Exercise sheet 2

Exercise 2.1: Schrödinger equation. A quatummechanical particle is governed by the complex-valued Schrödinger equation:

$$\mathrm{i}\frac{\partial}{\partial t}\Psi = -\alpha\Delta\Psi + V(x)\Psi\,. \tag{1}$$

with a constant $\alpha > 0$. The unknown function $\Psi : \mathbb{R} \times \mathbb{R}^3$ is called wave function.

a) Free particle: Let the potential $V = 0$ in (1). We look for solutions Ψ of the form $\Psi(t,x) = \gamma \exp(-a(t)|x|^2 + \sum_{i=1}^{d} b_i(t)x_i + c(t))$ for $t \in (0,\infty)$ and $x = (x_1,\ldots,x_d) \in \mathbb{R}^d$. Derive ordinary differential equations

$$\dot{a} = f(a,b,c)\,, \quad \dot{b}_i = g_i(a,b,c)\,, \quad \dot{c} = h(a,b,c) \tag{2}$$

for $a, b_i, c : \mathbb{R} \to \mathbb{C}$ with $i \in \{1,\ldots,d\}$, such that Ψ solves (1).

b) Provide a general solution of the ODE system (2).

c) Particle in a one-dimensional box: Let the potential

$$V(x) := \begin{cases} 0 & \text{if } 0 \le x \le L, \\ \infty & \text{otherwise.} \end{cases}$$

Provide continuous solutions of (1). Hint: separation of variables.

Exercise 2.2: Prove the following statement:
Let $\Omega \subset \mathbb{R}^3$ and $F \in \mathrm{C}([0,T]\times\Omega)$. Assume that

$$\int_\omega F(t,x)\,\mathrm{d}x = 0 \text{ for all } t \in [0,T] \text{ and every Lebesgue-measurable subset } \omega \subset \Omega\,.$$

This implies that $F(t,x) = 0$ for all $(t,x) \in [0,T]\times\Omega$.

Exercise 2.3: Determine the solution $u = u(t,x)$ of the following Cauchy problem with the method of characteristics:

$$\begin{aligned} \frac{\partial u}{\partial t} + x^2\frac{\partial u}{\partial x} &= 0 && \text{in } (0,\infty)\times\mathbb{R}\,, \\ u(0,x) &= u_0(x) && \text{in } \mathbb{R}\,. \end{aligned}$$

(please turn)

Exercise 2.4 (written): Differentiating the determinant. Let X and Y be Banach spaces. A mapping $f : X \to Y$ is differentiable at $A \in X$ if there is $f'(A) \in \mathcal{L}(X,Y)$ such that

$$f(A+H) = f(A) + f'(A)H + o(H)\,, \tag{3}$$

where $o(H) = \|H\|_X \varepsilon(H)$ with $\lim_{H\to 0} \varepsilon(H) = 0$ in Y. Here, $\mathcal{L}(X,Y)$ denotes the space of linear functionals $L : X \to Y$. The element $f'(A) \in \mathcal{L}(X,Y)$ is called the Fréchet derivative of f in the point $A \in X$.

a) Fréchet derivative of the determinant: Let $X = Y = \mathbb{R}^{3\times 3}$ and $f(A) = \det A$ for all $A \in \mathbb{R}^{3\times 3}$. Show that

$$A \text{ invertible} \quad \Rightarrow \quad f'(A)H = \det A \operatorname{tr}(A^{-1}H)\,. \tag{4}$$

Hint: Start from (3), exploit (and verify) the relation

$$\det(\mathrm{Id} + E) = 1 + \operatorname{tr} E + \{\text{monomials of degree} \geq 2\} \quad \text{for any } E \in \mathbb{R}^{3\times 3}.$$

Here Id denotes the identity matrix in $\mathbb{R}^{3\times 3}$.

b) Show the following statement:
Let $t \mapsto A(t) \in \mathbb{R}^{3\times 3}$ be continuously differentiable and $A(t)$ invertible. Then

$$\frac{\mathrm{d}}{\mathrm{d}t} \det A(t) = \det A(t) \operatorname{tr}\left(A^{-1} \frac{\mathrm{d}}{\mathrm{d}t} A(t)\right). \tag{5}$$

c) Consider a motion $\Phi : [0,\infty) \times \Omega_0 \to \mathbb{R}^3$, $(t,x) \mapsto \Phi(t,x)$ satisfying:
(Φ1) $\Phi(0,x) = x_0$,
(Φ2) $\Phi \in \mathrm{C}^1([0,\infty) \times \mathbb{R}^3)$,
(Φ3) the mapping $\Phi(t,\cdot) : \Omega_0 \to \Omega_t$ is invertible for all $t > 0$,
(Φ4) the Jacobian $\det \nabla_x \Phi(t,x)$ is positive for all $(t,x) \in [0,\infty) \times \Omega_0$.
Moreover, assume that the corresponding velocity field $v = \frac{\mathrm{d}}{\mathrm{d}t}\Phi(t,x)$ is continuously differentiable wrt. (t,x). Prove *Euler's expansion formula*:

$$\frac{\mathrm{d}}{\mathrm{d}t} \det \nabla\Phi(t,x) = \det \nabla\Phi(t,x) \operatorname{div}_y v(t,y)\big|_{y=\Phi(t,x)}\,. \tag{6}$$

For this, use (and verify) the relation $\operatorname{tr}(AB) = \operatorname{tr}(BA)$ for all $A, B \in \mathbb{R}^{3\times 3}$.

Ex. 2.4 is to be delivered in written form by teams of two persons each in the exercise lesson on 23/04/2012. It will be discussed in the subsequent week.

NEW room for the tutorial: RUD 25, 1.011