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NANYANG TECHNOLOGICAL UNIVERSITY

SEMESTER 2 EXAMINATION 2014-2015

PAP723–Advanced Numerical Methods for Physics

April/May 2015 Time Allowed: 3 Hours

INSTRUCTIONS TO CANDIDATES

1. This examination paper contains **FOUR (4)** questions and comprises **FIVE (5)** pages.
2. Answer **ALL FOUR (4)** questions.
3. Answer each question beginning on a **FRESH** page of the answer book.
4. This **IS NOT** an **OPEN BOOK** exam.

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1. **Finite-difference schemes** (35 marks total)

(a) Consider a non-relativistic spin-1/2 particle moving in 1D. The wavefunction at each point consists of two complex-valued components, $\{\psi_\uparrow(x), \psi_\downarrow(x)\}$, representing spin up and spin down respectively. In the presence of "spin-orbit interaction", the Schrödinger equation can take the form

$$-\frac{1}{2}\frac{d^2\psi_\uparrow}{dx^2} + V(x)\psi_\uparrow - \alpha\frac{d\psi_\downarrow}{dx} = E\psi_\uparrow(x)$$
$$-\frac{1}{2}\frac{d^2\psi_\downarrow}{dx^2} + V(x)\psi_\downarrow + \alpha\frac{d\psi_\uparrow}{dx} = E\psi_\downarrow(x),$$

where $V(x)$ is a real scalar potential and $\alpha \in \mathbb{R}$ is a spin-orbit parameter.

Formulate a finite-difference scheme for solving these coupled equations numerically. Assume Dirichlet boundary conditions: $\psi_\sigma(0) = \psi_\sigma(L) = 0$, where $\sigma \in \{\uparrow, \downarrow\}$ and L is the length of the computational cell.

In your answer, be sure to explain (i) your choice of spatial discretization points, (ii) how the discretized state vector relates to the wavefunctions $\{\psi_\uparrow(x), \psi_\downarrow(x)\}$, and (iii) the form of the Hamiltonian matrix.

(15 marks)

(b) Consider a spinless particle moving in 2D with zero scalar potential, and a 2D vector potential $\vec{A}(x, y)$. The Schrödinger equation takes the form

$$\left\{-\frac{1}{2}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right] + iA_x\frac{\partial}{\partial x} + iA_y\frac{\partial}{\partial y} + \frac{A_x^2 + A_y^2}{2}\right\}\psi(x, y) = E\psi(x, y).$$

Formulate a finite-difference scheme for solving this 2D differential equation numerically. Assume a square computational cell, $0 \le x \le L$ and $0 \le y \le L$, with Dirichlet boundary conditions at the boundaries of the cell. Do not make any assumptions about the form of $\vec{A}(x, y)$; in particular, note that it can vary from point to point.

In your answer, be sure to explain (i) your choice of spatial discretization points, (ii) how the discretized state vector relates to the wavefunction $\psi(x, y)$, and (iii) the form of the Hamiltonian matrix.

(20 marks)

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2. **Eigenvalues of a tridiagonal matrix** (15 marks total)

Consider the following $N \times N$ matrix:

$$\mathbf{A} = \begin{bmatrix} 1 & -1 & 0 & 0 & 0 & \cdots & 0 \\ -1 & 2 & -1 & 0 & 0 & \cdots & 0 \\ 0 & -1 & 2 & -1 & 0 & \cdots & 0 \\ \vdots & & \ddots & \ddots & \ddots & & \vdots \\ 0 & \cdots & 0 & -1 & 2 & -1 & 0 \\ 0 & \cdots & 0 & 0 & -1 & 2 & -1 \\ 0 & \cdots & 0 & 0 & 0 & -1 & 2 \end{bmatrix}$$

(Note that $A_{00} = 1$, but all the other entries on the diagonal are 2.)

For $N \gg 1$, estimate the three smallest eigenvalues. Explain your reasoning.

