1. The Figure show the output of vdp-rk4.c for the van der Pol oscillator with damping constant $\mu$. Sketch the phase space trajectory and explain why the oscillations do not damp to zero for this oscillator.

$$\frac{d^2x}{dt^2} - \mu(1 - x^2)\frac{dx}{dt} + x = 0$$

2. Describe in words an algorithm and code to solve the van der Pol equation.
1. Rahman’s MD simulation of Argon generates a microcanonical ensemble with fixed volume, energy and number of atoms. How would you set up an MD simulation to generate (1) a canonical ensemble? (2) a grand canonical ensemble?

2. Atoms obey quantum mechanics. Explain why an MD simulation using Newton’s classical equations works for Argon atoms. Under what conditions would such a simulation fail?
1. Explain Rahman’s Fig. 2. Pair-correlation function \( g(r) = \frac{V}{N} \frac{n(r)}{4\pi r^2 \Delta r} \) at 94.4°K and 1.374 g cm\(^{-3}\). The Fourier transform of this function has peaks at \( \kappa\sigma = 6.8, 12.5, 18.5, 24.8 \).

2. Why does cutting off the Lennard-Jones potential violate conservation of energy, and how does using the following modified potential correct for this?

\[
U_{\text{force shift}}(r) = U(r) - \frac{d}{dr} U(r_{\text{cut-off}})(r - r_{\text{cut-off}}).
\]
1. Explain the significance of the figure for MD simulations.

2. Find the Lagrangian which gives the third type of potential considered by FPU “Another case studied recently was

\[
\ddot{x}_i = \delta_1(x_{i+1} - x_i) - \delta_2(x_i - x_{i-1}) + c, \tag{3}
\]

where the parameters \(\delta_1, \delta_2, c\) were not constant but assumed different values depending on whether or not the quantities in parentheses were less than or greater than a certain value fixed in advance.”
1. Sketch FPU Fig. 1, and define $\delta t$, cycles and our units in their caption: The quantity plotted is the energy (kinetic plus potential in each of the first five modes). The units of energy are arbitrary. $N = 32$; $\alpha = 1/4$; $\delta t^2 = 1/8$. The initial form of the string was a single sine wave. The higher modes never exceeded in energy 20 of our units. About 30,000 computation cycles were calculated.

2. Outline the steps you might use to show that the long wavelength limit of the FPU $\beta$ model gives the Korteweg de Vries equation.

FPU: $\ddot{x}_i = (x_{i+1} + x_{i-1} - 2x_i) + \beta \left[ (x_{i+1} - x_i)^3 - (x_i - x_{i-1})^3 \right]$, KdV: $\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + \delta^2 \frac{\partial^3 u}{\partial x^3} = 0$
1. Plug Rayleigh's gravity wave function $u(x, t) = a \sech^2 [\beta (x - ct)]$ in the Zabusky-Kruskal version of the Korteweg-de Vries equation $u_t + uu_x + \delta^2 u_{xxx} = 0$ and determine the constants $a, \beta, c$.

2. Explain how the Korteweg-de Vries equation can be discretized in space and time, and how $u(x, t + dt)$ is computed from $u(x, t)$ after one time step $dt$ using the split-step Fourier transform method.
1. Explain how Liouville’s theorem in classical mechanics and Boltzmann’s Ergodic hypothesis in thermodynamics apply to the two-dimensional hard disk system. Are they equivalent or not? Explain.

2. Define and explain the essential differences between the following: (1) a random sampling of a probability distribution, (2) a random walk on the probability distribution, and (3) a pseudo-random number sequence on the probability distribution.
1. Explain how you would apply the Metropolis Monte Carlo algorithm to thermalize an ensemble of classical simple harmonic oscillators:

\[ E = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}. \]

2. Outline a code that converts `std::rand()` uniform deviates in the unit interval \([0, 1)\) to a Poisson distribution of integers for any given real number \(\lambda\)

\[ P(k) = \frac{\lambda^k e^{-\lambda}}{k!}. \]
1. Consider $N$ hard disks of diameter $d \ll 1$ in a unit square box. Find the $2N$-dimensional configuration space volume of allowed zero-energy configurations, i.e., the disks must be at rest and cannot overlap.

