Exercise Sheet 2 **Theoretische Physik 4: Quantenmechanik**

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Exercise 1 (10 points)

We are slowly coming to terms with interpreting the absolute square of the wavefunction of one particle $\rho(x) = |\phi(x)|^2 = \phi(x)^*\phi(x)$ as the probability density to find the particle in real space interval $[x, x + \mathrm{d}x]$, and by extension the integral $P(x_1, x_2) = \int\limits_{x_1}^{x_2} \mathrm{d}x\rho(x) = \int\limits_{x_1}^{x_2} \mathrm{d}x|\phi(x)|^2$ as the probability to find the the particle in the region $[x_1, x_2]$. This interpretation places physical constrains on the form and properties of $\phi(x)$. Lets examine these constrains in more detail.

1. (1/10) Argue why it must be the case that a physically meaningful wavefunction $\phi(x)$ is continuous.
   (Hint: Consider the left and right limits $\lim\limits_{x \to x_o^-} \phi(x)$ and $\lim\limits_{x \to x_o^+} \phi(x)$, and keep in mind that $\rho(x) = |\phi(x)|^2$ is being understood as a probability density.)
2. (1/10) Argue that it must be the case that any physically meaningful wavefunction must be normalized $\|\phi(x)\|^2 = (\phi(x), \phi(x)) = \int\limits_{-\infty}^{+\infty} \mathrm{d}x|\phi(x)|^2 = 1$.

Such wavefunctions are called square integrable. These functions abstractly live in a vector space of square integrable functions. For two "vectors" ϕ_1 and ϕ_2 of this vector space, the inner product is given by $(\phi_1(x), \phi_2(x)) = \int\limits_{-\infty}^{+\infty} \mathrm{d}x\phi_1^*(x)\phi_2(x)$ and is well defined (has the properties of the inner product, most importantly the integrals have a finite result) precisely when the wavefunctions are square integrable. This places limits on the $x \to \pm\infty$ behaviour of $\phi(x)$.

3. (1/10) Explain why $\lim\limits_{x \to \pm\infty} \phi(x) = 0$ is the only reasonable case for a physically sound wavefuction.
4. (1/10) What is the slowest α power decay $\phi(x) \sim x^\alpha$ allowed when $x \to \pm\infty$ so that the wavefuction is physically sound?

Now, let us consider a very simple set of wavefunctions, that of running waves with wavevector k

$$\phi_k(x) = N\mathrm{e}^{ikx} = N\mathrm{e}^{i\frac{px}{\hbar}} \tag{1}$$

where the momentum is $p = \hbar k$. The normalization constant N must be set such that ϕ_k is normalized to 1.

5. (1/10) Why is the running wave ill defined when applying the previous conclusions we reached?

This is only a problem of formality. We simply need to move into functionals. In the previous exercise sheet we saw precisely such a functional, the delta function.

6. (1/10) Generalizing the inner product of the two running waves as $(\phi_{k_1}(x), \phi_{k_2}(x)) = \int\limits_{-\infty}^{+\infty} \mathrm{d}x\phi_{k_1}^*(x)\phi_{k_2}(x) = \delta(p_1 - p_2)$ (take it as a given) show that the running wave wavefunctions are orthogonal when $k_1 \neq k_2$ and that $N = 1/\sqrt{2\pi\hbar}$

This is as far as we can get without considering a specific physical system. Let us return to the Hamiltonian $\hat{H} = \hat{p}^2/2m + V(\hat{x})$ that describes the dynamics of a particle under an external potential $V(x)$. The wavefunction must evolve according to the Schrödinger equation $i\hbar\partial_t\psi(x,t) = \hat{H}\psi(x,t)$. Very soon we will see that this can be reduced to the time independent Schrödinger equation $\hat{H}\phi_E(x) = E\phi_E(x)$ under the substitution $\psi(x,t) = \mathrm{e}^{-iEt/\hbar}\phi_E(x)$. Solving the time independent Schrödinger equation is the key to solving the Schrödinger equation. The time independent Schrödinger equation is a second order partial differential equation in space, and is uniquely solvable under appropriate boundary conditions. The previous analysis is crucial in setting the boundary conditions of $\phi_E(x)$. However, being a second order partial differential equation, we must also have boundary conditions for the first derivative $\partial_x\phi_E(x)$.

7. (1/10) Starting with the time independent Schrödinger equation, and regrouping it so as to isolate $\partial_x^2\phi_E(x)$ on the left, show that if $V(x)$ is everywhere continuous, then the first derivative $\partial_x\phi_E(x)$ must be everywhere continuous.

   (Hint: After regrouping, integrate both sides of the equation, in the region $[x_o - \epsilon, x_o + \epsilon]$, for arbitrary small $\epsilon > 0$. This allows you to access the first derivatives near arbitrary $x = x_o$.)

