FINAL EXAM

PHYS 401 (Fall 2006), 12/11/06

Name:

Signature:

Duration: 120 minutes

Show all your work for full/partial credit!

1.) *Multiple Choice* *(18 pts.)*

For each statement below, circle the correct answer (TRUE or FALSE, no reasoning required).

(a) The main objective of computational physics is to find the most elegant algorithm for solving a physics problem.
TRUE FALSE

(b) The main objective of computational physics is to provide solutions for analytically intractable physics problems.
TRUE FALSE

(c) The results of a computational solution to a physics problem should be sensitive to numerical input parameters (such as the numerical time-step width, Δt).
TRUE FALSE

(d) The equilibrium temperature of a molecular dynamics simulation depends on the initial speeds given to the molecules.
TRUE FALSE

(e) For given initial speeds of the molecules, the equilibrium temperature of a molecular dynamics simulation depends on the initial directions of the molecule velocities (assuming the total moment of the system to be zero).
TRUE FALSE

(f) Simulating a random walk is equivalent to solving a diffusion equation.
TRUE FALSE

No.	Points
1	
2	
3	
4	
5	
6	
7	
Sum	

2.) *Euler vs. Euler-Cromer Method* *(18 pts.)*

The ordinary, second order differential equation describing Simple Harmonic Motion is of the form

$$\frac{d^2\Theta}{dt^2} = -\Omega\ \Theta \tag{1}$$

where Ω is a given parameter.

(a) Decompose Eq. (1) into two first order differential equations and write down their discretized form using the Euler Method.

(b) What is the problem with using the Euler Method for the numerical solution of Eq. (1)?

(c) Write down the discretized solution to Eq. (1) using the Euler-Cromer Method. What is the essential improvement over the Euler Method?

3.) *Transition to Chaotic Motion* *(14 pts.)*

In class, two criteria for characterizing the transition from regular to chaotic motion have been introduced. For definiteness, consider a driven, damped, harmonic oscillator.

(a) Explain what is meant by "bifurcation" of the period of motion and how it relates to the transition to chaotic motion (*hint*: sketch a Poincaré section of the angular displacement $\Theta(t = nT_D)$ (T_D: period of the driving force, $n = 1, 2, \ldots$) as a function of driving force F_D.)

(b) Briefly explain another criterion for distinguishing chaotic and regular motion.

4.) *General Relativistic Correction to Newton's Gravitational Law* *(8 pts.)*

Upon including corrections due to general relativistic effects into Newton's universal law of gravitation, the force between two masses takes the form

$$F_G = \frac{GM_1M_2}{r^2}\left(1 + \frac{\alpha}{r^2}\right) \tag{2}$$

with a predicted $\alpha = 1.18AU^2$ (AU=astronomic units). The correction term predicts a precession frequency of Mercury's orbit around the Sun of about $\dot{\Theta}_p = \omega_p = 44\ arcsec/100y$, which is too small to be extracted by direct numerical simulation. Suppose you have a working code for simulating Mercury's orbit, briefly describe a numerical approach that allows to estimate the precession frequency for the physical value of α (a schematic graph will be helpful).

5.) *Poisson Equation* *(8 pts.)*

The Poisson equation for the electrostatic potential in 3 dimensions is given by

$$\vec{\nabla}^2 V = -\frac{\varrho}{\epsilon_0} \; . \tag{3}$$

Derive the symmetric finite-difference approximation to the second order derivatives in Cartesian coordinates and solve Eq. (3) for $V(i,j,k)$ in terms of its neighboring values and a given (discretized) charge density $\varrho(i,j,k)$.

6.) *Ising Model in Mean-Field Approximation* *(18 pts.)*

Consider the 2-D Ising model in an external magnetic field H; in the mean-field approximation, the energy of a single spin s_k is written as

$$E_k = -\mu H_{eff} s_k - \mu H s_k \ , \qquad (s_k = \pm 1). \tag{4}$$

where the "mean field", $H_{eff} \equiv zJ\langle s \rangle/\mu$, is induced by the z neighboring spins, and $\langle s \rangle$ is the average spin orientation.

(a) Using the definition of the average spin orientation, $\langle s \rangle = \sum_{k=\pm} P_k s_k$ with $P_k = C \exp(-E_k/k_B T)$, derive the mean field selfconsistency equation

$$\langle s \rangle = \tanh[\frac{\mu(H_{eff} + H)}{k_B T}] \tag{5}$$

(*hint*: use $P_+ + P_- = 1$ to determine C).

(b) For $H=0$, sketch the graphical solutions to the mean-field equation for large and small temperature T by plotting it's left- and right-hand-side versus $\langle s \rangle$.

(c) Show that the critical exponent β for the magnetization, defined by $\langle s \rangle \propto (T_c - T)^\beta$, has a value of $\beta = 0.5$ in the mean-field approximation (*hint*: use $\tanh(x) \simeq x - x^3/3$ for small x).

7.) *Ising Model and Monte Carlo Method* *(16 pts.)*

Consider the 2-D Ising model with a 10×10 configuration of spins at given temperature T, where each spin can point either up or down.

(a) When performing a Monte-Carlo sweep through the spin lattice, you have to decide for each spin whether to flip it or not. Suppose the energy change to flip a given spin is E_{flip}; describe how the Metropolis algorithm determines whether the spin should be flipped or not.

(b) Using the principle of detailed balance,

$$P_1 W(1 \to 2) = P_2 W(2 \to 1) \tag{6}$$

(P_i: occupation probability of state i, $W(i \to j)$: transition rate from state i to state j), identify the transition rates following from the Metropolis algorithm and show that the resulting occupation probabilities satisfy Boltzmann statistics, i.e.,

$$\frac{P_1}{P_2} = \frac{\mathrm{e}^{-E_1/k_B T}}{\mathrm{e}^{-E_2/k_B T}} \ . \tag{7}$$