Monte Carlo

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1. Write a Monte Carlo program to sample the configurations of a particle in 1D subject to a harmonic potential of stiffness k=1 at temperature $k_B T = 1$
$$U(q) = \frac{1}{2} q^2$$
(Hint: the probability distribution is $P(q)dq \propto e^{-\frac{q^2}{2}} dq$). Moves should be proposed using random numbers uniformly distributed in $[-\Delta, +\Delta]$ and accepted or rejected with a Metropolis procedure. Try different values of Δ (e.g. $\Delta = 0.01$, 0.1, 1) and different values of the initial condition q. Use any programming language you like (suggested: C, FORTRAN, awk, python).

2. Plot the resulting trajectory (i.e. q as a function of the number of iteration) for different values of Δ. Also compute the average acceptance as a function of Δ.

3. Compute the average value of q^2. The result should be equal to $\frac{1}{\sqrt{2\pi}} \int dq q^2 e^{-\frac{q^2}{2}}$. Check how many iterations you need to reach an estimate of this integral with a given accuracy. How is the accuracy scaling with the length of the simulation? How does the error depend on the initial condition for q? How does the error depend on the choice of Δ? Find the optimal value of Δ that allows to obtain the most accurate result in the shortest time.

4. Now modify the code such that you sample the position of two particles in 3D connected by a spring of equilibrium length L=4
$$U(\mathbf{q}_1, \mathbf{q}_2) = \frac{1}{2} \left(|\mathbf{q}_1 - \mathbf{q}_2| - L \right)^2$$
Notice that $\mathbf{q}_1$ and $\mathbf{q}_2$ are now vectors with three components each. *(Hint: at every iteration, choose randomly one of the two particles and one of the three possible components and displace it by a random displacement uniformly distributed in $[-\Delta, +\Delta]$).* Compute the average distance $|\mathbf{q}_1 - \mathbf{q}_2|$ between the two particles.