Moderne Theoretische Physik I
Grundlagen der Quantenmechanik

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Exercise Sheet 1

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

⋆ Problem 1 ⋆ Dirac Delta Distribution

We consider the family of functions $\delta_\sigma(x) = \alpha e^{-x^2/\sigma^2}$ and want to show that in the limit $\sigma \to 0$, it corresponds to the Dirac distribution $\delta(x)$. The latter is not a function in the strict sense but rather a probability distribution. It is defined such that the probability density is zero when $x \neq 0$. However, it is still normalized so that the integral over the real axis equals 1. This means that the probability distribution is non-zero at $x = 0$.

1. Determine α so that each function $\delta_\sigma(x)$ is normalized according to
$$\int_{-\infty}^{\infty} \mathrm{d}x \delta_\sigma(x) = 1. \tag{1}$$
2. Show that for each fixed x, the limit $\lim_{\sigma\to 0} \delta_\sigma(x) = \delta(x)$ is satisfied.
3. Determine, using the $\sigma \to 0$ limiting behavior (f is a smooth function)
$$\int_{-\infty}^{\infty} \mathrm{d}x \delta_\sigma(x) f(x) \to \int_{-\infty}^{\infty} \mathrm{d}x \delta(x) f(x) = f(0), \tag{2}$$
what is the analogous limiting behavior of $\int_{-\infty}^{\infty} \mathrm{d}x \delta'_\sigma(x) f(x)$.
4. Prove the relationship
$$\int_{-\infty}^{\infty} \mathrm{d}x\, \delta\left(f(x)\right) = \sum_i \frac{1}{|f'(x_i)|} \tag{3}$$
where x_i are the simple zeros of the function $f(x)$. (Simple zero means that the function's derivative is finite there. Assume f is smooth and has only simple zeros.)

Solution 1

1. The integral over the Gaussian distribution yields
$$\int_{-\infty}^{\infty} \mathrm{d}x \alpha e^{-x^2/\sigma^2} = \alpha\sigma\sqrt{\pi},,$$
which is normalized to 1 when $\alpha^{-1} = \sigma\sqrt{\pi}$.

2. First, we note that the normalization condition is fulfilled by choosing $\alpha^{-1} = \sigma\sqrt{\pi}$. Then, a case distinction is necessary: For $x = 0$, $\delta_\sigma(0) = \alpha = 1/(\sqrt{\pi}\sigma) \to \infty$. Otherwise, the limit is always dominated by the exponential behavior, and we find $\delta_\sigma(x) = (1/\sqrt{\pi}\sigma)e^{-x^2/\sigma^2} \to 0$. This can be demonstrated explicitly by:

$$e^x = \sum_n \frac{x^n}{n!} = 1 + x + ... \geq 1 + x \Leftrightarrow e^{-x} \leq \frac{1}{1+x}$$

$$\Rightarrow 0 \leq \lim_{\sigma\to 0} \frac{e^{-x^2/\sigma^2}}{\sigma} \leq \lim_{\sigma\to 0} \frac{\sigma}{\sigma^2 + x^2} = 0\,,$$

   if $x \neq 0$. Thus, in the limit $\sigma \to 0$, the family of functions $\delta_\sigma(x)$ converges point-wise towards the Dirac Delta Distribution.

   Math aside: point-wise convergence is not the same as convergence under the integral. This is a more involved thing to prove which we decided not to bother you with. Counterexample: the function

$$\Delta_\sigma(x) = \begin{cases} \sigma, & \text{for } x = 0, \\ \frac{1}{\sigma\sqrt{\pi}} e^{-x^2/\sigma^2}, & \text{for } x \neq 0, \end{cases}$$

   is also normalized to 1 (since points have zero measure) and converges point-wise to $\delta(x)$ when $\sigma \to +\infty$ (opposite limit), but under the integral it does not go to $\delta(x)$. The physical reason is that $\Delta_\sigma(x)$ gets broader instead of narrower as σ is increased.

3. Using integration by parts, we immediately find

$$\int_{-\infty}^{\infty} \mathrm{d}x\, \delta'_\sigma(x) f(x) = [\delta_\sigma(x) f(x)]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \mathrm{d}x\, \delta_\sigma(x) f'(x) \to -f'(0)\,.$$

   A slightly less elegant but still instructive derivation is based on the observation that $\delta'_\sigma(x) = (-2x/\sigma^2)\delta_\sigma(x)$. Since $\delta_\sigma(x)$ particularly emphasizes the values around $x = 0$, we can express $f(x)$ as a Taylor series. Thus,

$$\int_{-\infty}^{\infty} \mathrm{d}x\, \delta'_\sigma(x) f(x) \approx \int_{-\infty}^{\infty} \mathrm{d}x\, (-2x/\sigma^2)\delta_\sigma(x) \left[f(0) + f'(0)x\right]\,.$$

