1. Exercise sheet for Theoretical Femtosecond Physics

PD Dr. Frank Großmann, Sommersemester 2017

1: *Time-evolution operator I*
Verify the first three terms in the series for the time-evolution operator by collecting terms up to Δt^2 in the time-sliced expression

$$\hat{U}(t, t_0) = [\hat{1} - \frac{\mathrm{i}}{\hbar}\hat{H}(t_{N-1})\Delta t][\hat{1} - \frac{\mathrm{i}}{\hbar}\hat{H}(t_{N-2})\Delta t] \dots [\hat{1} - \frac{\mathrm{i}}{\hbar}\hat{H}(t_0)\Delta t]$$

and taking the limit $N \to \infty, \Delta t \to 0$ such that $N\Delta t = t - t_0$. Furthermore, show that $\hat{U}(t, t_0)$ is unitary, using the expression above.

2*: *Time-evolution operator II*
For the verification of the formal solution of the TDSE we need the time derivative of an operator of the form

$$\hat{U}(t) = \exp[\hat{B}(t)].$$

a) Calculate $\frac{\mathrm{d}\hat{U}}{\mathrm{d}t}$ by using Taylor expansion of the exponential function (keep in mind that, in general, an operator does not commute with its time derivative).

b) Consider the special case $\hat{B}(t) \equiv -\frac{\mathrm{i}}{\hbar}\hat{H}_0 t$ and give a closed form solution for $\frac{\mathrm{d}\hat{U}}{\mathrm{d}t}$.

c) Consider the special case $\hat{B}(t) \equiv -\frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t' \hat{H}(t')$ and convince yourself that a simple closed form expression for $\frac{\mathrm{d}\hat{U}}{\mathrm{d}t}$ can *not* be given!

d) Show that the construction $\hat{U}(t) = \hat{T}\exp[\hat{B}(t)]$ with the time ordering operator and the operator $\hat{B}$ from part c) allows for a closed form solution by proving that the relation

$$\hat{T}\hat{B}^n = n! \left(\frac{-\mathrm{i}}{\hbar}\right)^n \int_0^t \mathrm{d}t_n \int_0^{t_n} \mathrm{d}t_{n-1} \cdots \int_0^{t_2} \mathrm{d}t_1 \hat{H}(t_n)\hat{H}(t_{n-1}) \dots \hat{H}(t_1)$$

holds.

3: *Spectrum of the harmonic oscillator*
Use the propagator of the 1d harmonic oscillator with $V(x) = \frac{1}{2}m\omega_{\mathrm{e}}^2 x^2$, given by

$$K(x, t; x', 0) = \sqrt{\frac{m\omega_{\mathrm{e}}}{2\pi \mathrm{i}\hbar \sin(\omega_{\mathrm{e}} t)}} \exp\left\{\frac{\mathrm{i}m\omega_{\mathrm{e}}}{2\hbar \sin(\omega_{\mathrm{e}} t)}\left[(x^2 + x'^2)\cos(\omega_{\mathrm{e}} t) - 2xx'\right]\right\}$$

to derive the spectrum.
Hint: Use the geometric series.

bitte wenden

4*: *Gaussian Wavepacket Dynamics*
Use the GWD-Ansatz to solve the TDSE.

a) Use the differential equations for $q_t, p_t, \alpha_t, \delta_t$ in order to show that the Gaussian wavepacket fulfills the equation of continuity.

b) Solve the differential equations for $q_t, p_t, \alpha_t, \delta_t$ for the free particle case $V(x) = 0$.

c) Solve the differential equations for $q_t, p_t, \alpha_t, \delta_t$ for the harmonic oscillator case $V(x) = \frac{1}{2}m\omega_{\mathrm{e}}^2 x^2$.

d) Calculate $\langle\hat{x}\rangle$, $\langle\hat{p}\rangle$, and $\Delta x = \sqrt{\langle\hat{x}^2\rangle - \langle\hat{x}\rangle^2}$, $\Delta p = \sqrt{\langle\hat{p}^2\rangle - \langle\hat{p}\rangle^2}$ and from this the uncertainty product using the general Gaussian wavepacket. Discuss the special cases from b) und c). What do the results for the harmonic oscillator simplify to in the case $\alpha_{t=0} = m\omega_{\mathrm{e}}/(2\hbar)$?

To be discussed on 12.04.2017
exercises with an asterisk may be handed in for examination purposes