Moderne Theoretische Physik I
Grundlagen der Quantenmechanik

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Exercise Sheet 5

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The problems whose solutions you need to upload are designated with stars.

⋆ Problem 1 ⋆ Hermite's polynomials

The Hamiltonian of the simple harmonic oscillator (SHO) in the x-basis and its energy eigenvalues are given by

$$\Big(-\frac{\hbar^2}{2m}\partial_x^2+\frac{m\omega^2}{2}x^2\Big)\psi_n(x)=E_n\psi_n(x),\ E_n=\hbar\omega\Big(n+\frac{1}{2}\Big) \tag{1}$$

The eigenfunctions $\psi_n(x)$ are closely related to Hermite's polynomials

$$H_n(z)=(-1)^n e^{z^2}\partial_z^n e^{-z^2},\ \ n\geq 0 \tag{2}$$

1. First, show that the function e^{-t^2+2zt} is a generating function of Hermite polynomials, i.e.

$$e^{-t^2+2zt}=\sum_{n=0}^{\infty}\frac{t^n}{n!}H_n(z) \tag{3}$$

   (Hint: use the Taylor expansion of $e^{-(z-t)^2}$)

2. Using the above result, derive the following recursion relations for H_n:

$$\partial_z H_n(z)=2nH_{n-1}(z),\ \ n\geq 1 \tag{4}$$

   and

$$H_{n+1}(z)=2zH_n(z)-2nH_{n-1}(z),\ \ n\geq 1 \tag{5}$$

   Derive the following differential equation using Eqs. (4) and (5)

$$[\partial_z^2-2z\partial_z+2n]H_n(z)=0 \tag{6}$$

   (Hint: Eqs. (4) and (5) can be proven by differentiating Eq. (3) with respect to z or with respect to t)

3. Show the orthogonality of the Hermite polynomials,

$$\int_{-\infty}^{\infty}dze^{-z^2}H_n(z)H_m(z)=0,\ \text{for}\ n\neq m \tag{7}$$

   (Hint: manipulate Eq. (6) and integrate it over z)

Solution 1

1. First we show that the function e^{-t^2+2zt} is the generating function of the Hermitian polynomials, i.e.

$$F(z,t) \equiv e^{-t^2+2zt} = \sum_{n=0}^{\infty} \frac{t^n}{n!} H_n(z) \tag{8}$$

To do this, we use the hint suggested on the exercise sheet

$$\begin{aligned} e^{-t^2+2zt} &= e^{z^2} e^{-(z-t)^2} = e^{z^2} \sum_{n=0}^{\infty} \frac{t^n}{n!} \times \partial_t^n e^{-(z-t)^2}\Big|_{t=0} \\ &= e^{z^2} \sum_{n=0}^{\infty} \frac{t^n}{n!} \times (-1)^n \partial_z^n e^{-(z-t)^2}\Big|_{t=0} = \sum_{n=0}^{\infty} \frac{t^n}{n!} \times (-1)^n e^{z^2} \partial_z^n e^{-z^2} = \sum_{n=0}^{\infty} \frac{t^n}{n!} H_n(z) \end{aligned}$$

2. Again we use the hint to derive the recursion relations for H_n:

$$\begin{aligned} \partial_z F = 2tF &= \sum_{n=1}^{\infty} \frac{t^n}{n!} \partial_z H_n(z) = \sum_{n=0}^{\infty} \frac{t^{n+1}}{(n+1)!} \partial_z H_{n+1}(z) \\ \Rightarrow 2tF &= 2\sum_{n=0}^{\infty} \frac{t^{n+1}}{n!} H_n(z) = \sum_{n=0}^{\infty} \frac{t^{n+1}}{(n+1)!} \partial_z H_{n+1}(z) \end{aligned}$$