(15 marks)

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3. **Discrete Fourier transforms and wave propagation** (30 marks total)

Consider the time-*dependent* Schrödinger equation, in 1D space with zero potential:

$$i\frac{\partial \psi}{\partial t} = -\frac{1}{2}\frac{\partial^2 \psi}{\partial x^2}, \quad 0 \le x \le L.$$

Assume *periodic boundary conditions* with a cell of length L, i.e. $\psi(x) = \psi(x+L)$. Given an arbitrary initial wavefunction $\psi(x,0)$, defined for $0 \le x \le L$ at time $t = 0$, we wish to compute the wavefunction $\psi(x,T)$ at some later time $t = T$. This can be accomplished using the Discrete Fourier Transform (DFT).

(a) Due to the periodic boundary conditions, we can write the initial wavefunction as a Fourier series, $\psi(x,0) = \sum_p A_p e^{ik_p x}$, where the sum is taken over $p \in \mathbb{Z}$ (including negative integers), and $k_p \equiv 2\pi p/L$. Prove that

$$A_p = \frac{1}{L}\int_0^L dx\ \psi(x,0)\, e^{ik_p x}. \qquad \text{(3 marks)}$$

(b) Choose an appropriate set of N spatial discretization points, $\{x_0, x_1, \ldots, x_{N-1}\}$, and write down a formula for x_n in terms of L. Explain how to approximate the Fourier coefficients $\{A_p\}$ from part (a), in terms of the standard DFT formula

$$\mathcal{D}_k\{f\} = \sum_{m=0}^{N-1} e^{-2\pi i \frac{mk}{N}} f_m, \qquad \text{for } k = 0, \ldots, N-1. \qquad \text{(10 marks)}$$

(c) Using the time-dependent Schrödinger equation, derive an expression for the final wavefunction $\psi(x,T)$, in terms of the A_p's. (5 marks)

(d) Using your results from parts (a)–(c), formulate an algorithm that takes a discretized initial wavefunction $\{\psi(x_0,0), \psi(x_1,0), \ldots, \psi(x_{N-1},0)\}$ and computes the discretized final wavefunction $\{\psi(x_0,T), \psi(x_1,T), \ldots, \psi(x_{N-1},T)\}$. Your algorithm should be expressed in terms of the DFT formula given in part (c). (12 marks)

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4. **Monte Carlo simulations** (20 marks)

Consider the standard 2D Ising model, with the states given by the spins $\{s_{m,n}\}$ on an $N \times N$ lattice with site indices (m, n), where $s_{m,n} \in \{+1, -1\}$. The energy is

$$E = -H \sum_{(m,n)} s_{m,n} - J \sum_{\langle (m,n),(m',n') \rangle} s_{m,n} s_{m',n'},$$

where $\langle (m, n), (m', n') \rangle$ denotes pairs of nearest-neighbour sites without double-counting. As discussed in class, the thermodynamic properties can be found using a Metropolis Monte Carlo simulation.

(a) What is the size of the Markov chain's transition matrix? For the usual Metropolis Monte Carlo procedure, how many non-zero elements are there in the transition matrix, and why? (4 marks)

(b) How does the runtime to perform each step of the Monte Carlo simulation scale with N? Explain. (4 marks)

(c) We can start the Monte Carlo simulation by either assigning $s_{m,n} \in \{+1, -1\}$ randomly (and with equal probability) on each site, or setting $s_{m,n} = +1$ on each site. Explain why the initial choice should not matter, if we run the simulation for an extremely long time. Then explain why it *does* matter in practice, and which choice is preferable. (4 marks)

(d) Normally, on each Monte Carlo step we choose a random site, and either accept or reject a spin-flip on that site. As an alternative, we could randomly choose a number $1 \leq k \leq N^2$, randomly pick k lattice sites, and use the Metropolis criterion to decide whether to accept or reject flipping all k spins simultaneously. Is this a valid Monte Carlo scheme? Why or why not? (4 marks)

(e) As another alternative, we could update the lattice in "typewriter order": go through the sites one-by-one, in a cyclic sequence $(0, 0) \to (0, 1) \to (0, 2) \to \cdots \to (1, 0) \to (1, 1) \to (1, 2) \to \cdots \to (0, 0) \to \cdots$, and on each step either accept or reject the spin-flip on that site according to the Metropolis criterion. Is this a valid Monte Carlo scheme? Why or why not? (4 marks)

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