Questions SV 101.368

1) Show that the classical Newtonian dynamics of a spring-mass system governed by Hooke's law for the restoring force is given in the form of a Hamiltonian system for the variables $x, \dot{x}$ (x ... displacement).
Show that the Hamiltonian is conserved by the flow.

2) Show that the classical Newtonian dynamics of a particle in a force field $F = -\nabla V(q)$ (q ... position) is given in the form of a Hamiltonian system for the variables $q, p = m\dot{q}$.
Show that the Hamiltonian is conserved by the flow.

3) Consider a system of N particles interacting pairwise with potential forces which depend on the distances of the particles. This is a Hamiltonian system with

$$H(p,q) = \frac{1}{2}\sum_{i=1}^{N} \frac{1}{m_i} p_i^T p_i + \sum_{i=2}^{N}\sum_{j=1}^{i-1} V_{ij}(\|q_i - q_j\|),$$

q_i ... position of i-th particle

p_i ... momentum of i-th particle

V_{ij} ... interaction potential

(Q2)

Write down the equations of motion for q_i, p_i, and show that the linear momentum $p := \sum_{i=1}^{N} p_i$

and the angular momentum $L := \sum_{i=1}^{N} q_i \times p_i$

are conserved by the flow.

4) The time-dependent Schrödinger equation

$$i\dot{\psi} = H\psi$$

is defined with a self-adjoint operator H on a Hilbert space $\mathcal{H}$.

Show that the norm, $\|\psi\|$, and the energy, $\langle \psi | H | \psi \rangle$ are conserved along the flow.

What property is required of a self-adjoint operator A to ensure $\langle \psi | A | \psi \rangle \equiv \text{const.}$?

5) Derive an explicit formula for the solution of the free Schrödinger equation in $\mathbb{R}^D$

$$i\dot{\psi} = -\frac{1}{2}\Delta\psi, \quad \psi(0) = \psi_0$$

by using the Fourier transform.

Q3

6) Consider a one-parameter family $S(t)$ of linear operators on a Banach space X.
What conditions define a "strongly continuous semigroup of operators". Define the "infinitesimal generator" A of S, and show that

$$\frac{d}{dt} S(t) x = A S(t) x = S(t) A x \quad \forall x \in D(A).$$

Formulate the "Theorem of Stone".

7) Define the "position operator" q and the "momentum operator" p for $x \in \mathbb{R}$, and the quantum harmonic oscillator Hamiltonian H.
Moreover, define the "ladder operators" A, A^+.
Define the complete orthonormal system of eigenfunctions of AA^+, $\{\phi_j\}$, with $\phi_0(x) = \frac{1}{\sqrt[4]{\pi}} e^{-x^2/2}$.
Show that these correspond with eigenfunctions of H. Use this fact to show that the eigenvalues are real, and that $\phi_j \perp \phi_k$ for $\lambda_j \neq \lambda_k$.

8) Define the Hamiltonian of the molecular Schrödinger equation.

For <u>indistinguishable particles</u>,

$$\langle R\Psi|A|R\Psi\rangle = \langle \Psi|A|\Psi\rangle, \quad R\Psi(x_1,x_2;t) = \Psi(x_2,x_1;t),$$

holds for any observable A.

Show that this implies that the wave function is either symmetric or anti-symmetric under exchange of two particles, $\Psi(x_1,x_2;t) = \pm\Psi(x_2,x_1;t)$.

9) Consider $i\dot{\Psi} = H\Psi$, $\Psi(0) = \Psi_0$ on a Hilbert space $\mathcal{H}$.

Define a variational approximation on a submanifold $\mathcal{M} \subseteq \mathcal{H}$. Show that this conserves the average of any "<u>observable</u>" A with $[A,H] = 0$.

Particularly, the "<u>norm</u>" and "<u>energy</u>" are conserved.

10) Let u be defined as a variational approximation on a manifold $\mathcal{M}$, with $u(0) = \Psi(0)$. Show that

$$\|u(t) - \Psi(t)\| \leq \int_0^t \operatorname{dist}\left(\tfrac{1}{i} H u(s), T_{u(s)}\mathcal{M}\right) ds.$$

11) Consider a timedepent matrix $A(t) \in \mathbb{R}^{n \times n}$. (Q5)

We want to compute a variational approximation on the manifold of matrices of exactly rank r.
Give the variational principle, necessary additional orthogonality constraints and derive the equations of motion for S, where $A \approx Y = USV^T$.
($U, V \in \mathbb{R}^{n \times r}$ orthogonal, $S \in \mathbb{R}^{r \times r}$ nonsingular)

12) Define the method of "Variational Splitting", i.e. a symmetric second-order split-step time integrator.
What assumptions on the manifold M, variational approximation u, and kinetic and potential operators T and V are used to establish second-order convergence?

13) Define the approximation manifold used in Gaussian wavepacket dynamics, and formulate the error bound for the associated variational approximation.

Q6

14) Formulate the "Runge-Gross Theorem" underlying time-dependent density functional theory.
Give the "time-dependent Kohn-Sham equations" for the decoupled system.

15) Consider "pseudospectral space discretization" by the harmonic oscillator eigenfunctions φ_k. With the orthogonal projection $P_K f = \sum_{k<K} \langle \varphi_k | f \rangle \varphi_k$, derive an estimate for $\| f - P_K f \|$ for f in the Schwartz space S. Formulate the resulting error bound for the time-dependent Galerkin approximation on the space spanned by $\{ \varphi_k \}$.
Define a "hyperbolic reduced tensor grid" in $\mathbb{R}^d$.

16) Consider "collocation" based on trigonometric interpolation. Denote the trigonometric interpolation operator by $I_K f(x) = \sum_{k=-\frac{K}{2}}^{\frac{K}{2}-1} c_k e^{ikx}$, with the vector (c_k) the discrete Fourier transform of the vector of function values $(f(x_j))$.

Derive an estimate for $\| f - I_K f \|_{L^2}$.

Formulate the resulting error bound for the collocation approximation of the time-dependent problem.

17) Formulate the Chebyshev method for the computation of the matrix exponential $e^{-i\Delta t A}$, and give an error bound. What restriction is implied by this error bound? Formulate the recurrence relation for Chebyshev polynomials underlying "<u>Clenshaw's Algorithm</u>".

18) Formulate "<u>Lanczos Method</u>" for the computation of the matrix exponential $e^{-i\Delta t A}$. Formulate an error estimate for approximation on the m-th Krylov subspace associated with A and a vector v, when an approximation for $f(A)v$ is sought for a complex-valued function f. Discuss the implications on step-size choice in the approximation of $e^{-i\Delta t A}$

19) Define "Magnus integrators" for the approximation of $i\dot{\psi}(t) = H(t)\,\psi(t)$.
Give a simple example of a Magnus integrator.
Give three important "geometric properties" of these methods.

20) Consider "hierarchical matrices" for the approximation of the meanfield operator matrix
$V_{ij} := \int \phi_i V \phi_j$, ϕ_i, ϕ_j ... compactly supported.
Define a "cluster tree" and give one possible criterion to determine "admissible blocks".
Give the storage requirement and computational complexity for computations with hierarchical matrices.