Quantendynamik und Wellenpakete

Sommersemester 2016

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Problem Set No 1 Date: 19 April 2016

Problem 1.1 – Gaussian wave packets (10 points)

In the lecture, we have learned about Gaussian wave packets (see also Chapter 3 in Tannor's book, Eq.(3.28) and Problem 3.5). (a) Make a plot of the time-dependent parameters x_t, p_t and the widths

$$\Delta x_t^2 = \frac{1}{4\,\mathrm{Re}\,\alpha_t}\,, \qquad \Delta p_t^2 = \frac{\hbar^2 |\alpha_t|^2}{\mathrm{Re}\,\alpha_t}\,, \tag{1.1}$$

$$\langle x; p\rangle_t := \frac{1}{2}\big\langle xp + px\big\rangle_t - x_t p_t = -\frac{\hbar}{2}\frac{\mathrm{Im}\,\alpha_t}{\mathrm{Re}\,\alpha_t} \tag{1.2}$$

$$\alpha_t = a\frac{\alpha_0 \cos\omega t + \mathrm{i} a \sin\omega t}{a\cos\omega t + \mathrm{i}\alpha_0 \sin\omega t} \tag{1.3}$$

where $a = m\omega/2\hbar$ for a harmonic potential with frequency ω. (b) Consider the symmetric matrix

$$C_t = \begin{pmatrix} \Delta x_t^2 & \langle x; p\rangle_t \\ \langle x; p\rangle_t & \Delta p_t^2 \end{pmatrix} \tag{1.4}$$

and show that the product of its eigenvalues is $\hbar^2/4$. (This is the case for so-called pure states. The result illustrates that in phase space and for any time, one can find a rotated coordinate system where the Heisenberg uncertainty product $\Delta x'\Delta p'$ is minimal.)

(c) Compute the momentum distribution of the wave function

$$\Psi(x) = \exp\left[-\alpha_t(x - x_t)^2 + \mathrm{i}p_t(x - x_t) + \mathrm{i}\gamma_t\right] \tag{1.5}$$

where α_t and γ_t are complex-valued and ensure the normalization of $\Psi(x)$.

(d) Show that for $\alpha_t = a$, the Gaussian state (1.5) is the unique physical solution to the differential equation

$$\left(x + \frac{1}{2a}\frac{\mathrm{d}}{\mathrm{d}x}\right)\Psi(x) = \left(x_t + \frac{\mathrm{i}}{2\hbar a}p_t\right)\Psi(x) \tag{1.6}$$

Problem 1.2 – Quantum–classical correspondence (5 points)

In the lecture, we have learned about the hydrodynamical (or Madelung) formulation of the Schrödinger equation (see Tannor, Chapter 4) where the complex wave function is split into

$$\Psi(x,t) = A(x,t)\exp[\mathrm{i}S(x,t)/\hbar] \tag{1.7}$$

with real-valued functions A and S. (a) Show that the probability current

$$j(x,t) = \frac{\hbar}{m}\,\mathrm{Im}\left[\Psi^*(x,t)\frac{\mathrm{d}\Psi(x,t)}{\mathrm{d}x}\right] \tag{1.8}$$

takes the 'classical form'

$$j = \frac{1}{m}A^2\frac{\mathrm{d}S}{\mathrm{d}x} \tag{1.9}$$

with S/m playing the role of a 'velocity potential'. (b) Compute $j(x,t)$ for the wave packet (1.5) and make a sketch.

(c) The 'quantum potential' is given by the second derivative of the amplitude [Tannor Eq.(4.34)]

$$Q(x,t) = -\frac{\hbar^2}{2mA}\frac{\mathrm{d}^2A}{\mathrm{d}x^2} \tag{1.10}$$

Calculate and make a sketch for the gaussian wave packet. Write a few sentences on the impact of this potential on the '(semi)classical paths' that correspond to the flow lines of the hydrodynamic picture.

Problem 1.3 – Playing with eigenfunctions (5 points)

On the moodle platform, you can find the small Python program `play_eig.py` that computes the energy eigenstates in any potential. (a) Download it and try to execute it. (Look up 'Python Interpreter Mode' and the command `execfile`.) (b) Try to understand how the boundary conditions are handled and write a few sentences about your analysis. (c) Play with the numerically computed eigenstates and try for example to generate a 'movie' or a two-dimensional contour plot showing a time-dependent wave packet with arbitrary initial values.