{r}\partial_r\right) + V(r) - E\right]R(r) = \frac{1}{Y}\partial_\phi^2 Y(\phi) = -\mu^2,$$

where μ is constant because it cannot depend on either r or ϕ (notice how it equals functions which depend on only r and ϕ of the left-hand side so $\mu = f_r(r) = f_\phi(\phi)$ and thereby $\partial_r\mu = \partial_r f_\phi = 0$ and $\partial_\phi\mu = \partial_\phi f_r = 0$). $Y(\phi + 2\pi) = Y(\phi) = \mathrm{e}^{\mathrm{i}\mu\phi}$ must be periodic so $\mu \in \mathbb{Z}$ is an integer. Thus the radial Schrödinger equation is:

$$\left[\frac{-\hbar^2}{2m}\left(\partial_r^2 + \frac{1}{r}\partial_r\right) + \frac{\hbar^2\mu^2}{2mr^2} + V(r)\right]R(r) = E\,R(r).$$

2. For $R(r) = r^{-\alpha}u(r)$ we find that

$$R'' + \frac{1}{r}R' = \frac{1}{r^\alpha}\left[u'' + \frac{1-2\alpha}{r}u' + \frac{\alpha^2}{r^2}u\right],$$

so setting $\alpha = 1/2$ eliminates the second term. This gives the revised radial Schrödinger equation:

$$\left[\frac{-\hbar^2}{2m}\partial_r^2 + V_{\text{eff}}(r)\right]u(r) = E\,u(r),$$

where the effective potential equals

$$V_{\text{eff}}(r) = \frac{\hbar^2(\mu^2 - 1/4)}{2mr^2} + V(r).$$

3. If we set

$$\mu^2 - \frac{1}{4} = \ell(\ell+1) \implies \ell = -\frac{1}{2} + |\mu|$$

we obtain the same radial differential equation as in three dimensions. During the lectures we found that it has a bounded solution only when

$$n - \ell - 1 \equiv p$$

is a non-zero integer. The energies are therefore given by

$$E = -\frac{1}{n^2}\text{Ry} = -\frac{1}{(\ell+1+p)^2}\text{Ry} = -\frac{1}{(N+\frac{1}{2})^2}\text{Ry},$$

where $N = |\mu| + p \in \{0, 1, 2, \ldots\}$ spans the non-zero integers.

Problem 3 Particle in a modified Coulomb potential

Consider a particle in three dimensions subject to the spherically symmetric potential:

$$V(r) = -\frac{Ze^2}{r} + \frac{\gamma}{r^2}. \tag{10}$$

Find the energies of the bound states for this modified Coulomb potential. What happens when $\gamma < 0$? (Hint: follow the steps you went through when solving the hydrogen atom problem during class.)

Solution 3

The only difference in the calculation compared to the Coulomb case is in the differential equation for the radial part of the wave function:

$$\left[\frac{1}{2m}\widehat{p}_r^2 + V_{\text{eff}}(r)\right]R(r) = ER(r),$$

where $\widehat{p}_r = -\mathrm{i}\hbar\frac{1}{r}\frac{\partial}{\partial r}r$ and now

$$V_{\text{eff}}(r) = -\frac{Ze^2}{r} + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2} + \frac{\gamma}{r^2}.$$

Thus we need to do two changes. First we notice that

$$\frac{\hbar^2}{2m}\ell(\ell+1) \to \frac{\hbar^2}{2m}\ell(\ell+1) + \gamma$$

and therefore it will be useful to define

$$\lambda(\lambda+1) = \ell(\ell+1) + \frac{2m\gamma}{\hbar^2}$$

to obtain a formally identical equation. Second, the natural length scale has been changed to

$$\tilde{a} = \frac{\hbar^2}{Zme^2}$$

so that in terms of

$$x = \frac{2}{n}\frac{r}{\tilde{a}}, \qquad E = -\frac{Z^2}{n^2}\mathrm{Ry}$$

for $R(r) = r^{-1}u(r)$ we obtain the same differential equation from the lectures:

$$u''(x) - \frac{\lambda(\lambda+1)}{x^2}u + \left(\frac{n}{x} - \frac{1}{4}\right)u = 0.$$

In the lectures we showed that

$$n - \lambda - 1 \equiv p$$

has to be a non-zero integer for $u(x)$ not to diverge at infinity. Thus the energies are given by

$$E_{p,\ell} = -\frac{Z^2}{\left(p + \frac{1}{2} + \frac{1}{2}\sqrt{(2\ell+1)^2 + \frac{8m\gamma}{\hbar^2}}\right)^2}\mathrm{Ry}$$

where $p, \ell \in \{0, 1, 2, \ldots\}$. Notice that

$$\lambda = -\frac{1}{2} + \frac{1}{2}\sqrt{(2\ell+1)^2 + \frac{8m\gamma}{\hbar^2}}$$

can become negative for small enough ℓ and sufficiently negative γ. A negative λ would give a $R(r) \sim r^\lambda$ that diverges at $r = 0$, which isn't allowed.