Here we took advantage of the fact that $\partial_z H_0 = 0$. A coefficient comparison provides the first recursion equation

$$\partial_z H_n(z) = 2nH_{n-1}(z) \tag{9}$$

Differentiating F with respect to t gives

$$\begin{aligned} \partial_t F = (-2t+2z)e^{-t^2+2zt} &= \sum_{n=0}^{\infty} \Big(-\frac{2t^{n+1}}{n!} H_n(z) + \frac{2zt^n}{n!} H_n(z) \Big) = \sum_{n=0}^{\infty} \frac{nt^{n-1}}{n!} H_n(z) \\ \Rightarrow \sum_{n=0}^{\infty} \frac{-2t^n}{(n-1)!} H_{n-1}(z) &+ \frac{2zt^n}{n!} H_n(z) - \frac{(n+1)t^n}{(n+1)!} H_{n+1}(z) = 0 \end{aligned}$$

Here H_{-1} and H_{-2} are not defined. We therefore set this to zero as a matter of form. A coefficient comparison immediately gives

$$H_{n+1}(z) = 2zH_n(z) - 2nH_{n-1}(z) \tag{10}$$

With the help of the two recursion equations, the differential equation for the Hermite polynomials can be derived

$$\begin{aligned} \partial_z^2 H_n &= 2n\partial_z H_{n-1} = 4n(n-1)H_{n-2}, \\ -2z\partial_z H_n &= -4nzH_{n-1} \end{aligned}$$

With Eq. (10) we then get

$$4n(n-1)H_{n-2} - 4nzH_{n-1} + 2nH_n = [\partial_z^2 - 2z\partial_z + 2n]H_n(z) = 0 \tag{11}$$

3. If we multiply $e^{-z^2}H_m$ to the left of the Eq. (11) and integrate over z, it gives

$$\int_{-\infty}^{\infty} dz e^{-z^2} H_m(\partial_z^2 - 2z\partial_z)H_n = -2n \int_{-\infty}^{\infty} dz e^{-z^2} H_m(z)H_n(z) \tag{12}$$

The partial integration of the left side gives

$$\int_{-\infty}^{\infty} dz e^{-z^2} H_m(\partial_z^2 - 2z\partial_z)H_n = e^{-z^2} H_m \partial_z H_n \Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} dz \Big(\partial_z e^{-z^2} H_m\Big)\partial_z H_n$$
$$+ \int_{-\infty}^{\infty} dz e^{-z^2} H_m(-2z\partial_z)H_n$$
$$= -\int_{-\infty}^{\infty} dz e^{-z^2} (\partial_z H_m)(\partial_z H_n)$$

Then,

$$-\int_{-\infty}^{\infty} dz e^{-z^2} (\partial_z H_m)(\partial_z H_n) = -2n \int_{-\infty}^{\infty} dz e^{-z^2} H_m(z) H_n(z) \tag{13}$$

If we swap m and n, we have

$$-\int_{-\infty}^{\infty} dz e^{-z^2} (\partial_z H_n)(\partial_z H_m) = -2m \int_{-\infty}^{\infty} dz e^{-z^2} H_m(z) H_n(z) \tag{14}$$

If we subtract both equations, we get:

$$(2n - 2m) \int_{-\infty}^{\infty} dz e^{-z^2} H_m(z) H_n(z) = 0 \tag{15}$$

This means that for $m \neq n$

$$\int_{-\infty}^{\infty} dz e^{-z^2} H_m(z) H_n(z) = 0 \tag{16}$$

⋆ Problem 2 ⋆ Two-dimensional harmonic oscillator

We consider the two-dimensional harmonic oscillator with the Hamilton operator

$$\hat{H} = \frac{\hat{p}_1^2 + \hat{p}_2^2}{2m} + \frac{m\omega^2}{2}(\hat{x}_1^2 + \hat{x}_2^2) \tag{17}$$

where $\hat{x}_i$ and $\hat{p}_i$ satisfy the commutation relations: $[\hat{x}_i, \hat{x}_j] = [\hat{p}_i, \hat{p}_j] = 0$ and $[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$ where i, j=1,2.

1. Based on Heisenberg's uncertainty relation, derive a lower bound of the ground state energy.
2. From the position and momentum operators $\hat{x}_i$, $\hat{p}_j$, we define creation and annihilation operators $\hat{a}_i^\dagger$ and $\hat{a}_i$ as follows:

$$\hat{a}_i = \alpha\hat{x}_i + i\beta\hat{p}_i, \tag{18}$$
$$\hat{a}_i^\dagger = \alpha\hat{x}_i - i\beta\hat{p}_j \tag{19}$$

where α and β are real numbers.