   The first term in the square brackets yields an odd integrand (thus, the integral vanishes). The second term is even and yields

$$\int_{-\infty}^{\infty} \mathrm{d}x\, \delta'_\sigma(x) f(x) \approx \int_{-\infty}^{\infty} \mathrm{d}x\, \frac{-f'(0)}{\sqrt{\pi}} \frac{\partial}{\partial\sigma} e^{-x^2/\sigma^2} = \frac{\partial}{\partial\sigma} \int_{-\infty}^{\infty} \mathrm{d}x\, \frac{-f'(0)}{\sqrt{\pi}} e^{-x^2/\sigma^2} = -f'(0).$$

4. Since the δ distribution, according to our definition, is zero when its argument is non-zero, we can confine ourselves to a region of length $2\epsilon > 0$ around each respective zero. In this region, the function is well described by its linear Taylor expansion, i.e., $f(x) = (x - x_i)f'(x_i)$, thus,

$$\int_{-\infty}^{\infty} \mathrm{d}x\, \delta\left(f(x)\right) = \sum_i \int_{x_i-\epsilon}^{x_i+\epsilon} \mathrm{d}x\, \delta\left(f(x)\right) = \sum_i \int_{x_i-\epsilon}^{x_i+\epsilon} \mathrm{d}x\, \delta\left((x - x_i)f'(x_i)\right)$$

   Next, we use the substitution $y = (x - x_i)f'(x_i)$ and obtain

$$\sum_i \int_{x_i-\epsilon}^{x_i+\epsilon} \mathrm{d}x\, \delta\left((x - x_i)f'(x_i)\right) = \sum_i \int_{-f'(x_i)\epsilon}^{f'(x_i)\epsilon} \frac{\mathrm{d}y}{f'(x_i)} \delta(y) = \sum_i \frac{\operatorname{sign}\left(f'(x_i)\right)}{f'(x_i)} = \sum_i \frac{1}{|f'(x_i)|}\,,$$

   where we have used that depending on the sign of $f'(x_i)$, the interval is traversed straightly or in reverse.

⋆ Problem 2 ⋆ Expectation values of a Gaussian wave function

Consider the wave function ($\sigma > 0$):

$$\psi(x) = \frac{1}{(2\pi\sigma^2)^{1/4}} e^{-\frac{(x-x_0)^2}{4\sigma^2}} \tag{4}$$

1. Show that the given wave function is normalized: $\int_{-\infty}^{\infty} |\psi(x)|^2 = 1$.
2. Calculate the expectation value of x:
$$\langle \hat{x} \rangle = \int_{-\infty}^{\infty} \mathrm{d}x |\psi(x)|^2 x. \tag{5}$$
This is the first moment of the distribution, also called the mean.
3. Calculate the expectation value of x^2:
$$\langle \hat{x}^2 \rangle = \int_{-\infty}^{\infty} \mathrm{d}x |\psi(x)|^2 x^2. \tag{6}$$
Using these two quantities, we can calculate the second moment of the distribution, $\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$. This quantity is also called the standard deviation.
4. Calculate the expectation value of the momentum $\hat{p}$:
$$\langle \hat{p} \rangle = \int_{-\infty}^{\infty} dx \psi^*(x) \frac{\hbar}{i} \partial_x \psi(x). \tag{7}$$
5. Calculate the expectation value of $\hat{p}^2$ and standard deviation of the $\hat{p}$:
$$\langle \hat{p}^2 \rangle = \int_{-\infty}^{\infty} dx \psi^*(x) \left(\frac{\hbar}{i}\right)^2 \partial_x^2 \psi(x), \tag{8}$$
$$\Delta p = \sqrt{\langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2} \tag{9}$$
6. Calculate the product $\Delta x \cdot \Delta p$. Compare it with Heisenberg's uncertainty relation $\Delta x \cdot \Delta p \geq \hbar/2$.

