2. Exercise sheet for Theoretical Femtosecond Physics

PD Dr. Frank Großmann, Summer 2017

1*: *Short-time propagator*

a) Derive the short-time propagator starting from

$$\hat{U}(\Delta t) = \exp\{-\mathrm{i}\hat{H}\Delta t/\hbar\}$$

for the infinitesimal time-evolution operator.
Hint: Use first order Taylor expansion of the exponential function

b) Use the short time propagator in order to propagate an arbitrary wavefunction $\Psi(x,t)$ over an infinitesimal time interval Δt via

$$\Psi(x, t+\Delta t) = \int \mathrm{d}y K(x, \Delta t; y, 0)\Psi(y,t).$$

and derive the TDSE!
Hint: To this integral only a small intervall of y centered around x is contributing. Expansion of the expression above to first order in Δt and up to second order in $\eta = y - x$ leads to a linear partial differential equation for $\Psi(x,t)$. Use Gaussian integrals, where appropriate.

2*: *Short action and van Vleck propagator*
Use the Legendre transform of the time-dependent action $S(t)$, the so-called short action

$$W(E) = S(t) + Et,$$

in order to show the equivalence of

$$K(x_f, t; x_i, 0) = \exp\left\{\frac{\mathrm{i}}{\hbar}S[x_{\mathrm{cl}}]\right\}\sqrt{\frac{m}{2\pi\mathrm{i}\hbar\dot{x}_{\mathrm{cl}}(0)\dot{x}_{\mathrm{cl}}(t)\int_0^t \frac{\mathrm{d}t'}{\dot{x}^2_{\mathrm{cl}}(t')}}}$$

with the van Vleck expression for the propagator from the lecture.

a) Show that all three $\dot{x}$-dependent terms can be written as second derivatives of W.
Hint: $W(E) = \int_{x(0)}^{x(t)} m\dot{x}\mathrm{d}x$

b) Express the mixed second derivative of S wrt $x_{\mathrm{cl}}(0) = x_i$ und $x_{\mathrm{cl}}(t) = x_f$ by derivatives of W.
Hint: $\frac{\partial S}{\partial t} = -E$

3: *Time-evolution operator III*
Verify that the time evolution operator in the interaction representation $\hat{U}_{\mathrm{I}}(t,0) = \hat{U}_0^+(t,0)\hat{U}(t,0)$ fulfills the appropriate differential equation.

4: *Magnus expansion*
Verify the second order expression $\hat{\mathrm{H}}_2$ of the Magnus expansion in the exponent of the time-evolution operator in the interaction picture.

to be discussed on 26.04.2017
exercises with an asterisk may be handed in for examination purposes