Determine α and β so that:

$$[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}, \tag{20}$$
$$[\hat{a}_i, \hat{a}_j] = [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0 \tag{21}$$
$$\hat{H} = \sum_{j=1}^{2} \hbar\omega\Big(\hat{N}_j + \frac{1}{2}\Big) \tag{22}$$

where $\hat{N}_i = \hat{a}_i^\dagger \hat{a}_i$.

3. Prove the following identities:

$$[\hat{N}_i, \hat{a}_j] = -\hat{a}_j \delta_{ij}, \tag{23}$$
$$[\hat{N}_i, \hat{a}_j^\dagger] = \hat{a}_j^\dagger \delta_{ij}, \tag{24}$$
$$[\hat{N}_i, \hat{N}_j] = 0 \tag{25}$$

4. Because $[\hat{N}_1, \hat{N}_2] = 0$ we can find common eigenstates for $\hat{N}_1$ and $\hat{N}_2$

$$\hat{N}_1 |n_1, n_2\rangle = n_1 |n_1, n_2\rangle, \tag{26}$$
$$\hat{N}_2 |n_1, n_2\rangle = n_2 |n_1, n_2\rangle \tag{27}$$

Calculate the effect of $\hat{a}_1$, $\hat{a}_2$, $\hat{a}_1^\dagger$, $\hat{a}_2^\dagger$ on the state $|n_1, n_2\rangle$. To do this, calculate the eigenvalues of $\hat{N}_1$ and $\hat{N}_2$ from the respective states $\hat{a}_1|n_1, n_2\rangle$, $\hat{a}_2|n_1, n_2\rangle$, $\hat{a}_1^\dagger|n_1, n_2\rangle$, $\hat{a}_2^\dagger|n_1, n_2\rangle$.

5. Now what are the eigenstates and eigenenergies of the two-dimensional harmonic oscillator? Why does $n_1, n_2 \in N_0$ have to apply? (Hint: you can use the result of part 1 of this assignment that the energy eigenvalues are bounded from below)

Solution 2

1. Since the harmonic oscillator potential is symmetric about 0, the ground state should also be symmetric (or anti-symmetric) and therefore $\langle \hat{x}_i \rangle = \langle \hat{p}_i \rangle = 0$. This means that for $i = 1, 2$

$$\Delta x_i^2 \equiv \langle \hat{x}_i^2 \rangle - \langle \hat{x}_i \rangle^2 = \langle \hat{x}_i^2 \rangle, \ \Delta p_i^2 \equiv \langle \hat{p}_i^2 \rangle - \langle \hat{p}_i \rangle^2 = \langle \hat{p}_i^2 \rangle \tag{28}$$

Using Heisenberg's uncertainty relation,

$$\Delta x_i^2 \Delta p_i^2 \geq \frac{|\langle [\hat{x}_i, \hat{p}_i] \rangle|^2}{4} = \frac{\hbar^2}{4} \tag{29}$$

Combining Eqs. (28) and (29) gives

$$\langle \hat{p}_i^2 \rangle \geq \frac{\hbar^2}{4 \langle \hat{x}_i^2 \rangle} \tag{30}$$

The energy is given by the expectation value of the Hamilton operator

$$\begin{aligned} E = \langle \hat{H} \rangle &= \frac{\langle \hat{p}_1^2 \rangle + \langle \hat{p}_2^2 \rangle}{2m} + \frac{m\omega^2}{2} (\langle \hat{x}_1^2 \rangle + \langle \hat{x}_2^2 \rangle) \\ &\geq \frac{\hbar^2}{8m} \left[\frac{1}{\langle \hat{x}_1^2 \rangle} + \frac{1}{\langle \hat{x}_2^2 \rangle} \right] + \frac{m\omega^2}{2} (\langle \hat{x}_1^2 \rangle + \langle \hat{x}_2^2 \rangle) \end{aligned} \tag{31}$$