Solution 2

1. Using the Gaussian integral formula: $\int_{-\infty}^{\infty} e^{-ax^2} = \sqrt{\frac{\pi}{a}}$ $(a > 0)$,
$$\int_{-\infty}^{\infty} dx |\psi(x)|^2 = \frac{1}{(2\pi\sigma^2)^{1/2}} \int_{-\infty}^{\infty} dx e^{-\frac{(x-x_0)^2}{2\sigma^2}} = \frac{1}{(2\pi\sigma^2)^{1/2}} \int_{-\infty}^{\infty} dy e^{-\frac{y^2}{2\sigma^2}} \ (\because y = x - x_0) = 1.$$
2.
$$\langle \hat{x} \rangle = \int_{-\infty}^{\infty} dx x |\psi(x)|^2 = \frac{1}{(2\pi\sigma^2)^{1/2}} \int_{-\infty}^{\infty} dx\ x e^{-\frac{(x-x_0)^2}{2\sigma^2}} = \frac{1}{(2\pi\sigma^2)^{1/2}} \int_{-\infty}^{\infty} dy\ (y + x_0) e^{-\frac{y^2}{2\sigma^2}} \ (\because y = x - x_0)$$
$$= \frac{1}{(2\pi\sigma^2)^{1/2}} \int_{-\infty}^{\infty} dy\ x_0 e^{-\frac{y^2}{2\sigma^2}} = x_0.$$
3. As in the previous solution, we first perform a change of variables, $y = x - x_0$, and do the integral.
$$\langle \hat{x}^2 \rangle = \frac{1}{(2\pi\sigma^2)^{1/2}} \int_{-\infty}^{\infty} dy\ (y + x_0)^2 e^{-\frac{y^2}{2\sigma^2}} = \frac{1}{(2\pi\sigma^2)^{1/2}} \int_{-\infty}^{\infty} dy (y^2 + 2x_0 y + x_0^2) e^{-\frac{y^2}{2\sigma^2}}$$
$$= \frac{1}{(2\pi\sigma^2)^{1/2}} \int_{-\infty}^{\infty} dy (y^2 + x_0^2) e^{-\frac{y^2}{2\sigma^2}} = \sigma^2 + x_0^2$$

where we used the following identity:

$$
\begin{aligned}
-\frac{\partial}{\partial a}\int_{-\infty}^{\infty} dx e^{-ax^2} &= \int_{-\infty}^{\infty} dx\; x^2 e^{-ax^2} = -\frac{\partial}{\partial a}\sqrt{\frac{\pi}{a}} = \frac{1}{2}\frac{\pi^{1/2}}{a^{3/2}} \\
\Rightarrow \int_{-\infty}^{\infty} dx\; x^2 e^{-ax^2} &= \frac{1}{2}\frac{\pi^{1/2}}{a^{3/2}}.
\end{aligned}
$$

Then the standard deviation is given by:

$$\Delta x = \sqrt{\langle \hat{x}^2\rangle - \langle \hat{x}\rangle^2} = \sigma.$$

4.

$$\langle \hat{p}\rangle = -\frac{\hbar}{i}\frac{1}{(2\pi\sigma^2)^{1/2}}\int_{-\infty}^{\infty} dx \frac{x-x_0}{2\sigma^2} e^{-\frac{(x-x_0)^2}{4\sigma^2}} = -\frac{\hbar}{i}\frac{1}{2\sigma^2}\Big(\langle \hat{x}\rangle - x_0\Big) = 0$$

5.

$$
\begin{aligned}
\partial_x^2 \psi(x) &= \frac{1}{(2\pi\sigma^2)^{1/4}}\partial_x\Big(-\frac{x-x_0}{2\sigma^2}e^{-\frac{(x-x_0)^2}{4\sigma^2}}\Big) = \frac{1}{(2\pi\sigma^2)^{1/4}}\Big(-\frac{1}{2\sigma^2} + \frac{(x-x_0)^2}{4\sigma^4}\Big)e^{-\frac{(x-x_0)^2}{4\sigma^2}} \\
&= \Big(-\frac{1}{2\sigma^2} + \frac{(x-x_0)^2}{4\sigma^4}\Big)\psi(x).
\end{aligned}
$$

Therefore

$$
\begin{aligned}
\langle \hat{p}^2\rangle &= \hbar^2\int_{-\infty}^{\infty} dx \frac{1}{2\sigma^2}\Big(1 - \frac{(x-x_0)^2}{2\sigma^2}\Big)|\psi(x)|^2 = \frac{\hbar^2}{2\sigma^2}\Big(1 - \frac{1}{2\sigma^2}(\langle \hat{x}^2\rangle + x_0^2 - 2x_0\langle \hat{x}\rangle)\Big) \\
&= \frac{\hbar^2}{4\sigma^2}\;(\because \langle \hat{x}^2\rangle = \sigma^2 + x_0^2,\; \langle \hat{x}\rangle = x_0)
\end{aligned}
$$

Then

$$\Delta p = \sqrt{\langle \hat{p}^2\rangle - \langle \hat{p}\rangle^2} = \frac{\hbar}{2\sigma}$$

6. Combining with the results for Δx of part 3, we get

$$\Delta x \cdot \Delta p = \frac{\hbar}{2}$$

which is as small as it can get, in light of Heisenberg's uncertainty relation. So Gaussian wave functions realize the extremum of the lower bound on the x and p uncertainties.