2. Find (1) the magnetization and (2) total energy of the 2-D Ising spin configuration shown below?

\[ M = \sum_i s_i \]
\[ E = -J \sum_{\langle ij \rangle} s_i s_j - H \sum_i s_i \]
1. Define the quantities in the following formula and explain their physical significance:

\[ m = \lim_{N \to \infty} \frac{\langle \sum_i s_i \rangle}{N} = \begin{cases} 
1 - \left\{ \sinh \left( \frac{2J}{k_B T} \right) \right\}^{-1/2}, & \text{for } T \leq T_c \\
0, & \text{for } T > T_c
\end{cases} \]

2. What is \( \chi \)? Which theorem (1) Ergodic, (2) Fluctuation-Dissipation, or (3) Equipartition, does the formula represent? Explain.

\[ \chi = \left( \frac{\partial \langle m \rangle}{\partial H} \right)_T = \left( \frac{\partial \langle \sum_i s_i \rangle}{\partial H} \right)_T = \frac{1}{k_B T} \left[ \langle \frac{1}{N} \left( \sum_{i=1}^{N} s_i \right)^2 \rangle - \left( \frac{1}{N} \langle \sum_i s_i \rangle \right)^2 \right]. \]
1. Explain the difference between first and second order phase transitions. How are they identified numerically in a Metropolis Monte Carlo simulation of the 2-D Ising model?

2. Define the symbols and briefly explain the significance of the following formulas for simulating the Ising model:

\[
g(r) = \langle s_0 s_n \rangle - \langle s_0 \rangle \langle s_n \rangle \sim e^{-r/\xi} \left( \frac{1}{p(d-2+\eta)} \right), \quad \tau \sim \xi^z \sim \frac{1}{|T - T_c|^\nu z}.
\]
1. The symmetry groups $O(2)$ and $U(1)$ are mathematically isomorphic. Explain the difference between global $O(2)$ invariance of the XY Model and the local $U(1)$ invariance of a 2-D superconductor.

2. Write down an XY Model Hamiltonian for the “One-volt NIST Josephson Junction array standard having 3020 junctions” shown in the Figure.
1. Identify the Ising model observables and supply the missing critical index values:

\[ M \sim (T_c - T)^\beta \quad \beta = 1/8 \]
\[ g(r) \sim e^{-r/\xi} / r^{d-2+\eta} \quad \eta = 1/4 \]
\[ \xi \sim (T - T_c)^{-\nu} \quad \nu = \]
\[ \chi \sim (T - T_c)^{-\gamma} \quad \gamma = \]
\[ C \sim (T - T_c)^{-\alpha} \quad \alpha = \]
\[ M \sim B^{1/\delta}, (T = T_c) \quad \delta = \]

2. How does the Wolff cluster algorithm differ from the Newman-Ziff cluster algorithm?
1. Explain the significance of the three configurations for enumerating polymer configurations:

2. What are possible advantages of using a C++ deque object to represent a polymer, and a separate C++ set object to represent the sites occupied by the polymer?
1. Explain the Metropolis Monte Carlo algorithm used by Shakhnovich et al. to simulate a 27-monomer chain on the cubic lattice shown in the figure.

![Cubic lattice diagram](image)

**FIG. 1.** An example of CSA on a $3\times3\times3$ fragment of a cubic lattice (fat line).

2. Explain the physical meaning of the terms in the energy function used by Shakhnovich et al.

\[
E = B_0 \sum_{ij} \Delta(r_i - r_j) + \sum_{ij} B_{ij} \Delta(r_i - r_j) + D_2 \sum_{ij} \delta(r_i - r_j) + D_3 \sum_{ijk} \delta(r_i - r_j) \delta(r_i - r_k)
\]

\[
P(B_{ij}) = \sqrt{\frac{1}{2\pi B^2}} \exp \left[ -\frac{B_{ij}^2}{2B^2} \right]
\]
1. Give brief pseudo-code outlines of (1) simulated annealing, and (2) genetic algorithm, applied to the 2-D lattice protein folding problem.