We now minimize the above energy with respect to $\langle \hat{x}_i^2 \rangle$

$$\frac{\hbar^2}{8m} \frac{1}{\langle \hat{x}_i^2 \rangle} + \frac{m\omega^2}{2} \langle \hat{x}_i^2 \rangle \geq \frac{\hbar\omega}{2} \tag{32}$$

Then

$$E = \langle \hat{H} \rangle \geq \sum_{i=1}^{2} \frac{\hbar\omega}{2} = \hbar\omega \tag{33}$$

2.

$$[\hat{a}_i, \hat{a}_j] = [\alpha \hat{x}_i + i\beta \hat{p}_i, \alpha \hat{x}_j + i\beta \hat{p}_j] = i\alpha\beta([\hat{x}_i, \hat{p}_j] + [\hat{p}_j, \hat{x}_i]) = 0 \tag{34}$$
$$[\hat{a}_i^\dagger, \hat{a}_j^\dagger] = ([\hat{a}_j, \hat{a}_i])^\dagger = 0 \tag{35}$$
$$[\hat{a}_i, \hat{a}_j^\dagger] = [\alpha \hat{x}_i + i\beta \hat{p}_i, \alpha \hat{x}_j - i\beta \hat{p}_j] = -2i\alpha\beta[\hat{x}_i, \hat{p}_j] = 2\hbar\alpha\beta\delta_{ij} = \delta_{ij} \tag{36}$$

As a result, $\alpha\beta = \frac{1}{2\hbar}$.

$\hat{x}_i$ and $\hat{p}_i$ in terms of $\hat{a}_i$ and $\hat{a}_i^\dagger$ are given by

$$\hat{x}_i = \frac{\hat{a}_i + \hat{a}_i^\dagger}{2\alpha}, \tag{37}$$

$$\hat{p}_i = \frac{\hbar\alpha}{i}(\hat{a}_i^\dagger - \hat{a}_j^\dagger) \tag{38}$$

Plug this into the Hamiltonian:

$$\begin{aligned}
\hat{H} &= \sum_i^2 \Big[-\frac{\hbar^2\alpha^2}{2m}(\hat{a}_i - \hat{a}_i^\dagger)^2 + \frac{m\omega^2}{8\alpha^2}(\hat{a}_i + \hat{a}_i^\dagger)^2 \Big] \\
&= \sum_{i=1}^2 \Big[\Big(\frac{m\omega^2}{8\alpha^2} - \frac{\hbar^2\alpha^2}{2m}\Big)(\hat{a}_i\hat{a}_i + \hat{a}_i^\dagger\hat{a}_i^\dagger) + \Big(\frac{m\omega^2}{8\alpha^2} + \frac{\hbar^2\alpha^2}{2m}\Big)(\hat{a}_i\hat{a}_i^\dagger + \hat{a}_i^\dagger\hat{a}_i) \Big] \\
&= \sum_{i=1}^2 \Big[\Big(\frac{m\omega^2}{8\alpha^2} - \frac{\hbar^2\alpha^2}{2m}\Big)(\hat{a}_i\hat{a}_i + \hat{a}_i^\dagger\hat{a}_i^\dagger) + \Big(\frac{m\omega^2}{8\alpha^2} + \frac{\hbar^2\alpha^2}{2m}\Big)(2\hat{a}_i^\dagger\hat{a}_i + 1) \Big] \\
&= \sum_{i=1}^2 \Big[\Big(\frac{m\omega^2}{8\alpha^2} - \frac{\hbar^2\alpha^2}{2m}\Big)(\hat{a}_i\hat{a}_i + \hat{a}_i^\dagger\hat{a}_i^\dagger) + 2\Big(\frac{m\omega^2}{8\alpha^2} + \frac{\hbar^2\alpha^2}{2m}\Big)(\hat{a}_i^\dagger\hat{a}_i + 1/2) \Big] \stackrel{!}{=} \sum_{j=1}^2 \hbar\omega\Big[\hat{N}_j + 1/2\Big]
\end{aligned}$$

By comparison, we see that the following must apply

$$\frac{m\omega^2}{8\alpha^2} - \frac{\hbar\alpha^2}{2m} = 0 \Rightarrow \alpha = \sqrt{\frac{m\omega}{2\hbar}}. \tag{39}$$

Thus α has the dimensions of inverse length, and β of inverse momentum. Up to a factor, this could have also been derived by dimensional analysis.

