Task 6 Phi-4 Model

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Problem 71

Split the Hamiltonian of the two-dimension Φ^4 model

$$H = \sum_{i=1}^{N} v(\phi_i) + H_I$$

in local and interaction terms

$$\beta v(\phi_i) = -\frac{b}{2}\phi_i^2 + \frac{u}{4}\phi_i^4 \qquad \beta H_I = -\sum_{\langle ij \rangle} \phi_i \phi_j$$

Devise a Monte Carlo method where the proposal $g(\phi_i) = C^{-1}e^{-\beta v(\phi_i)}$ depends on the local term and find an appropriate expression for the acceptance probability h. Use this method to plot the order parameter $m = \left| \frac{\sum_{i=1}^{N} \phi_i}{N} \right|$ as a function of $b \in (-3, -2)$ for $u = 1$ and a two-dimensional system with $N = 10 \times 10$ variables.

Initially I define the ϕ_i's as Gaussian numbers with 0 mean and variance 1 (this is arbitrary, this is what I chose). Then we thermalize the system for each value of b and to propose ϕ_i' (i randomly chosen) we must first figure out how to generate the proposals according to $g(\phi_i) = C^{-1}e^{-\beta v(\phi_i)}$. The simplest method is the acceptance/rejection method: the function $g(\phi_i)$ is split into the product of a proposal probability $\tilde{g}(\phi_i)$ and an acceptance probability $\tilde{h}(\phi_i)$:

$$g(\phi_i) = C^{-1}e^{-\beta v(\phi_i)} = C^{-1}e^{\frac{b}{2}\phi_i^2 - \frac{1}{4}\phi_i^4} \propto \tilde{g}(\phi_i)\tilde{h}(\phi_i)$$

Since b is negative the simplest election for the proposal probability is a Gaussian centered at 0 with variance $\sigma = \sqrt{-1/b}$ ($g(\phi_i) = \frac{1}{\sqrt{2\pi}\sigma}e^{-\phi_i^2/2\sigma^2}$) and the acceptance is $\tilde{h}(\phi_i) = e^{-\frac{\phi^4}{4}}$. The algorithm is as follows: we generate a Gaussian number $g = G(0, \sqrt{-1/b})$ and if $u < h(g)$ (u is a uniform random number between 0 and 1 as usual) the number is accepted; otherwise another one is proposed until it is accept. In this problem we cannot leave the proposals ϕ_i' unaccepted because in this way we cannot jump to the next step, which is the Metropolis algorithm. In Python this is done by simply defining a counter for the wanted number of updates and a while loop.

Once $\phi_i' = G(0, \sqrt{-1/b})$ is proposed we will accept it in the Metropolis step according to another acceptance probability h (not to be confused with the previous one $\tilde{h}$). If we replace the proposal $g(\phi_i)$ in the detailed balance condition we get:

$$e^{-\beta v(\phi_i')}h(\phi'|\phi)e^{-\beta v(\phi_i)}e^{-\beta H_I(\phi)} = e^{-\beta v(\phi_i)}h(\phi|\phi')e^{\beta v(\phi_i')}e^{-\beta H_I(\phi')}$$

and thus

$$h(\phi'|\phi)e^{\beta H_I(\phi)} = h(\phi|\phi')e^{\beta H_I(\phi')}$$

Although our proposal $g(\phi_i)$ is not symmetrical we get the same form for the detailed balance condition for symmetrical proposals due to the fact that the proposal pdf depends only on the interaction term H_I. We can hence use the Metropolis solution for h considering only the interaction Hamiltonian:

$$h(\phi'|\phi) = \min(1, e^{-\beta\Delta H_I(\phi')})$$

The change in the interaction Hamiltonian is:

$$\beta\Delta H_I = -\sum_{\langle ij\rangle} \phi_i'\phi_j + \sum_{\langle ij\rangle} \phi_i\phi_j = (\phi_i - \phi_i')\sum_{\mu=1}^{4} \phi_{i\mu}$$

being $\phi_{i\mu}$ the 4 neighbors of ϕ_i. The code of the Metropolis algorithm is quite simple: the value $\phi' = G(0, \sqrt{-1/b})$ will be always accepted if the change in energy $\beta\Delta H_I$ is negative, otherwise it will be accepted with probability $e^{-\beta\Delta H_I}$, for which a second random uniform number must be generated.

