NANYANG TECHNOLOGICAL UNIVERSITY

SEMESTER 2 EXAMINATION 2013-2014

PAP723 – Advanced Numerical Methods for Physicists

MAY 2014 TIME ALLOWED: 3 HOURS

INSTRUCTIONS TO CANDIDATES

1. This examination paper contains **FOUR (4)** questions and comprises **SIX (6)** pages.

2. Answer **ALL** questions.

3. Answer each question beginning on a **FRESH** page of the answer book.

4. Candidates may use calculators. However, they should write down systematically the steps in the workings.

5. This is a **CLOSED BOOK** exam.

1. **Finite-Difference Schemes in 1D** (20 marks total)

Consider the Schrödinger wave equation with a constant potential V_0, in a one-dimensional space of length L (with $\hbar = m = 1$):

$$\left[-\frac{1}{2}\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\psi(x), \qquad 0 \le x \le L.$$

Following the finite-difference method, we discretize space into N points $\{x_0, x_1, \cdots, x_{N-1}\}$, which are equally-spaced with $\Delta x \equiv x_{j+1} - x_j$.

(a) Consider Dirichlet boundary conditions: $\psi(0) = \psi(L) = 0$. Define a set of finite-difference points $\{x_j\}$, in terms of N and L. Hence, find the finite-difference matrix equation.

(3 marks)

(b) Consider "Robin boundary conditions": for independent constants α and β,

$$\begin{aligned} \psi'(x=0) + \alpha\,\psi(x=0) &= 0, \\ \psi'(x=L) + \beta\,\psi(x=L) &= 0. \end{aligned}$$

Define $\{x_j\}$ in terms of N and L, and find the finite-difference matrix equation. Under what circumstances is the finite-difference matrix Hermitian?

(5 marks)

(c) Consider "twisted boundary conditions": for some constant K,

$$\psi(L) = \psi(0)\, e^{iKL}.$$

Define $\{x_j\}$ in terms of N and L, and find the finite-difference matrix equation. Under what circumstances is the finite-difference matrix Hermitian?

(5 marks)

(d) Consider "outgoing boundary conditions",

$$\begin{aligned} \psi'(0) &= -ik\psi(0) \\ \psi'(L) &= +ik\psi(L), \end{aligned}$$

where k is a constant. Define $\{x_j\}$ in terms of N and L, and find the finite-difference matrix equation. Under what circumstances is the finite-difference matrix Hermitian?

(7 marks)

2. **Finite-Difference Schemes in 2D** (30 marks total)

In two dimensions, a finite-difference grid is labeled by two indices (m, n) where $0 \le m < M$ and $0 \le n < N$. The field at grid index (m, n) is denoted $\psi_{m,n}$. Consider Schrödinger's wave equation

$$\left[-\frac{1}{2}\nabla^2 + V(x, y)\right] \psi(x, y) = E\psi(x, y).$$

This can be written as a finite-difference equation of the form

$$\sum_{m'n'} H_{mn,m'n'}\, \psi_{m'n'} = E\psi_{mn}.$$

(a) For 2D Cartesian coordinates, let m be the x index, with grid spacing Δx; let n be the y index, with grid spacing Δy. Derive $H_{mn,m'n'}$, expressing it in terms of Kronecker deltas (δ_{pq}). Ignore boundary conditions.

(6 marks)

(b) Consider a grid with $M = 4$ and $N = 3$, defined in a rectangular domain $x \in [0, L_x]$, $y \in [0, L_y]$ with Dirichlet conditions at the boundaries. Define an appropriate set of grid points, stating clearly the (x, y) coordinates of grid point (m, n). Hence, write down the 12×12 finite-difference matrix H.

(7 marks)

(c) In polar coordinates (r, ϕ), the Laplacian can be written as

$$\nabla^2\psi = \frac{1}{r}\frac{\partial\psi}{\partial r} + \frac{\partial^2\psi}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2\psi}{\partial\phi^2}.$$

Consider Dirichlet boundary conditions at radius R, i.e. $\psi(R, \phi) = 0$. Define an appropriate set of polar grid points indexed by (m, n), where m is the radial index and n is the azimuthal index. State the (r, ϕ) coordinates of grid index (m, n). Hence, derive $H_{mn,m'n'}$, expressing it in terms of Kronecker deltas.

(12 marks)

(d) For $M = 4$ and $N = 3$, write down the finite-difference matrix.

