P653 HW10

Due Nov 22, 2005

Problem 1. Single particle density matrix of an ideal gas

Consider an ideal gas of particles of mass m in a large three-dimensional volume V at temperature T connected with a reservoir of chemical potential μ. The single particle density matrix can be taken to be $\rho_1(r,r') = \frac{1}{V}\sum_k n_k e^{ik\cdot(r-r')}$, where n_k is the number of particles of momentum k.

1.1. For Boltzmann particles, where $n_k = e^{-\beta(k^2/2m-\mu)}$, calculate $n_1(r,r')$.

Hint: Use Cartesian coordinates for the integral.

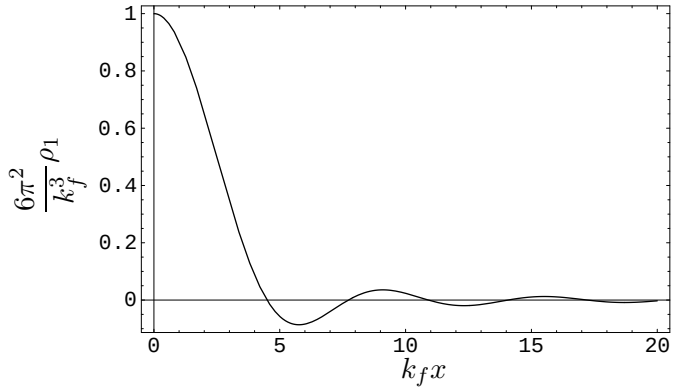
Solution 1.1. The result only depends on $\mathbf{x} = \mathbf{r} - \mathbf{r}'$. Choose Cartesian coordinates with the $\hat{z}$ axis aligned with $\mathbf{x}$ so that

$$\begin{aligned}\rho_1(x) &= \frac{e^{\beta\mu}}{(2\pi)^3}\int dk_x\, e^{-\beta k_x^2/2m}\int dk_y\, e^{-\beta k_x^2/2m}\int dk_z\, e^{-\beta k_z^2/2m+ik_z x}\\ &= e^{\beta\mu}\left(\frac{m}{2\pi\beta}\right)^{3/2} e^{-mx^2/2\beta}.\end{aligned}$$

1.2. For zero temperature Fermi particles, where $n_k = 1$, for $k^2/2m < \mu$, but $n_k = 0$ for $k^2/2m > \mu$ calculate $\rho_1(r,r')$ in terms of $k_f = \sqrt{2m\mu}$. Plot ρ_1 as a function of $r - r'$.

Solution 1.2. The result only depends on $x = r - r'$, so

$$\begin{aligned}
\rho_1(x) &= \frac{1}{(2\pi)^3}\int_{|k|<k_f} d^3k\, e^{i\mathbf{k}\cdot\mathbf{x}} \\
&= \frac{1}{(2\pi)^2}\int_{-1}^{1} d\cos\theta \int_0^{k_f} dk\, k^2 e^{ikx\cos(\theta)} \\
&= \frac{1}{2\pi^2}\int_0^{k_f} dk \frac{k}{x}\sin(kx) \\
&= \frac{1}{2\pi^2 x^3}\left(\sin(k_f x) - k_f x\cos(k_f x)\right).
\end{aligned}$$



1.3. For Bose-condensed particles, $\mu = 0$ and $n_k = 1/(e^{\beta k^2/2m} - 1)$ for $k > 0$, and $n_0 = N_0$ is the number of condensed atoms, which is extensive. Here the integrals cannot be done in closed form. What does ρ_1 approach for large $x = r - r'$? Over what length scale does it approach this value

Solution 1.3. The contribution from the noncondensed particles falls off on a length-scale of order $\sqrt{\beta/m}$, and it approaches N_0/V.

Problem 2. Longitundinal and Transverse velocities In two dimensions, we can always decompose $\mathbf{v}(\mathbf{r}) = \mathbf{v}_\parallel(\mathbf{r}) + \mathbf{v}_\perp(\mathbf{r})$, where $\nabla \times v_\parallel(r) = 0$ and $\nabla \cdot v_\perp(r) = 0$.

2.1. Argue that there exists a smooth θ such that $v_\parallel(r) = \nabla\theta(r)$.

Solution 2.1. This is a consequence of $\nabla \times v_\parallel(r) = 0$.

2.2. Show that if $n(r) = \nabla \times v_\perp(r)/(2\pi)$, then $v_\perp(r) = \nabla \int dr' n(r')\mathrm{Im}\log(z - z')$. Assume that $n(r)$ is well behaved.