Figure 1 depicts the dependence of the order parameter m for 20 different values of b in the interval (-3,-2). The errors ϵ_m take into account the correlation time τ, and let's briefly recall the expressions for the error:

$$\sigma_m^2[\hat{m}] = \frac{\sum_{i=1}^{M} m_i^2}{M} - \left(\frac{\sum_{i=1}^{M} m_i}{M}\right)^2 \qquad \epsilon_m = \frac{\hat{\sigma}_m[\hat{m}]}{\sqrt{M}}\sqrt{2\tau+1}$$

The correlation time τ is approximated considering the correlation between two consecutive measurements $\rho(1)$:

$$\tau = \frac{\rho(1)}{1-\rho(1)}; \qquad \rho(1) = \frac{\langle m_i m_{i+1}\rangle - \langle m_i\rangle\langle m_{i+1}\rangle}{\sigma_m[\hat{m}]}$$

This τ is indeed very important because I got large negative values for τ if I did not separate enough the measurements. Finally I realized that 100 Metropolis steps between measures was enough to get reasonable positive and small values for τ. The thermalization for each value of b was even more important: 10^4 updates were made before the first measure so that we ensure that we are in equilibrium. In practical terms it is easy to know if we are in the steady state by checking:

$$\langle e^{-\beta\Delta H_I}\rangle_{st} = 1$$

With 10^4 thermalization iterations the obtained value for this average was always bigger than 0.99 and for some b's larger than 0.999. Another thing that can be noticed is that the arrors are relatively large, and that is because I took $M = 10^4$ measures for each b. If I considered a larger value the errors would be smaller but let's point out that it took me 51 minutes to get these 20 points. In all this time the program had to make, for each b, 10^4 thermalization steps and separate the 10^4 measures 100 Metropolis steps to avoid large correlations between measures. I tried to increase M at least up to 10^5 but it turned out to be an unbearable burden that my 4GB RAM laptop refused to carry despite letting the program run for hours.

Finally it is graphically evident that m does not follow a special dependence with b, but it does seem to increase as b is increased. At the beginning m seems to be irregularly constant

and then it grows as b is decreased in absolute value, and this could be predicted a priori: after all the acceptance-rejection steps in the Metropolis algorithm, let's not forget that our ϕ_i are Gaussians with 0 mean and width $\sigma = \sqrt{-1/b}$. As the width is made larger by decreasing the absolute value of b, larger values around 0 are proposed for ϕ_i' (either positive or negative, that is, in absolute value). Thus, if we considered negative values of b near 0, our proposals would be very wide Gaussian distributions centered at 0 and hence the ϕ_i' (and the order parameters) would be large in absolute value too. On the other hand, had we taken large negative values of b, the proposals would resemble a delta distribution centered at 0 (very narrow Gaussian functions) and consequently the ϕ's and the m's would be approximately 0.

The last thing to be pointed out is why the errors increase with b, and that has to do with the correlations. Note that from approximately $b = -2.7$ hereunder the order parameter m increases, i.e the correlation is positive and therefore the errors increase. If there is not a clear correlation like in the interval (-3,-2.7), the next value of m cannot be estimated from the previous one and consequently the correlation times are smaller.

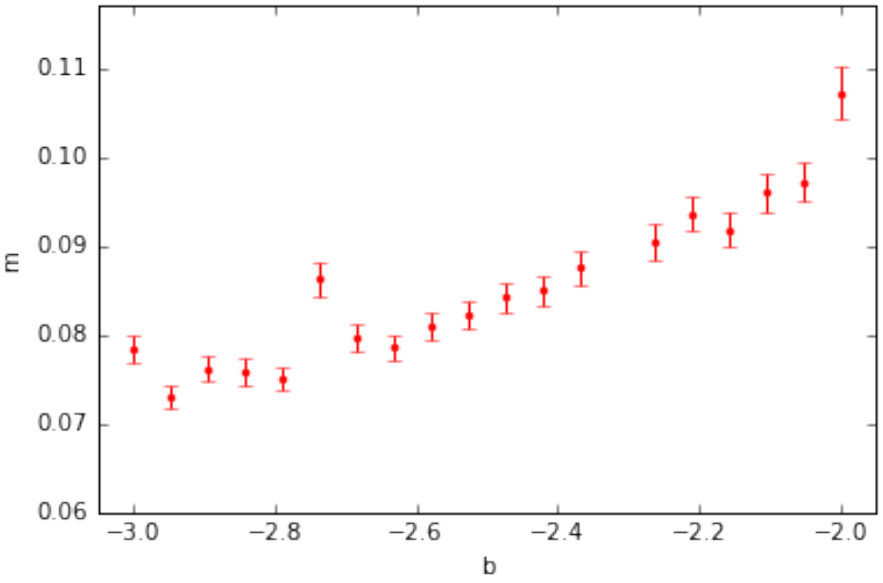

Figure 1: Order parameter m in terms of the parameter b.