2. Find the energies of the three configurations

\[ V = - \sum_{\langle B_i, B_j \rangle} \Delta(r_i - r_j) \]

(A)                     (B)                     (C)
1. Explain the meaning of the symbols in the Hodgkin-Huxley neuron model equation with the help of a circuit diagram:

\[ I = C_M \frac{dV}{dt} + \bar{g}_K n^4 (V - V_K) + \bar{g}_{Na} m^3 h (V - V_{Na}) + \bar{g}_l (V - V_l) \]

2. An action potential propagates along a nerve fiber like a soliton. Can you see any similarities between the Hodgkin-Huxley equation above and the Korteweg - de Vries equation below?

\[ \frac{\partial u}{\partial t} + (1 + u) \frac{\partial u}{\partial x} + \frac{\partial^3 u}{\partial x^3} = 0 \]
1. Explain “Fig. 1 Two-dimensional representation of motion in state space.” from Hopfield’s article in Scholarpedia, giving a possible application:

2. Prove Hopfield’s claim that $E$ is a monotonically decreasing function if $T_{ij} = T_{ji}$, i.e., $\Delta E < 0$ where

$$E = -\frac{1}{2} \sum_{i,j \neq i} T_{ij} V_i V_j , \quad \Delta E = -\Delta V_i \sum_{j \neq i} T_{ij} V_j$$
1. Briefly explain how to find the global minimum of a complicated function in a multidimensional space using (1) a genetic algorithm and (2) a neural network.

2. Explain the difference between the architectures in the figure and give the form of the connection strength matrix $w_{ij}$ for each type:

(a) [Diagram of feed-forward architecture]

(b) [Diagram of feed-back architecture]

Figure 2.3: (a) Feed-forward and (b) feed-back architectures
1. Explain how to reduce the generalized eigenvalue problem to an ordinary eigenvalue problem:

$$\mathbf{HC} = E\mathbf{SC}, \quad \sum_{q=1}^{N} H_{pq} C_q = E \sum_{q=1}^{N} S_{pq} C_q, \quad p = 1, \ldots, N.$$ 

2. Compare the Gaussian orbital expectation value of the Coulomb potential with the exact hydrogen ground state expectation value:

$$V_{ij} = -e^2 \int d^3r \ e^{-\alpha_i r^2} \frac{1}{r} e^{-\alpha_j r^2} = -\frac{2\pi e^2}{\alpha_i + \alpha_j}.$$
1. Explain the meaning of the terms in the Hartree-Fock equation for Helium
\[
\left[-\frac{1}{2} \nabla^2 - \frac{1}{r} + \sum_{r,s} c_r c_s \int d^3r' \frac{\chi(r')\chi(r)}{|r-r'|} \right] \sum_q c_q \chi_q(r) = E' \sum_q c_q \chi_q(r).
\]

2. By considering plane wave states in a box show that the Fermi momentum of a free electron gas is related to the electron density by
\[
k_F = \left[3\pi^2 n(r)\right]^{1/3}.
\]
1. State and explain the two density functional theorems of Hohenberg and Kohn, with one or two sentences and one equation for each theorem.

2. Prove the Hellmann-Feynman theorem

\[ \nabla_n \left[ \frac{\langle \Psi(\mathbf{R})|H(\mathbf{R})|\Psi(\mathbf{R})\rangle}{\langle \Psi(\mathbf{R})|\Psi(\mathbf{R})\rangle} \right] = \frac{\langle \Psi(\mathbf{R})|\nabla_n H(\mathbf{R})|\Psi(\mathbf{R})\rangle}{\langle \Psi(\mathbf{R})|\Psi(\mathbf{R})\rangle} \]
1. Explain the symbols in the Car-Parinello Lagrangian

\[ \mathcal{L}(\{\psi_k\}, \mathcal{R}) = \frac{1}{2} \sum_\ell M_\ell \dot{\mathbf{R}}_\ell^2 + \frac{\mu}{2} \int d^3 \mathbf{r} \sum_k |\dot{\psi}_k|^2 - E_{\text{tot}}(\{\psi_k\}, \mathcal{R}) + \sum_{kk'} \Lambda_{kk'} [\langle \psi_k | \psi_{k'} \rangle - \delta_{kk'}]. \]

2. Give an example of a reasonable one-electron orbital wavefunction in each of (1) atomic hydrogen, (2) molecular hydrogen, and (3) conduction band in copper.
1. Draw a diagram of the Kronig-Penney potential and explain how Bloch’s theorem applies:

\[ \psi_k(x) = e^{ikx} \sum_K e^{iKx} C_{k+K} = e^{ikx} u_k(x) , \quad u_k(x + na) = u_k(x) . \]

2. Explain the symbols in the APW basis function and sketch the \( l = 0 \) component as a function of \( r \):

\[ \psi^\text{APW}_q(r) = 4\pi \sum_{lm} i^l \left[ \frac{ji(qr)}{\mathcal{R}_l(r)} \right] Y^*_l m(\theta_q, \phi_q) \ Y_l m(\theta, \phi) . \]
1. Explain the difference between the Variational Method of Topic 4 to find the electronic ground state energy, and the Variational Monte Carlo Method of Topic 5 to compute the same quantity.