3. We calculate

$$[\hat{N}_i, \hat{a}_j] = [\hat{a}_i^\dagger\hat{a}_i, \hat{a}_j] = \hat{a}_i^\dagger[\hat{a}_i, \hat{a}_j] + [\hat{a}_i^\dagger, \hat{a}_j]\hat{a}_i = -\delta_{ij}\hat{a}_i, \tag{40}$$

$$[\hat{N}_i, \hat{a}_j^\dagger] = (-[\hat{N}_i, \hat{a}_j])^\dagger = \delta_{ij}\hat{a}_i^\dagger, \tag{41}$$

$$[\hat{N}_i, \hat{N}_j] = [\hat{N}_i, \hat{a}_j^\dagger\hat{a}_j] = [\hat{N}_i, \hat{a}_j^\dagger]\hat{a}_j + \hat{a}_j^\dagger[\hat{N}_i, \hat{a}_j] = \delta_{ij}(\hat{N}_j - \hat{N}_j) = 0 \tag{42}$$

4. From the above commuation relations (Eqs. (40) and (41)), we can guess the effect of $\hat{a}_j$ on the state $|n_1, n_2\rangle$ as follows:

$$\hat{a}_1|n_1, n_2\rangle = c_1|n_1 - 1, n_2\rangle, \tag{43}$$

$$\hat{a}_2|n_1, n_2\rangle = c_2|n_1, n_2 - 1\rangle \tag{44}$$

The annihilation operators $\hat{a}_1$, $\hat{a}_2$ reduce their respective quantum numbers by 1. We now want to determine c_1 and c_2. We can do this via

$$\langle n_1, n_2|\hat{a}_1^\dagger\hat{a}_1|n_1, n_2\rangle = |c_1|^2\langle n_1 - 1, n_2|n_1 - 1, n_2\rangle, \tag{45}$$

$$\Rightarrow \langle n_1, n_2|\hat{N}_1|n_1, n_2\rangle = |c_1|^2 = n_1 \tag{46}$$

$$\therefore c_1 = \sqrt{n_1} \tag{47}$$

Similarly, we can obtain $c_2 = \sqrt{n_2}$. Therefore

$$\hat{a}_1|n_1, n_2\rangle = \sqrt{n_1}|n_1 - 1, n_2\rangle \tag{48}$$

$$\hat{a}_2|n_1, n_2\rangle = \sqrt{n_2}|n_1, n_2 - 1\rangle \tag{49}$$

In the same way we find

$$\hat{a}_1^\dagger|n_1, n_2\rangle = \sqrt{n_1 + 1}|n_1 + 1, n_2\rangle \tag{50}$$

$$\hat{a}_2^\dagger|n_1, n_2\rangle = \sqrt{n_2 + 1}|n_1, n_2 + 1\rangle \tag{51}$$

5. The common eigenstates $|n_1, n_2\rangle$ of $\hat{N}_1$ and $\hat{N}_2$ are also the eigenstates of $\hat{H}$

$$\hat{H}|n_1, n_2\rangle = \sum_{i=1}^{2} \hbar\omega[\hat{N}_i + 1/2]|n_1, n_2\rangle = \sum_{i=1}^{2} \hbar\omega[n_i + 1/2]|n_1, n_2\rangle \equiv E_{n_1,n_2}|n_1, n_2\rangle \tag{52}$$

where

$$E_{n_1,n_2} = \sum_{i=1}^{2} \hbar\omega[n_i + 1/2] = \hbar\omega[n_1 + n_2 + 1]. \tag{53}$$

We had shown that the intrinsic energies are bounded from below: $E \geq \hbar\omega$. As a result, n_1 and n_2 obey a lower bound: $n_1 \geq 0$ and $n_2 \geq 0$. Additionally, we can also show that n_1 and n_2 must be integer numbers larger than -1 by applying the annihilation operators to the state several times:

$$\hat{a}_1^{n_1+1}|n_1, n_2\rangle = \sqrt{n_1}\hat{a}_1^{n_1}|n_1 - 1, n_2\rangle = \cdots = \sqrt{n_1!}a_1|0, n_2\rangle = 0. \tag{54}$$

If n_i were not integer, then there would be states with negative n_i which implies negative energy. This would contradict the results of part 1.

