NANYANG TECHNOLOGICAL UNIVERSITY

SEMESTER 2 EXAMINATION 2012-2013

PAP723 – Advanced Numerical Methods for Physicists

MAY 2013 TIME ALLOWED: 3 HOURS

INSTRUCTIONS TO CANDIDATES

1. This examination paper contains **TWO (2)** questions and comprises **FIVE (5)** 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. <u>**The Transfer Matrix Method**</u> (28 marks total)

(a) For the 1D Schrödinger equation, the transfer matrix M satisfies

$$\begin{bmatrix} M_{00} & M_{01} \\ M_{10} & M_{11} \end{bmatrix} \begin{bmatrix} \psi_R(x_0) \\ \psi_L(x_0) \end{bmatrix} = \begin{bmatrix} \psi_R(x_1) \\ \psi_L(x_1) \end{bmatrix},$$

where x_0 and x_1 are spatial positions, and $\psi_{L,R}(x)$ are the left- and right-moving components of the wavefunction. The scattering matrix S satisfies:

$$S \begin{bmatrix} \psi_R(x_0) \\ \psi_L(x_1) \end{bmatrix} = \begin{bmatrix} \psi_L(x_0) \\ \psi_R(x_1) \end{bmatrix}.$$

Write down an explicit expression for the S matrix, in terms of the transfer matrix elements M_{ij}. (6 marks)

(b) Write the S matrix in terms of r, t, r', and t', where r and t are the reflection and transmission coefficients for waves incident from the left, and r' and t' are the reflection and transmission coefficients for waves incident from the right.

(4 marks)

(c) In class, we derived the transfer matrix across a constant-potential region, and across a finite potential step. Now consider the delta-function potential

$$V(x) = V_0 + A\delta(x - x_0),$$

where V_0 and A are constants and $\delta(x - x_0)$ is a delta function centered at x_0. Using the 1D Schrödinger equation, derive the transfer matrix from x_0^- to x_0^+ (i.e. across the delta-function spike). (10 marks)

Hint: the wavefunction remains continuous at x_0, but not its first derivative. Also, the delta-function potential satisfies

$$\int_{x_0^-}^{x_0^+} dx\, V(x) = A.$$

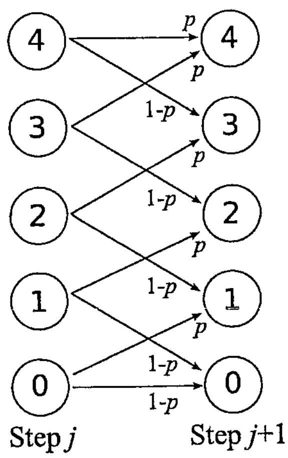
(d) For the above delta-function potential, sketch a graph of the transmittance $T = |t|^2$ versus the energy E, for $E > V_0$. Indicate clearly the limiting values of T for $E \to V_0$ and for $E \to \infty$. (8 marks)

2. Markov chains (72 marks total)

Consider a Markov chain defined with N states, labeled $\{x_0, x_1, \cdots x_{N-1}\}$, and transition probabilities

$$\begin{aligned} P_t(x_m|x_n) &= \left\{ \begin{array}{ll} p & \text{if } m = n+1 \\ 1-p & \text{if } m = n-1 \\ 0 & \text{otherwise} \end{array} \right\} \quad \text{for } 1 \le n \le N-2 \\ P_t(x_0|x_0) &= P_t(x_{N-2}|x_{N-1}) = 1-p, \\ P_t(x_1|x_0) &= P_t(x_{N-1}|x_{N-1}) = p. \end{aligned}$$

This is illustrated in the following figure, for the $N = 4$ case:



Let $\vec{p}_j \equiv [p_j(x_0), \cdots, p_j(x_{N-1})]$ be the probability distribution of the states at step j. The Markov step can be written as a matrix equation

$$\vec{p}_{j+1} = \mathcal{P}\,\vec{p}_j,$$

where $\mathcal{P}$ is an $N \times N$ matrix (the transition matrix), such that $\mathcal{P}_{ij} = P_t(x_i|x_j)$. (Note that i is the matrix's row index and j is the column index.)