(5 marks)

3. **Fourier Analysis** (30 marks total)

Consider the truncated Fourier integral

$$F(\omega;T) = \int_0^T dt\, e^{-i\omega t} f(t).$$

(a) Let $f(t) = A\,e^{i\omega_0 t}$, where $\omega_0 \in \mathbb{R}$. Calculate $F(\omega;T)$.

(4 marks)

(b) Sketch $|F(\omega;T)|$ versus ω. On this sketch, indicate and state: (i) the height of the main Fourier peak, and (ii) the frequencies of the sidelobe peaks.

(4 marks)

(c) Is it possible to resolve the peaks and troughs of these sidelobes with a single discrete Fourier transform? If so, find the required Δt. If not, explain why not.

(4 marks)

(d) Consider a Fourier integral with an exponential window function:

$$F(\omega;T,\gamma) = \int_0^T dt\, e^{-i\omega t}\, e^{-\gamma|t-\frac{T}{2}|}\, f(t).$$

Sketch the window function as a function of t.

(2 marks)

(e) Find $F(\omega;T,\gamma)$ for $f(t) = A\,e^{i\omega_0 t}$. Hence, sketch $|F(\omega;T,\gamma)|$ versus ω for $\gamma \gg T$. State the Fourier peak's width and height, and the area under the curve. Express your answers in terms of A, γ, T, and/or ω_0.

(8 marks)

(f) The discrete Fourier transform's standard definition is

$$X_k = \sum_{n=0}^{N-1} x_n \cdot e^{-2\pi i k n/N}.$$

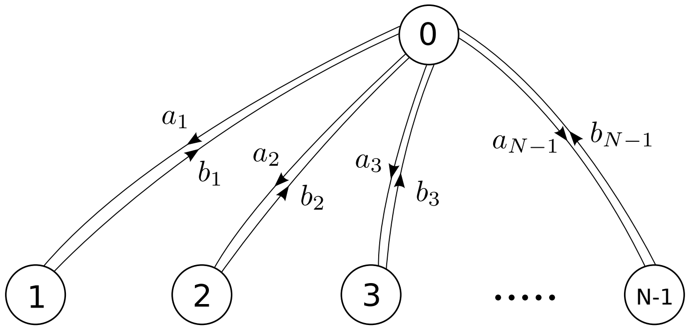
Let $[f(t_0), f(t_1), \dots f(t_{N-1})]$ be N sampled values of $f(t)$, taken at equal time intervals $\Delta t = t_{n+1} - t_n$. We wish to find the Fourier transform $F(\omega;T)$, for a frequency range centered at zero: $\omega \in [-\Omega, \Omega]$ for some Ω.

Derive an appropriate set of discretized frequencies ω_k, which includes both positive and negative values centered at zero. Hence, derive $F(\omega_k;T)$ in terms of $[f(t_0), f(t_1), \dots f(t_{N-1})]$. For the case where $f(t)$ is real, derive the symmetry of the resulting discrete Fourier spectrum.

(8 marks)

4. **Markov chains** (20 marks total)

Consider a Markov chain of N states, with the following state diagram:



(a) For $N = 5$, write down the transition matrix $P_{mn} \equiv P(m|n)$.

(3 marks)

(b) Find the steady-state probability distribution $\{p_n\}$, in terms of the transition probabilities a_m and b_m.

(3 marks)

(c) Suppose the Markov chain represents a thermodynamic system with state energies $E_0, E_1, \ldots, E_{N-1}$, at temperature T. What conditions should the transition probabilities a_m, and b_m satisfy?

(4 marks)

(d) Suppose we wish to perform a Monte Carlo simulation of this thermodynamic system, following this rule:

- If the system is in state 0, then during the next Monte Carlo step, it transitions to one of the states $\{1, 2, \ldots, N-1\}$, with equal probability.

If the system is in state $n > 0$, what is the rule for choosing the next step?

(4 marks)

Note: Question no. 4 continues on Page 6.

(e) Fill in the Scipy code to perform a simulation based on the above Monte Carlo scheme, starting with the lines below. The simulation should calculate the thermodynamic average of a quantity X. The variable `N` is the number of states, `nsteps` is the number of Monte Carlo steps, `E` is an array containing the state energies, and `X` is an array containing the X values for the various states. You can use the function `random.randrange(a,b)`, which returns a random integer $a \leq m < b$.

(6 marks)

```
N, nsteps = 100, 1000
E = linspace(0, 20, N)        # State energies
X = random.random(N)          # Value of X for each state
```

- End of paper -