Exercise Sheet 1 **Theoretische Physik 4: Quantenmechanik**

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Exercise 1 (10 points)

Let us examine the properties of the delta function $\delta(x)$. The intuitive definition of the delta function is a function that is almost everywhere zero, except at $x = 0$ where it is infinity, but in such way that the total area under the curve is unity. This somewhat singular notion can be defined as a functional, i.e., a function that is defined under integration, and the full definition reads

$$\delta(x) = 0 \text{ if } x \neq 0, \text{ and } \int_{\eta_1}^{\eta_2} \mathrm{d}x\ \delta(x) = 1 \text{ for any } \eta_1, \eta_2 \text{ such that } \eta_1 < 0 < \eta_2, \tag{1}$$

where "for any η_1, η_2" also includes the limit $\eta_1 \to -\infty$, $\eta_2 \to +\infty$. Suppose that we have a well behaved test function $f(x)$, in other words any possible random function which is continuous and finite, and differentiable as often as needed.

1. (1/10) Calling the dimensions of length $[x] = L$, and using the definition Eq. (1), what are the dimensions of the delta function $\delta(x)$? If we where working with the three dimensional generalization : $\int_V \mathrm{d}^3\mathbf{x}\delta(\mathbf{x}) = 1$ for any volume V that contains the origin $(0, 0, 0)$, what are the dimensions of $\delta(\mathbf{x})$?
2. (1/10) Argue from the definition Eq. (1) that, for any well behaved test function $f(x)$, it must be the case that
$$\int_a^b \mathrm{d}x\ f(x)\delta(x) = \begin{cases} f(0) & a < 0 < b \\ 0 & \text{otherwise} \end{cases}$$
assuming that the integration bounds always respect the ordering $a < b$.
3. (1/10) Show that
$$\int_a^b \mathrm{d}x\ f(x)\delta(x - x_o) = \begin{cases} f(x_o) & x_o \in (a, b) \\ 0 & \text{otherwise} \end{cases}$$
assuming that the integration bounds always respect the ordering $a < b$.
4. (1/10) Show that $\delta(-x) = \delta(x)$
5. (1/10) For any $c \in \mathbb{R}$, $c \neq 0$, show that $\delta(cx) = \frac{1}{|c|}\delta(x)$.
6. (1/10) Given a function $g(x)$ that has no coincident roots at $x_1, x_2, ..., x_n$, i.e. $g(x_i) = 0$ for every i in $\{1, 2, ..., n\}$ and all x_i are different, show that $\delta(g(x)) = \sum_{i=1}^{n} \frac{\delta(x - x_i)}{|g'(x_i)|}$.

The delta function cannot be represented by any smooth function, however, it can be "reached" by a smooth function $\Delta(\epsilon, x)$ against some control parameter ϵ in an appropriate limit. The key is to engineer this procedure such that the total area under the curve is unity in the limit. In practical applications, we some times use these "smooth" approximations, but some care must be taken to make the approximation respect the delta function definitions. Such considerations also bring up questions about the behaviour of the test function in the extrema cases where $\eta_1 \to -\infty$, $\eta_2 \to +\infty$.

7. (1/10) Show that the Gaussian $\Delta_1(\epsilon, x) = \dfrac{\mathrm{e}^{-x^2/\epsilon^2}}{\epsilon\sqrt{\pi}}$ will become the delta function $\delta(x)$ in the limit $\lim\limits_{\epsilon\to 0} \Delta_1(\epsilon, x)$, by showing that the limit follows the definition Eq. (1).

   $\left(\text{Hint: } \int\limits_{-\infty}^{+\infty} \mathrm{d}x \mathrm{e}^{-x^2} = \sqrt{\pi}\right)$

8. (1/10) Show that the Lorentzian $\Delta_2(\epsilon, x) = \dfrac{\epsilon/\pi}{x^2 + \epsilon^2}$ will become the delta function $\delta(x)$ in the limit $\lim\limits_{\epsilon\to 0} \Delta(\epsilon, x)$ in the similar way.

   $\left(\text{Hint: } \int\limits_{-\infty}^{+\infty} \mathrm{d}x \frac{1}{x^2+1} = \pi\right)$

9. (1/10) Argue about the asymptotic restrictions of $f(x)$ so that $\int\limits_{-\infty}^{+\infty} \mathrm{d}x\, f(x)\delta(x) = 1$ make sense when approaching $\delta(x)$ from the Lorentzian representation $\Delta_2(\epsilon, x)$.

10. (1/10) Find the Fourier transform $\tilde{\Delta}_2(\epsilon, k) = \dfrac{1}{\sqrt{2\pi}} \int\limits_{-\infty}^{+\infty} \mathrm{d}x\, \Delta_2(\epsilon, x)\mathrm{e}^{-ikx}$, and considering the limit $\epsilon \to 0$ argue that $\delta(x) = \dfrac{1}{2\pi} \int\limits_{-\infty}^{+\infty} \mathrm{d}k\ \mathrm{e}^{ikx}$.