(a) Write down the transition matrix for $N = 4$. (4 marks)

(b) Write down the transition matrix for $N = 8$. (4 marks)

Note: Question no. 2 continues on Page 4.

(c) Fill in the Python code to construct the transition matrix for general N. Start from the code given below. (8 marks)

```
from scipy import *
import scipy.sparse as sp
N, p = 500, 0.25
H = sp.lil_matrix(N, N) # Creates an empty sparse NxN matrix.
## Fill in the rest of the code below.
## Do not copy out this starting code in your answer.
```

(d) Suppose the states $\{x_0, x_1, \cdots x_{N-1}\}$ correspond to evenly-spaced positions, with spacing $\Delta x \equiv x_{j+1} - x_j$. The Markov transition matrix equation can be regarded as the finite difference limit of a differential equation,

$$p_{j+1}(x) = D\frac{d^2 p_j}{dx^2} + \mu\frac{dp_j}{dx} + Cp_j(x).$$

Write down the finite difference matrix equation corresponding to this differential equation. Hence, by comparison to the Markov transition equation, find appropriate values of D, μ, and C, in terms of p and Δx. (12 marks)

(e) To be consistent with P_t, the differential equation in (d) must satisfy certain boundary conditions. On the left boundary, we can write

$$p'(x_L) + \alpha\, p(x_L) = 0,$$

where p' denotes the first derivative of $p(x)$. Find appropriate values of α and x_L, in terms of p and Δx. (10 marks)

(f) Suppose we treat the Markov chain steps as time steps, and define

$$p_j(x) = p(x, t_j), \quad t_j \equiv t_0 + j\Delta t$$
$$p_{j+1}(x) - p_j(x) = \Delta t \cdot \frac{\partial}{\partial t}\Big[p(x,t)\Big]_{t=t_j}.$$

The differential equation in (d) becomes a partial differential equation in x and t. Write down the partial differential equation, in terms of the parameters Δx, Δt, and p. (2 marks)

Note: Question no. 2 continues on Page 5.

(g) If we ignore the boundary conditions and normalization, one solution to the above partial differential equation is

$$p(x,t) = \frac{1}{\sqrt{t}} \exp\left[-A\frac{(x-vt)^2}{t}\right].$$

Find the values of A and v in terms of Δx, Δt, and p. (10 marks)

(h) Suppose we wish to use the states $\{x_0, x_1, \cdots x_{N-1}\}$ in a Monte Carlo simulation, assigning them energies $\{E_0, \cdots, E_{N-1}\}$. In each Monte Carlo step, we propose a trial move and then choose to accept or reject the trial move with probability

$$P_a(x_i|x_j) = \text{probability of accepting a trial move from } x_i \text{ to } x_j.$$

However, unlike the usual Metropolis algorithm, we do not generate trial moves using an unbiased random walk. Instead, we generate trial moves using the Markov chain P_t. State the relationship between P_a, P_t, and the inverse temperature β, in order to satisfy detailed balance. (6 marks)

(i) Suppose the Markov chain used to generate the trial moves is the one described at the beginning of this problem, i.e. with transition probabilities P_t. For the $N = 4$ case, find an explicit matrix $P_a(x_i|x_j)$ satisfying detailed balance.

(8 marks)

(j) Find a matrix $P_a(x_i|x_j)$ satisfying detailed balance, for general N. (8 marks)

- End of paper -

Please read the following instructions carefully:

1. **PLEASE DO NOT TURN OVER THE QUESTION PAPER UNTIL YOU ARE TOLD TO DO SO. DISCIPLINARY ACTION MAY BE TAKEN AGAINST YOU IF YOU DO SO.**

2. You may raise your hand if you need to communicate with the invigilator.

3. Please write your **Matriculation Number** on the front of the answer book.

4. Please indicate clearly in the answer book (at the appropriate place) if you are continuing the answer to a question elsewhere in the book.