Problem 3 Spectral density in a box

Consider an electromagnetic field in a cubic box with volume $V = L^3$. A simple estimate for the number of free electromagnetic modes can be obtained by requiring periodic boundary conditions on the vector potential ($\omega_{\mathbf{k}} = c|\mathbf{k}|$)

$$\mathbf{A}(\mathbf{r}, t) = \sum_{\mathbf{k}} \mathbf{A}_{\mathbf{k}} e^{i(\mathbf{k}\cdot\mathbf{x} - \omega_{\mathbf{k}} t)} \tag{10}$$

1. Show that this condition leads to a quantization of the k-states and determine this. Specifically, show that $k = \frac{2\pi}{L}(n_x, n_y, n_z)$ with $n_x, n_y, n_z \in \mathbb{Z}$.
2. Use the quantization condition from 1 to derive an expression for the number of modes dN in the interval $[k, k+dk]$; here $k = |\mathbf{k}|$. Keep in mind that the vector potential is transverse to the k-vector, i.e., $\mathbf{A}\cdot\mathbf{k} = 0$.

3. Calculate the spectral energy density $u(\omega)$ ($u(\omega)d\omega$ is the energy per volume in the interval $[\omega, \omega + d\omega]$) in thermal equilibrium. To do this, use the classic equipartition principle, which states that each mode contributes the energy $k_B T$. Explain why this assumption is problematic.

4. Planck's law of radiation
$$u(\omega) = \frac{\eta\omega^3}{\pi^2 c^3} \frac{1}{e^{\eta\omega/k_B T} - 1} \tag{11}$$
avoids the problem mentioned above. Determine the behavior of this radiation law at small and large frequencies and compare with the results of part 3. Specify the units of η and interpret the quantity $\eta\omega$.

Solution 3

1. From the periodic boundary condition,
$$\begin{aligned} \mathbf{A}(x = 0, y, z, t) &= \mathbf{A}(x = L, y, z, t), \\ \mathbf{A}(x, y = 0, z, t) &= \mathbf{A}(x, y = L, z, t), \\ \mathbf{A}(x, y, z = 0, t) &= \mathbf{A}(x, y, z = L, t). \end{aligned}$$
Using Eq. (10) and the above conditions, we can obtain following conditions for the momentum $\mathbf{k}$:
$$\begin{aligned} & e^{ik_x L} = e^{ik_y L} = e^{ik_z L} = 1 \\ & \Rightarrow k_{x,y,z} = \frac{2\pi n_{x,y,z}}{L}, \; n_{x,y,z} \in Z. \end{aligned}$$
Overall, the k-space is quantized with each k-value taking up a cubic volume $\Delta k_x \Delta k_x \Delta k_x = (2\pi/L)^3$.

2. The interval $[k, k + dk]$ describes a spherical shell in k-space with volume $4\pi k^2 dk$. The number of modes within this volume is given by
$$dN = 2(4\pi k^2 dk)/(\Delta k)^3 = \frac{V k^2 dk}{\pi^2}$$
where the factor 2 comes from the fact that there are two transverse mode for each $\mathbf{k}$.

3. In thermal equilibrium, every classical mode carries an energy $k_B T$. We also use the dispersion relation $\omega_{\mathbf{k}} = c|\mathbf{k}|$. From this we conclude that
$$u(\omega)d\omega = k_B T dN/V = k_B T \frac{k^2 dk}{\pi^2} = \frac{k_B T}{\pi^2 c^3} \omega^2 d\omega.$$
Therefore $u(\omega) = \frac{k_B T}{\pi^2 c^3} \omega^2$. This energy density is not bounded and leads to a UV catastrophe (divergence at large frequencies).

4. At low frequencies, a Taylor expansion in ω of Eq. (11) provides the classic result which is obtained in 3:
$$u_{cl}(\omega) = u(\omega) = \frac{k_B T}{\pi^2 c^3} \omega^2.$$
At high frequencies one instead finds
$$u(\omega) = \frac{\eta\omega^3}{\pi^2 c^3} e^{-\eta\omega/k_B T} = \frac{\eta\omega}{k_B T} e^{-\eta\omega/k_B T} u_{cl}(\omega).$$
Here, $\eta\omega$ has the dimensions of energy, whereas η has the dimension of an action. The exponential suppression of mode contributions for frequencies $\omega \gg k_B T/\eta$ indicates thermal activation of a discrete excitation spectrum. $\eta\omega$ is the energy quantum of modes with frequency ω.