3. Exercise sheet for Theoretical Femtosecond Physics

PD Dr. Frank Großmann, Summer 2017

1: *Split-operator method*
Show that the Strang splitting of the time-evolution operator leads to a second order method.
Hint: use the Zassenhaus as well as the BCH formula

2*: *Poisson bracket operation*
The Poisson bracket operation with the Hamiltonian is denoted by

$$\hat{H}\boldsymbol{\eta} = \{H, \boldsymbol{\eta}\}.$$

By expanding up to second order in Δt show that there is a difference between $\exp\{-\Delta t \hat{H}\}$ and $\exp\{-\Delta t \hat{T}_{\mathrm{k}}\} \exp\{-\Delta t \hat{V}\}$.

3: *Symplecticity*
Prove the symplectic property

$$\mathbf{M}^{\mathrm{T}}\mathbf{J}\mathbf{M} = \mathbf{J} \qquad \forall t$$

of the stability matrix with the skew symmetric matrix $\mathbf{J}$.
Hint: Consider the time derivative of $\mathbf{M}^{\mathrm{T}}\mathbf{J}\mathbf{M}$.

4*: *Stability matrix and width parameter*
The TGWD width parameter allows for a reformulation of the HK prefactor.

a) Show that the nonlinear differential equation

$$\dot{\gamma}_t = -\frac{\mathrm{i}\hbar}{m}\gamma_t^2 - \frac{1}{\mathrm{i}\hbar}V''$$

is fulfilled by the width parameter.

b) Writing the width parameter in the log-derivative form

$$\gamma_t = \frac{m}{\mathrm{i}\hbar}\frac{\dot{Q}}{Q},$$

with $Q = m_{22} + \mathrm{i}\hbar\gamma m_{21}$, show that the HK prefactor can be entirely formulated in terms of γ_t via

$$R^* = \sqrt{\frac{1}{2}(1 + \gamma_t/\gamma)} \exp\left\{\frac{1}{2}\int_0^t \mathrm{d}t' \frac{\mathrm{i}\hbar}{m}\gamma_{t'}\right\}.$$

5: *Van Vleck-Gutzwiller propagator from Herman-Kluk propagator*
Derive the 1d van Vleck-Gutzwiller propagator

$$K^{\mathrm{VVG}}(x'', t; x', 0) = (2\pi i\hbar)^{-\frac{1}{2}} \sum_j \left(\frac{\partial^2 S_j}{\partial x'' \partial x'}\right)^{\frac{1}{2}} \exp\left\{\frac{i}{\hbar} S_j[x'', x']\right\}$$

from the Herman-Kluk(HK) propagator

$$K^{\mathrm{HK}}(x'', t; x', 0) = \int \frac{\mathrm{d}p'\mathrm{d}q'}{2\pi\hbar} \langle x''|\tilde{z}_t\rangle R(p', q', t) \exp\left\{\frac{i}{\hbar} S(p', q', t)\right\} \langle \tilde{z}'|x'\rangle$$

by taking the limit $\gamma \to \infty$. The 1d analoga of the quantities given in the lectures are

$$\langle x|\tilde{z}\rangle = \left(\frac{\gamma}{\pi}\right)^{1/4} \exp\left\{-\frac{\gamma}{2}(x-q)^2 + \frac{i}{\hbar} p(x-q)\right\}$$

$$R(p', q', t) = \sqrt{\frac{1}{2}\left(m_{11} + m_{22} - i\hbar\gamma m_{21} - \frac{1}{i\hbar\gamma} m_{12}\right)}.$$

a) First take the following limits

$$\lim_{\gamma\to\infty} \langle x''|\tilde{z}_t\rangle, \qquad \lim_{\gamma\to\infty} \langle \tilde{z}|x'\rangle.$$

Can these be written using δ-functions?

b) Now perfrom the integrations over q' and p'.

to be discussed on 10.05.2017

exercises with an asterisk may be handed in for examination purposes