Exercise 2 (5 points)

In the lectures we learned how observables in classical mechanics A become hermitian operators $\hat{A}$ (hermitian operator: $\hat{A}^\dagger = \hat{A}$) in quantum mechanics, that operate on wavefunctions $\psi(\mathbf{r})$. We saw that we can make the corresponding operators by promoting the position $r_j \to \hat{r}_j = r_j$ and the conjugate momentum $p_j \to \hat{p}_j = -i\hbar\partial_{r_j}$. We can use this correspondence to build other operators. One particularly important operator is the angular momentum $\mathbf{L}$, and in classical mechanics we have $\mathbf{L} = \mathbf{r} \times \mathbf{p}$.

1. (1/5) Using the correspondence principle to promote to operators, show that the angular momentum operators $\hat{L}_j$ are written as $\hat{L}_x = -i\hbar(y\partial_z - z\partial_y)$, $\hat{L}_y = -i\hbar(z\partial_x - x\partial_z)$, $\hat{L}_z = -i\hbar(x\partial_y - y\partial_x)$.

The most important property of the quantum operators are its commutation relations to other operators. This defines its behavior.

2. (1/5) Using the differential operators above, show that $[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z$.

   (Hint: Take the commutator and apply it to a trial wavefunction $[\hat{L}_x, \hat{L}_y]\psi(\mathbf{r})$, which is just a complex function of the position $\mathbf{r}$. From there you can expand and replace the differential form of the operators, and doing the algebra you need to show that it will be equal to $i\hbar\hat{L}_z\psi(\mathbf{r})$. Showing this for any random trial wavefunction $\psi(\mathbf{r})$ means the operator identity hold true in all cases and you have proven the equality.)

This commutation relation you proved above also holds for cyclic permutations of the indexes, in other words it is also true that $[\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x$ and $[\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y$. The algebra to show them is completely analogous to the above derivation. From here we can built other commutation relations using only the commutator identities, without expanding the operators into differential form.

3. (1/5) For any three operators, $\hat{A}$, $\hat{B}$, and $\hat{C}$, show that $[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]$.

Following the same algebra we would also find that $[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$. These two identities let you decompose commutators of string of multiplications until only simple commutators remain. Lets make use of them bellow.

4. (1/5) Show that $[\hat{L}^2, \hat{L}_z] = 0$, where $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$ is the square of the total angular momentum.

Following the same algebra you could also show that $[\hat{L}^2, \hat{L}_x] = [\hat{L}^2, \hat{L}_y] = 0$. All the commutators we found completely define the relations of angular momentum set of operators $\{\hat{L}_x, \hat{L}_y, \hat{L}_z, \hat{L}^2\}$.

5. (1/5) Using the commutator relations of the set $\{\hat{L}_x, \hat{L}_y, \hat{L}_z, \hat{L}^2\}$, and remembering the result you showed in the previous week (Ex.3.4 of exercise sheet 00), discuss the implications for what operators out of the set share or do not share eigenstates. What is the maximal set of commuting operators you can construct out of these? Is it a unique choice?

Exercise 3 (5 points)

In quantum mechanics, the Hamiltonian that defines all the dynamics of the system is promoted to a hermitian operator, and we generally wrote a one dimensional, one particle, Hamiltonian $\hat{H} = \hat{p}/2m + V(\hat{x})$ where $\hat{p} = -i\hbar\partial_x$ and $V(\hat{x})$ is a real function of x describing some external field acting on the particle. Consider the case where the Hamiltonian is modified as

$$\hat{H} = \hat{p}/2m + V(\hat{x}) - iW(\hat{x}) \tag{2}$$

where $W(x)$ is also a real function of x. This makes the Hamiltonian non-hermitian.

1. (1/5) For the Hamiltonian of the form Eq. (2), show that the continuity equation now becomes
$$\frac{\partial\rho(x,t)}{\partial t} + \frac{\partial J(x,t)}{\partial x} = -\frac{2}{\hbar}W(x)\rho(x,t),$$
where $\rho(x,t) = |\psi(x,t)|^2$ the probability density and $J = \frac{\hbar}{2im}\left(\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial x} - \psi(x,t)\frac{\partial\psi^*(x,t)}{\partial x}\right)$ the probability current.
2. (1/5) Find the time evolution equation of the total probability $P_{\text{tot}}(t)$, where by total probability we mean the probability of being anywhere in space at a given time $P_{\text{tot}}(t) = \int_{-\infty}^{+\infty} \mathrm{d}x\rho(x,t)$.

   (Hint: There should be no losses at infinity, in other words $J(\pm\infty, t) = 0$)
3. (1/5) Consider the simplified case where $W(\hat{x}) = w$ just a constant $w \in \mathbb{R}$, and show that $P_{\text{tot}}(t) = P_{\text{tot}}(0)\mathrm{e}^{-t/\tau}$, where $\tau = \hbar/(2w)$.
4. (1/5) If $W(\hat{x}) = 0$ we recover the familiar Hamiltonian of a free particle under an external potential. In this case, what is the above telling us about the behavior of the total probability over time?
5. (1/5) Now return to the case $W(\hat{x}) = w$ but with $w \neq 0$, what is the above telling us about the behavior of the total probability over time? What type of system could this non-hermitian Hamiltonian describe for $w > 0$ and $w < 0$?