Problem 3 Cauchy-Schwarz inequality

1. Derive the Cauchy-Schwarz inequality

$$|\mathbf{v}|^2|\mathbf{u}|^2 \geq |\mathbf{v} \cdot \mathbf{u}|^2 \tag{55}$$

by using the fact that

$$(\mathbf{v} - \lambda\mathbf{u})^2 \geq 0 \tag{56}$$

and minimizing $(\mathbf{v} - \lambda\mathbf{u})^2$ with respect to λ. Here $\mathbf{v}$ and $\mathbf{u}$ are real-valued vectors and λ is a real number.

2. Can we extend the above result to the complex-valued vector case?

$$(\mathbf{v}^* \cdot \mathbf{v})|(\mathbf{u}^* \cdot \mathbf{u})| \geq |\mathbf{v}^* \cdot \mathbf{u}|^2 \tag{57}$$

Solution 3

1. Set $f(\lambda) = (\mathbf{v} - \lambda\mathbf{u})^2$.

$$\frac{df(\lambda)}{d\lambda} = 2\lambda|\mathbf{u}|^2 - 2\lambda\mathbf{u} \cdot \mathbf{v} \tag{58}$$

Therefore the value of λ minimizing $f(\lambda)$ is $\frac{\mathbf{u}\cdot\mathbf{v}}{|\mathbf{u}|^2}$.

$$f(\lambda) \geq f(\lambda = \frac{\mathbf{u} \cdot \mathbf{v}}{|\mathbf{u}|^2}) = \left(\mathbf{v} - \frac{\mathbf{u} \cdot \mathbf{v}}{|\mathbf{u}|^2}\mathbf{u}\right)^2 = |\mathbf{v}|^2 - \frac{|\mathbf{u} \cdot \mathbf{v}|^2}{|\mathbf{u}|^2} \geq 0 \Rightarrow |\mathbf{v}|^2|\mathbf{u}|^2 \geq |\mathbf{v} \cdot \mathbf{u}|^2 \tag{59}$$

2. For complex valued case, we can consider λ as two parameters: $\operatorname{Re}\lambda$ and $\operatorname{Im}\lambda$ then,

$$g(\operatorname{Re}\lambda, \operatorname{Im}\lambda) = (\mathbf{v}^* - \lambda^*\mathbf{u}^*) \cdot (\mathbf{v} - \lambda\mathbf{u}) \tag{60}$$

$$\frac{\partial g}{\partial \operatorname{Re}\lambda} = 2\operatorname{Re}\lambda|\mathbf{u}|^2 - \mathbf{u}^* \cdot \mathbf{v} - \mathbf{u} \cdot \mathbf{v}^* = 0, \tag{61}$$

$$\frac{\partial g}{\partial \operatorname{Im}\lambda} = 2\operatorname{Im}\lambda|\mathbf{u}|^2 + i(\mathbf{u}^* \cdot \mathbf{v} - \mathbf{u} \cdot \mathbf{v}^*) = 0 \tag{62}$$

Therefore the value λ minimizing $g(\operatorname{Re}\lambda, \operatorname{Im}\lambda)$ is $\frac{\mathbf{u}^*\cdot\mathbf{v}}{|\mathbf{u}|^2}$.

$$g(\lambda) \geq g(\lambda = \frac{\mathbf{u}^* \cdot \mathbf{v}}{|\mathbf{u}|^2}) = \left|\mathbf{v} - \frac{\mathbf{u}^* \cdot \mathbf{v}}{|\mathbf{u}|^2}\mathbf{u}\right|^2 = |\mathbf{v}|^2 - \frac{|\mathbf{u}^* \cdot \mathbf{v}|^2}{|\mathbf{u}|^2} \geq 0 \Rightarrow (\mathbf{v}^* \cdot \mathbf{v})|(\mathbf{u}^* \cdot \mathbf{u})| \geq |\mathbf{v}^* \cdot \mathbf{u}|^2 \tag{63}$$