Solution 2.2. Taking the gradient of the suggested expression

$$\nabla v_\perp(r) = \int dr' n(r')\nabla^2 \mathrm{Im}\log(z - z').$$

Recognizing that $\nabla^2\mathrm{Im}\log(z - z') = 2\pi\delta^2(r - r')$ gives the desired result.

2.3. Show that there exists a smooth ϕ such that $v_\perp(r) = \nabla \times (\hat{z}\phi(r))$. How is ϕ related to n?

Hint: You may wish to remember the connection between stream functions and potential functions [Cauchy-Riemann].

Solution 2.3. If $f(z)$ is an analytic function then

$$\nabla f(z) = [\hat{x}u - \hat{y}v] + i\,[\hat{x}v + \hat{y}u]\,,$$

where u and v are respectively the real and imaginary part of $f'(z)$. Thus the gradient of the real and imaginary part of $f(z)$ are perpendicular to one another. In particular $\phi(r) = -\int dr' n(r') \mathrm{Re}\log(z - z')$.

2.4. Since θ is smooth we can write $\theta(r) = \sum_q e^{iq\cdot r}\theta_q$. Differentiate to prove that $(v\ \|)_a(\mathbf{q}) = q_a f(\mathbf{q})$. How is $f(\mathbf{q})$ related to θ_q?

2.5. Still assuming that $n(r)$ is well behaved, we can write $n(r) = \sum_q e^{iq\cdot r} n_q$. Using that $\nabla \times v_\perp = n$, show that $(v_\|)_a(\mathbf{q}) = \epsilon_{ab} q_b g(\mathbf{q})$, where $\epsilon_{xy} = 1$, $\epsilon_{yx} = -1$, and $\epsilon_{xx} = \epsilon_{yy} = 0$. How is $g(\mathbf{q})$ related to n_q?

We now see that the $\|$ and $\perp$ refer to whether the Fourier momenta of the velocity are parallel or perpendicular to the velocity. These are known as the longitudinal and transverse velocities respectively.

Problem 3. Wolff Algorithm This problem illustrates that Monte-Carlo update moves need not be just simple local updates. The following algorithm does not suffer from the critical slowing down of the metropolis algorithm.

Consider an $N \times N$ square lattice Ising model. Given a spin configuration $\{\sigma_i^{(0)}\}$ we will generate a new configuration by the following "cluster" algorithm. In this algorithm we generate a cluster, and flip it. Note that we always flip something [unlike the Metropolis algorithm where we often refuse to make a change].

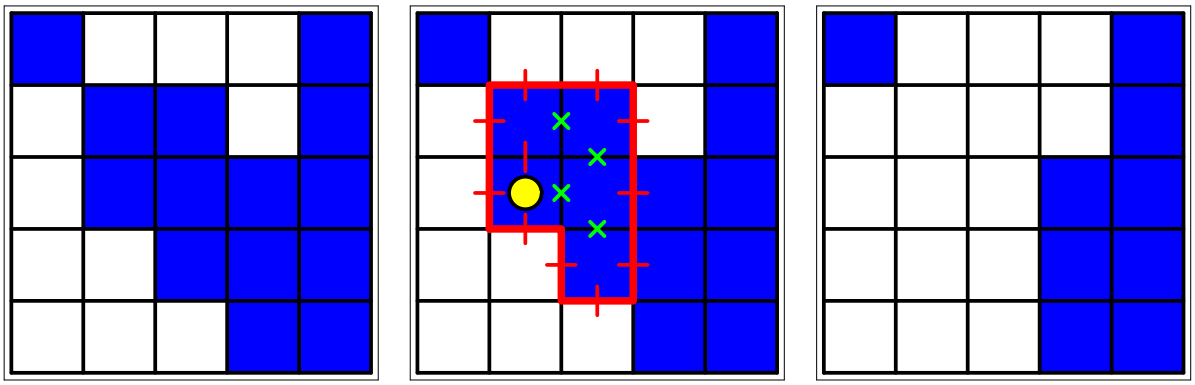
To start the cluster, we choose a random site i. We grow the cluster by looking at each of its neighbors j_1, j_2, j_3, j_4. If the nieghbors are aligned with i we add them to the cluster with probability $1 - e^{-2\beta J}$. If they are not aligned we never add them. Bonds where a spin is successfully added are referred to as "accepted", bonds which are considered, but where a spin is not added are referred to as "rejected".

We further grow the cluster by looking at each of the neighbors of the newly added sites. Again we add them with probability $1 - e^{-2\beta J}$ if they are aligned with the cluster spins, and never add them if they are not aligned.

We repeat until no spins are added to the cluster.