2. Find and sketch the local energy for the Hydrogen atom with Gaussian trial function

\[ H = -\frac{1}{2} \left( \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) - \frac{1}{r}, \quad E_{L}(r) = \frac{1}{\psi_{T,\alpha}} H \psi_{T,\alpha}(r), \quad \psi_{T,\alpha}(r) = e^{-\alpha r^2} \]
1. Explain the motivation for using the Slater-Jastrow wavefunction in a VMC determination of the Helium atom ground state

\[ \Psi(r_1, r_2) = e^{-2r_1}e^{-2r_2}e^{\frac{r_{12}}{2(1+\alpha r_{12})}}. \]

2. Transform the diffusion equation and its Green’s function to the case of the one dimensional time-dependent Schrodinger equation:

\[ \frac{\partial \psi(x, \tau)}{\partial \tau} = \frac{1}{2} \frac{\partial^2 \psi(x, \tau)}{\partial x^2} - V(x)\psi(x, \tau), \quad G(x, y; \tau) = \frac{1}{\sqrt{2\pi \tau}}e^{-\frac{(x-y)^2}{2\tau}}. \]
1. Why does the number of random walkers in Diffusion Monte Carlo (DMC) need to be changed at each time step and how does the parameter $E_T$ determine the number of walkers to be added or removed?

$$\frac{\partial \psi(x, \tau)}{\partial \tau} = \frac{1}{2} \frac{\partial^2 \psi(x, \tau)}{\partial x^2} - (V(x) - E_T)\psi(x, \tau)$$

2. Define the variables and explain the physical meaning of Eq. (2.5.47) in Sakurai Quantum Mechanics:

$$\langle x_N, t_N | x_1, t_1 \rangle = \lim_{N \to \infty} \left( \frac{m}{2\pi\hbar\Delta t} \right)^{(N-1)/2} \int dx_{N-1} \ldots \int dx_2 \Pi_{j=2}^N \exp \left[ \frac{iS(j, j - 1)}{\hbar} \right]$$
1. Evaluate the free particle Green’s function by inserting a complete set \( \sum_p |p\rangle \langle p| \) of momentum eigenstates (plane waves)
\[
\langle x' | \exp \left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right] | x \rangle.
\]

2. Prove the virial theorem in classical mechanics for the kinetic energy \( T \) of \( N \) particles with positions \( \mathbf{r}_k \) and net forces \( \mathbf{F}_k \)
\[
2\langle T \rangle = - \sum_{k=1}^{N} \langle \mathbf{r}_k \cdot \mathbf{F}_k \rangle.
\]
1. Define the symbols and explain the motivation for the VEGAS step probability function

\[ p(x) = \frac{1}{N\Delta x_i}, \quad x_i - \Delta x_i \leq x \leq x_i, \quad i = 1, \ldots, N, \quad \sum_{i=1}^{N} \Delta x_i = 1. \]

2. Give examples in your research area for which VEGAS is being used, or if not, for which you think it might be useful and why.
1. Draw a diagram of a Compton scattering event and explain the symbols in the Klein-Nishina cross section formula

\[
\frac{1}{r_e^2} \frac{d\sigma}{d\Omega} = \left( \frac{\omega'}{\omega} \right)^2 \left[ |\epsilon^* \cdot \epsilon_0|^2 + \frac{(\omega - \omega')^2}{4\omega\omega'} \left( 1 + |\epsilon^* \cdot \epsilon_0|^2 - |\epsilon \cdot \epsilon_0|^2 \right) \right]
\]

2. Write a few lines of code to integrate a function \( f(x) \) using VEGAS from the GNU Scientific Library.
1. Explain the variables in the Drell-Yan cross section formula
\[ \frac{d\sigma}{d\Omega} = \sum_{a_1,a_2} \int_0^1 dx_2 dx_1 f_{a_1}^{h_1}(x_1,M^2) f_{a_2}^{h_2}(x_2,M^2) E_Q \frac{d\sigma_{a_1a_2}}{d^3Q}(x_1 P_1, x_2 P_2, M^2). \]