8. (1/10) Potentials need not be continuous. If $V(x)$ has a simple discontinuity of the form

$$V(x) = \begin{cases} V_1(x) & x < x_d \\ V_2(x) & x > x_d \end{cases}, \; V_1(x_d) \neq V_2(x_d),$$

   where the branches $V_1(x)$ and $V_2(x)$ are continuous, but the entire potential $V(x)$ is not continuous. Show that the first derivative $\partial_x\phi_E(x)$ must be everywhere continuous including $x = x_d$.

9. (1/10) Now lets consider a potential $V(x)$ with an aggressive discontinuity, something like $V(x = x_d) = \infty$ but everywhere else well behaved. Show that the first derivative $\partial_x\phi(x)$ must be everywhere continuous except for $x = x_d$ where it is discontinuous, with the discontinuous jump of $\partial_x\phi_E(x)|_{x=x_d}$ scaling as $-\frac{2m}{\hbar}\int\limits_{x_d-\epsilon}^{x_d+\epsilon} \mathrm{d}x V(x)\phi_E(x)$ for arbitrary small $\epsilon > 0$.

10. (1/10) For the previously considered case of the aggressively discontinuous potential, is it physically reasonable to consider cases where the discontinuous jump of $\partial_x\phi_E(x)|_{x=x_d}$ is infinity large?

Exercise 2 (5 points)

We want to construct a wavefunction which is a localized wave packet in a region of width L. We may attempt to do this by

$$\psi_k(x) = \begin{cases} N\mathrm{e}^{ikx} & |x| < L/2 \\ 0 & \text{else} \end{cases} \tag{2}$$

1. (1/10) Argue from the continuity at $x = \pm L/2$ that such a construction is not physically meaningful.

To amend this, lets alter the construction with two running waves

$$\psi_k(x) = \begin{cases} N_+\mathrm{e}^{ikx} + N_-\mathrm{e}^{-ikx} & |x| < L/2 \\ 0 & \text{else} \end{cases} \tag{3}$$

2. (1/10) What are the boundary conditions at $x = \pm L/2$ to make this a physically meaningful wavefunction? Is the condition at $x = L/2$ different than at $x = -L/2$ or are they somehow related and equivalent?

3. (1.5/10) Solve the boundary conditions and show that the solutions give us three cases: i) $N_+ = N_- = 0$ which is trivially $\psi(x) = 0$ everywhere, ii) $k = 2n\pi/L$ with $n \in \mathbb{Z}$ and $N_+ = -N_-$, iii) $k = (2n+1)\pi/L$ with $n \in \mathbb{Z}$ and $N_+ = N_-$. (Note how the continuity of our trial wavefunction of running waves forced k to be quantized.)

4. (1.5/10) For the non-trivial solutions, normalize the wavefunction.

Exercise 3 (5 points)

Consider the wavefunction that is constant value within width L, and everywhere else is zero

$$\psi(x) = \begin{cases} N & |x| < L/2 \\ 0 & \text{else} \end{cases} \tag{4}$$

1. (1/10) Normalize the wavefunction and show that $N = 1/\sqrt{L}$.

2. (1/10) Show that the Fourier transform is $\widetilde{\psi}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \mathrm{d}x \psi(x) \mathrm{e}^{ikx} = \sqrt{\frac{L}{2\pi}} \frac{\sin(kL/2)}{kL/2}$.

3. (1/10) What is the value of $\widetilde{\psi}(0)$? Argue that it is the global maxima. $\widetilde{\psi}(k)$ hosts a collection of nodes ($\psi(x) = 0$), at what k are they?

4. (1/10) Along with the global maxima of $\widetilde{\psi}(k)$, there is a collection of local maxima and minima as a result of the oscillating sin term. These should continue on to infinity. In the limit $|k|L/2 \gg 1$ approximately where can we find these local maxima and where the local minima?

5. (1/10) Working in units of $L = 1$ (in other words setting $L = 1$) plot $\psi(x)$ for $x \in [-2, 2]$ and $\widetilde{\psi}(k)$ for $k \in [-10\pi, 10\pi]$. Label the x-axis and y-axis. On the x-axis indicate with ticks and labels the locations of the nodes. On the y-axis indicate with ticks and labels the global maxima. For $\widetilde{\psi}(k)$ plot only, also indicate with solid vertical grid lines the locations of the approximate maxima you found (as many as can fit in the plot range $k \in [-10\pi, 10\pi]$), and do the same for the approximate minima but with dashed lines.

   Argue from the plots graphically that the spreads must be approximately $\Delta x \sim L$, and $\Delta p = \hbar \Delta k \sim 2\pi\hbar/L$. What can you say about the bound on $\Delta x \Delta p$? Also comment about how good are the approximate locations of the approximate maxima and minima you found and how/when do they fail?