Having generated the cluster we then flip it. This sequence of steps: generating a cluster and flipping it, constitutes one step of a Markov process.

3.1. As a concrete example, consider the spin configuration depicted below on the left. Dark (blue) squares represent spin up sites, and light squares represent spin down sites. Consider the cluster illustrated in the middle. The red lines outline the cluster. Green x's represent accepted bonds, while bars represent rejected bonds. The starting site is marked with a yellow disk. The configuration to the right represents what happens the configuration looks like after this cluster is flipped.



Given that the temperature is T, what is the probability P that this cluster was generated (starting from that particular starting square with that particular pattern of accepted and rejected bonds)?

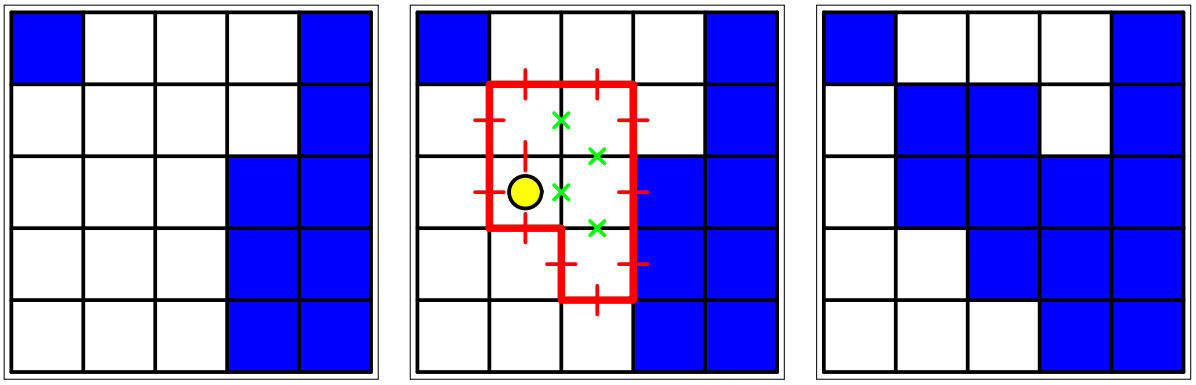
Solution 3.1. The probability of choosing that particular starting square is 1/25. Each rejected bond linking two blue squares occurs with probability $e^{-2\beta J}$. Each accepted bond linking two blue squares occurs with probability $(1-e^{-2\beta J})$. There are 3 rejected bonds between blue squares [note the red dash above the yellow circle] and four accepted bonds. The total probability of this particular sequence is then

$$P = \frac{1}{25} e^{-6\beta J}(1 - e^{-2\beta J})^4.$$

3.2. What is the energy difference between the final and initial configuration, $E_f - E_0$.

Solution 3.2. The difference in energy can only be due to the boundary of the cluster. We go from having 8 dissastisfied bonds and two sattisfied to having 8 sattisfied and 2 dissatisfied. So $E_f - E_0 = -12J$.

3.3. Using the same notation, the reverse move is illustrated below. Note that not only is the cluster the same, but the pattern of accepted and rejected bonds is the same.



What is the probability $\bar{P}$ that this reverse cluster is generated?

Solution 3.3. Using the previous argument,

$$\bar{P} = \frac{1}{25} e^{-18\beta J}(1 - e^{-2\beta J})^4.$$

3.4. What is the ratio $P/\bar{P}$? Show that detailed balance is satisfied. Argue that it will be satisfied for an arbitrary cluster, not just the one considered here.

Solution 3.4.

$$\frac{P}{\bar{P}} = e^{12\beta J} = \frac{e^{-\beta E_f}}{e^{-\beta E_i}},$$

as required by detailed balance.
Generically all of the terms from bonds in the middle of the cluster will cancel between the cluster and the reverse cluster, leaving only the surface bonds. Counting the contribution from the surface bonds is exactly the same as counting the energy difference from flipping the cluster. Therefore we always sattisfy

3.5. Argue that this process is ergodic: ie. one can generate any spin configuration by repeatedly applying these cluster moves.

Solution 3.5. There is always some possiblity that only a single spin is flipped. We know that single spin flips can generate any configuration. Hence one can generate any configurations with this algorithm.

3.6. Suppose at $T = 0$ all of the spins are aligned up. What does a single Markov step do to the configuration? How does this compare to the Metropolis algorithm?

Solution 3.6. All spins automatically flip. Conversely in the Metropolis algorithm no spins flip.

3.7. At $T = \infty$ what does a single Markov step do to the configuration? How does this compare to the Metropolis algorithm?

Solution 3.7. A single spin randomly flips at each step. The same thing happens in the Metropolis algorithm.