2. The effective QED coupling \( \alpha(Q) \) is found to increase slowly with energy from \( 1/137.036 \) at zero energy to approximately \( 1/128 \) at the mass of the Z boson. The QCD coupling \( \alpha_s(Q) \) decreases with energy. Why do these couplings depend on energy and why do they change in opposite directions?
1. Show that the QED Lagrangian density is gauge invariant

\[ \mathcal{L}_{\text{QED}} = \bar{\psi} \left[ \gamma^\mu (i\partial_\mu - eA_\mu) - m \right] \psi - \frac{1}{4} F_{\mu\nu} F^{\mu\nu}, \ A_\mu(x) \rightarrow A_\mu(x) - \partial_\mu \chi(x), \ \psi(x) \rightarrow e^{ie\chi} \psi(x). \]

2. The Coulomb potential \( V(r) \sim 1/r \) in \( D = 3 \) dimensions. How does it depend on \( r \) in \( D = 1 \) and \( D = 2 \) dimensions? Hint: Use Gauss' Law to get the \( r \) dependence of the electric field.
1. Explain the concepts (1) Wilson loop, (2) plaquette, and (3) path ordered, in lattice gauge theory.

2. Explain the significance of the figure

**FIG. 8.** Square Wilson loops of sides one and two for the group $Z_2$. 
1. Explain the significance of the following equation in lattice QCD

\[ V(R) = C + \frac{B}{R} + \sigma R + \lambda \left( \frac{1}{R_{\text{lat}}} - \frac{1}{R} \right). \]

2. What are some of differences between Monte Carlo simulation of lattice QED and lattice QCD?
1. Explain the significance of the two metrics, and an application for each:

\[ ds^2 = dt^2 + a^2(t) \left[ \frac{dr^2}{1 - kr^2} - r^2 \left( d\theta^2 + \sin^2 \theta d\phi^2 \right) \right], \]

\[ ds^2 = a^2(\mu, t) dt^2 - b^2(\mu, t) d\mu^2 - R^2(\mu, t) d\Omega^2, \quad 4\pi \rho R^2 b = 1. \]

2. If \( \mathbf{u}(r, t) \) represent fluid velocity, explain the physical meaning of each of the three terms:

\[ \frac{d\mathbf{u}}{dt} = \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u}, \]
1. What is the Riemann problem for the equation $\frac{\partial}{\partial t} u(x, t) + c \frac{\partial}{\partial x} u(x, t) = 0$. Why is it a problem and what is its solution?

2. Identify the shock and two contact discontinuities in Sod’s shock tube problem. In which direction does each move, and which has the fastest and which the slowest speeds?
1. Explain the variables and the basic physics that follows from
\[ E_F + E_G = \frac{\hbar c N^{1/3}}{R} - \frac{G N m_B}{R}. \]

2. Find the non-relativistic limit of the TOV equation and give a simple interpretation for a shell of matter at radius \( r \) with thickness \( dr \):
\[ \frac{dP(r)}{dr} = -\frac{G}{r^2} \left[ \rho(r) + \frac{P(r)}{c^2} \right] \left[ m(r) + \frac{4\pi r^3 P(r)}{c^2} \right] \left[ 1 - \frac{2Gm(r)}{rc^2} \right]^{-1}. \]
1. Explain the figure from Baym-Pethick-Sutherland identifying stable regions and type of star in each:

![Graph showing stable regions and type of star](image)

2. Describe the types of matter modeled by the (1) Fermi-Metropolis-Teller, (2) Baym-Pethick-Sutherland, (3) Baym-Bethe-Pethick, and (4) Pandharipande, equations of state.
1. Explain the symbols in the equations for gravitational collapse:

\[ D_t R = U, \]
\[ D_t m = -4\pi R^2 p U, \]
\[ D_t U = - \left[ \frac{1 + U^2 - 2m/R}{\epsilon + p} \right] \left( \frac{\partial p}{\partial R} \right)_t - \frac{m + 4\pi R^3 p}{R^2}, \]
\[ \left( \frac{\partial m}{\partial R} \right)_t = 4\pi R^2 \epsilon. \]

2. Explain the significance of the collapse simulation in the figure: