PROBLEM SET 6

Physics 219A, Spring 2014

Due Wednesday, June 11

[1.] For a system of non–interacting one–dimensional classical particles in a harmonic oscillator potential:

a. Calculate the grand potential.

b. Obtain $\langle N \rangle$ and $\langle E \rangle$ and show they obey the equipartition theorem.

[2.] Massless particles have energy–momentum relationship $E = cp$. For a system of spinless one–dimensional Fermi–Dirac massless particles, determine the relationships between $\langle N \rangle$, $\langle E \rangle$, μ, and T.

[3.] Consider a gas of He^3 atoms at pressure P and temperature T in equilibrium with an adsorbed surface layer of He^3 atoms. The surface He^3 atoms have their translational degrees of freedom, as well as spin, and are bound with an energy ϵ_0. Find the dependence of the surface density of He^3 as a function of P and T in

a. the classical limit.

b. in a limit where the gas is classical and the adsorbed layer is not.

[4.] Write down the path integral expression for the *quantum* partition function for the $d = 1$ Ising model in a transverse field

$$\hat{H} = -J \sum_{i=1}^{N} \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z - \Gamma \sum_{i=1}^{N} \hat{\sigma}_i^x$$

and show it is identical to that of the $d = 2$ *classical* Ising model (with anisotropic coupling $J_x \neq J_y$).

1-1

N particles have partition function of 1 particle to Nth power

a) $$Q = \sum_N e^{\beta\mu N} \left[\int dx \int dp\; e^{-\beta p^2/2m}\; e^{-\beta \frac{1}{2} m\omega^2 x^2} \right]^N 1/N!$$

$$= \sum_N e^{\beta\mu N} \frac{1}{N!} \left(\sqrt{2\pi m/\beta}\, \sqrt{2\pi/\beta m\omega^2} \right)^N$$

$$= \sum_N e^{\beta\mu N} \frac{1}{N!} \left(\frac{2\pi}{\beta\omega} \right)^N$$

need this even for classical particles!

$$Q = \exp\left[e^{\beta\mu} \frac{2\pi}{\beta\omega} \right]$$

b) $$Q = \mathrm{Tr}\, e^{-\beta(H-\mu N)}$$

$$\frac{1}{\beta} \frac{\partial}{\partial\mu} \ln Q = \frac{1}{Q} \mathrm{Tr}\, N e^{-\beta(H-\mu N)} = \langle N \rangle$$

$$-\partial/\partial\beta \ln Q = \frac{1}{Q} \mathrm{Tr}\,(H-\mu N) e^{-\beta(H-\mu N)} = \langle E \rangle - \mu \langle N \rangle$$

$$\langle N \rangle = \frac{1}{\beta} \partial/\partial\mu \left[e^{\beta\mu} \frac{2\pi}{\beta\omega} \right] = e^{\beta\mu} \frac{2\pi}{\beta\omega}$$

$$\langle E \rangle = -\partial/\partial\beta \ln Q + \mu \langle N \rangle = -\partial/\partial\beta \left[e^{\beta\mu} \frac{2\pi}{\beta\omega} \right] + \mu \langle N \rangle$$

$$= -\mu e^{\beta\mu} \frac{2\pi}{\beta\omega} + e^{\beta\mu} \frac{2\pi}{\beta^2\omega} + \mu e^{\beta\mu} \frac{2\pi}{\beta\omega}$$

$$\therefore \quad \langle E \rangle = \frac{1}{\beta^2} \frac{2\pi}{\omega} e^{\beta\mu} \qquad \langle N \rangle = \frac{2\pi}{\beta\omega} e^{\beta\mu}$$

clearly $$\langle E \rangle = \frac{1}{\beta} \langle N \rangle = \langle N \rangle k_B T$$

as expected $\frac{1}{2} k_B T$ for each of the two quadratic terms in H.

Following the discussion in class and applying it to 1-d and $E = cp$ we have

$$Q = \prod_p \left(1 + e^{-\beta(cp - \mu)}\right)$$

$$\ln Q = \int dp \, \ln\left(1 + e^{-\beta(cp-\mu)}\right) \frac{L}{\hbar}$$

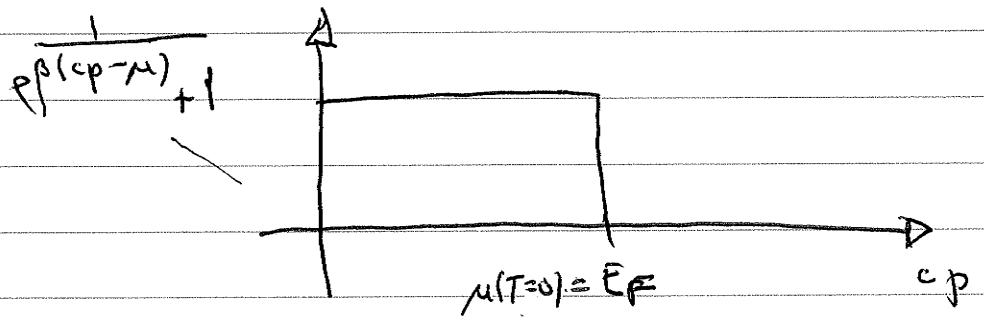
The $\frac{L}{\hbar}$ factors come from $\int dx$, assuming particle moves in interval $(0, L)$, and $1/\hbar$ from dimensionless phase space integration $dx\,dp/\hbar$

$$\langle N \rangle = \frac{1}{\beta}\frac{\partial}{\partial \mu} \ln Q = \int \frac{dp\,L}{\hbar} \left[e^{\beta(cp-\mu)} + 1\right]^{-1}$$

$$\langle E \rangle = -\frac{\partial}{\partial \beta} \ln Q + \mu \langle N \rangle = \int \frac{dp\,L}{\hbar} \, cp \left[e^{\beta(cp-\mu)} + 1\right]^{-1}$$

These two equations relate $\langle E \rangle$, $\langle N \rangle$, T, and μ.

We usually like to eliminate μ. Suppose $T = 0$ and then denote μ by E_F. In this case the FD distribution factor looks like:



Then $\langle N \rangle = L E_F / c\hbar$

Meanwhile

$$\langle E \rangle = \frac{L}{h} \frac{1}{2} c p^2 \Big|_0^{E_F/c} = \frac{L}{2hc} E_F^2$$

Putting together

$$\langle E \rangle = \frac{1}{2} \langle N \rangle E_F$$

On average each of $\langle N \rangle$ particles has $\frac{1}{2} E_F$ of energy. Slightly different result in 2-d, 3-d due to phase space factors.

Actually, the integral for $\langle N \rangle$ can be done analytically even if $T \neq 0$ using

$$\int \frac{dx}{a e^{bx} + 1} = \frac{1}{b} \ln\left(\frac{e^{bx}}{1 + a e^{bx}}\right)$$

so

$$\langle N \rangle = \frac{L}{h} \int dp \; \frac{1}{e^{-\beta\mu} e^{cp\beta} + 1}$$

$$= \frac{L}{hc\beta} \ln\left(1 + e^{\beta\mu}\right)$$

But I do not think $\langle E \rangle$ integral is doable.

See Ashcroft and Mermin for an approach to doing low, but nonzero, temperatures.

The Sommerfeld expansion states

$$\int_0^\infty H(E) f(E)\,dE = \int_0^\mu H(E)\,dE + \frac{\pi^2}{6}(k_B T)^2 H'(\mu) + \cdots$$

f: fermi function

H: other (smooth) function

So $$\langle N\rangle = \int_0^\infty \frac{L}{\hbar c}\,dE\, f(E) = \int_0^\mu \frac{L}{\hbar c}\,dE + \frac{\pi^2}{6}(k_B T)^2 \cdot 0$$

$$= \underbrace{\int_0^{E_F} \frac{L}{\hbar c}\,dE}_{\text{This is just } \langle N\rangle} + (E_F - \mu)\frac{L}{\hbar c}$$

as can be seen by looking at $T = 0$.

conclusion: $\mu(T) = E_F$ through order T^2

(This is not true in 2-d and 3-d where there is a T^2 correction)

Meanwhile $$\langle E\rangle = \int_0^\infty \frac{L}{\hbar c} E\, f(E)\,dE$$

$$\approx \frac{L}{\hbar c}\int_0^\mu E\,dE + \frac{\pi^2}{6}(k_B T)^2 \cdot 1 \cdot \frac{L}{\hbar c}$$

use $\mu = E_F$ ↳

$$= \frac{L}{\hbar c}\left(\frac{E_F^2}{2} + \frac{\pi^2}{6}(k_B T)^2\right)$$

$$= \langle N\rangle\left[\frac{1}{2}E_F + \frac{\pi^2 (k_B T)^2}{6\, E_F}\right]$$

$$C = \frac{\pi^2}{3}\langle N\rangle \frac{k_B T}{E_F} k_B$$

This shows electronic contribution to specific heat of solids is $\sim T^1$.

a) First, review the results for Q for a 3-d classical gas such as exists above the surface

$$Q_{3d} = \sum_{n=0}^{\infty} \frac{1}{n!} e^{\beta \mu n} Z_n$$

$$Z_n = V^n / \lambda_T^{3n} \qquad \lambda_T = h(2\pi m k_B T)^{-1/2}$$

$$Q_{3d} = \exp\left(e^{\beta\mu} V / \lambda_T^3\right)$$

$$\ln Q_{3d} = e^{\beta\mu} V / \lambda_T^3$$

We can compute $\langle N \rangle$ and P via

$$\langle N \rangle = \frac{1}{\beta} \frac{\partial}{\partial \mu} \ln Q = e^{\beta\mu} V / \lambda_T^3$$

$$P = \frac{1}{\beta} \frac{\partial}{\partial V} \ln Q = \frac{1}{\beta} e^{\beta\mu} / \lambda_T^3 = \langle N \rangle / V \quad 1/\beta$$

$$PV = \langle N \rangle k_B T.$$

another way to express these relations is

$$e^{\beta\mu} = \frac{\langle N \rangle}{V} \lambda_T^3 = \frac{P}{k_B T} \lambda_T^3$$

The same calculation goes for the surface, except V gets replaced by A, there are only 2 momentum integrals for each particle, and also each particle feels an energy $-\epsilon_0$ at the surface

3-2

$$Q_{2d} = \sum_{n=0}^{\infty} \frac{1}{n!} e^{\beta\mu n} Z_n$$

Here I use same symbols μ and T as before, understanding that since surface is in contact with gas, the temperatures and chemical potentials must be equal.

$$Z_n = \frac{A^n}{\lambda_T^{2n}} e^{+\beta\epsilon_0 n}$$

$$Q_{2d} = \exp\left(e^{\beta\mu} \frac{A}{\lambda_T^2} e^{\beta\epsilon_0} \right)$$

The number of particles on the surface is

$$\langle N_{2d} \rangle = \frac{1}{\beta} \frac{\partial}{\partial \mu} \ln Q_{2d} = e^{\beta\mu} \frac{A}{\lambda_T^2} e^{\beta\epsilon_0}$$

$$\frac{\langle N_{2d} \rangle}{A} = e^{\beta\epsilon_0} \frac{P}{k_B T} \lambda_T^3 = e^{\beta\epsilon_0} \frac{P}{k_B T} \lambda_T$$

b) If the surface is treated quantum mechanically

$$\langle N_{2d} \rangle = \int \frac{dp_x\, dp_y\, dx\, dy}{h^2} \underbrace{\frac{1}{e^{\beta(p^2/2m - \epsilon_0 - \mu)} + 1}}_{\text{Fermi-Dirac function}}$$

$$= \frac{A}{h^2} \int_0^{\infty} 2\pi p\, dp \frac{1}{e^{-\beta\epsilon_0} e^{-\beta\mu} e^{\beta p^2/2m} + 1}$$

Let $x = \beta p^2/2m \qquad dx = \beta p/m\, dp$

$$= \frac{A}{h^2} 2\pi \frac{m}{\beta} \int_0^{\infty} dx \frac{1}{e^{-\beta(\epsilon_0+\mu)} e^{x} + 1}$$

This integral can be done analytically

$$\int \frac{dx}{a e^{bx} + 1} = \frac{1}{b} \ln\left[\frac{e^{bx}}{1 + a e^{bx}}\right]$$

$$\frac{\langle N_{2d} \rangle}{A} = \frac{2\pi m}{\beta h^2} \ln\left(\frac{e^{x}}{1 + e^{-\beta(\epsilon_0 + \mu)} e^{x}}\right)_0^{\infty}$$

$$= \frac{2\pi m}{\beta h^2} \ln\left(1 + e^{-\beta(\epsilon_0 + \mu)}\right)$$

We can write the prefactor as $1/\lambda_T^2$

$$\frac{\langle N_{2d} \rangle}{A} = \frac{\ln\left(1 + e^{\beta(\epsilon_0 + \mu)}\right)}{\lambda_T^2}$$

This reduces to (a) in the usual classical limit where $e^{\beta\mu} \to 0$. As in part (a) we can replace $e^{\beta\mu}$ by $P\lambda_T^3/k_BT$ to get

$$\frac{\langle N_{2d} \rangle}{A} = \frac{1}{\lambda_T^2} \ln\left[1 + e^{\beta\epsilon_0} \frac{P\lambda_T^3}{k_BT}\right]$$

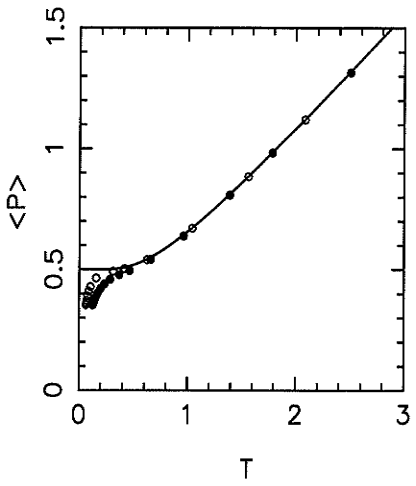


Figure 5. The potential energy of a single Quantum Oscillator as a function of temperature. Here $m = 1$ and $\omega = 2$. The full line is the exact result for $\Delta\tau = 0$ while the closed and open circles are for fixed $L = 8$ and $L = 16$ respectively.

The quantum mechanical operators $\hat{X}_n$ generate a set of classical variables $x_{n,l}$ with an additional imaginary time index. Thus the partition function of the one dimensional quantum problem maps onto a classical problem in $1 + 1$ dimensions. Anisotropic couplings distinguish correlations in space and imaginary time.

3. The One–Dimensional Ising Model in a Transverse Field

In the previous section we described the world–line approach for a single quantum oscillator and collections of quantum oscillators. These models provide the most simple illustration of the technique, and are also solvable analytically, in the absence of anharmonicity. The bulk of the applications of the world–line approach, however, has been to quantum spins and interacting bosons and fermions. In this section we will describe the Ising model in a transverse magnetic field. Here, the effective classical model is especially simple, and, in fact, the world–line mapping allows us to determine much of the physics even before performing simulations. This model, with the addition of randomness to the couplings, has revealed some remarkable features of disordered quantum systems, partially through numerical work.[10, 11]

The Ising model provides a simple description of magnetic phase transitions. Classical "spin" degrees of freedom $S_{\mathbf{i}}^z$ which can take on the values $S_{\mathbf{i}}^z = \pm 1$ exist on the sites $\mathbf{i}$ of a lattice. Spins on different lattice sites interact via a coupling constant J,

$$H_0 = J \sum_{\langle \mathbf{ij} \rangle} S_{\mathbf{i}}^z S_{\mathbf{j}}^z. \tag{21}$$

The symbol $\langle \mathbf{ij} \rangle$ indicates a sum over near–neighbor sites, the case most often considered. For a ferromagnetic coupling $J < 0$, spins $S_{\mathbf{i}}^z$ and $S_{\mathbf{j}}^z$ with the same value have lower energy and hence order is favored. On the other hand, the entropy favors random spin configurations. This model has a finite temperature phase transition in two and higher dimensions in which the global up–down symmetry of the spins is broken and a non–zero spontaneous magnetization $m = \langle S_{\mathbf{i}}^z \rangle$ exists below the critical temperature T_c. For a two–dimensional square lattice in which the couplings J_x and J_y between neighbors in the x and y directions are identical, $T_c \approx 2.269J$. More generally, if J_x and J_y differ, T_c is given by

$$2\tanh[\frac{2J_x}{kT_c}]\tanh[\frac{2J_y}{kT_c}] = 1. \tag{22}$$

The Ising model Eq. 22 has been very extensively studied by classical monte carlo methods.[12] However, if a *transverse* magnetic field, $H_1 = -B \sum_{\mathbf{i}} S_{\mathbf{i}}^x$, is added, quantum simulation methods must be employed owing to the non–commutivity of the operators. We proceed as for the quantum harmonic oscillator, beginning with the partition function, discretizing the inverse temperature β, and separating the two non–commuting pieces of the Hamiltonian.

$$Z = \mathrm{Tr} e^{-\beta \hat{H}} = \mathrm{Tr}[e^{-\Delta\tau \hat{H}}]^L \approx Z_{\mathrm{tr}} = \mathrm{Tr}[e^{-\Delta\tau \hat{H}_0} e^{-\Delta\tau \hat{H}_1}]^L. \tag{23}$$

Complete sets of states $|S_1^z\, S_2^z \ldots S_N^z\rangle$ which are eigenstates of the z component of spin on each of the N sites of the spatial lattice are then inserted.

$$\begin{aligned} Z \approx \sum_{S_{il}^z} \quad & \langle S_{11}^z S_{21}^z \ldots S_{N1}^z | e^{-\Delta\tau H_0} e^{-\Delta\tau H_1} | S_{12}^z S_{22}^z \ldots S_{N2}^z \rangle \\ & \langle S_{12}^z S_{22}^z \ldots S_{N2}^z | e^{-\Delta\tau H_0} e^{-\Delta\tau H_1} | S_{13}^z S_{23}^z \ldots S_{N3}^z \rangle \ldots \\ & \langle S_{1L}^z S_{2L}^z \ldots S_{NL}^z | e^{-\Delta\tau H_0} e^{-\Delta\tau H_1} | S_{11}^z S_{21}^z \ldots S_{N1}^z \rangle. \end{aligned} \tag{24}$$

The eigenvalues S_{il}^z have a second label l to specify the imaginary time slice. Like the potential energy operator in our quantum oscillator example, the

operator $\exp(-\Delta\tau H_0)$ is diagonal in the basis chosen for the intermediate states, and immediately comes out of the expectation values.

$$\begin{aligned} Z \approx \quad & \sum_{S^z_{\mathbf{i}l}} \exp[J\Delta\tau \sum_{\langle \mathbf{ij}\rangle, l} S^z_{\mathbf{i}l} S^z_{\mathbf{j}l}] \, \langle S^z_{11} S^z_{21} \dots S^z_{N1} | e^{-\Delta\tau \hat{H}_1} | S^z_{12} S^z_{22} \dots S^z_{N2} \rangle \\ & \langle \; S^z_{12} S^z_{22} \dots S^z_{N2} | e^{-\Delta\tau \hat{H}_1} | S^z_{13} S^z_{23} \dots S^z_{N3} \rangle \dots \\ & \langle \; S^z_{1L} S^z_{2L} \dots S^z_{NL} | e^{-\Delta\tau \hat{H}_1} | S^z_{11} S^z_{21} \dots S^z_{N1} \rangle \end{aligned} \tag{25}$$

The remaining expectation values of the operators of x component of spin are easily evaluated, since $\hat{H}_1$ is the sum of pieces which commute. Each matrix element factorizes,

$$\begin{aligned} & \langle S^z_{1l} S^z_{2l} \dots S^z_{Nl} | e^{-\Delta\tau \hat{H}_1} | S^z_{1,l+1} S^z_{2,l+1} \dots S^z_{N,l+1} \rangle \\ & \qquad = \prod_{\mathbf{i}} \langle S^z_{\mathbf{i},l} | e^{\Delta\tau B S^x_{\mathbf{i}}} | S^z_{\mathbf{i},l+1} \rangle . \end{aligned} \tag{26}$$

These single site matrix elements are,

$$\langle S^z_{\mathbf{i}l} | e^{\Delta\tau B S^x_{\mathbf{i}}} | S^z_{\mathbf{i}l+1} \rangle = e^{-\lambda S^z_{\mathbf{i}l} S^z_{\mathbf{i}l+1}}, \tag{27}$$

where $\lambda = -\frac{1}{2}\ln[\tanh\Delta\tau B]$. Thus the effect of the transverse magnetic field is to introduce an Ising–like coupling in the imaginary time direction. This is in close analogy to the kinetic energy operator in the quantum oscillator case, which coupled positions at different imaginary times.

With the matrix elements evaluated, we have,

$$Z_{\rm tr} = \sum_{S^z_{\mathbf{i}l}} e^{-E} \tag{28}$$

$$E = -J\Delta\tau \sum_{\langle \mathbf{ij}\rangle, l} S^z_{\mathbf{i}l} S^z_{\mathbf{j}l} - \lambda \sum_{\mathbf{i},l} S^z_{\mathbf{i}l} S^z_{\mathbf{i}l+1}, \tag{29}$$

which is identical to that of a $(d+1)$–dimensional classical Ising model with one direction having a different coupling constant, λ, from the other d dimensions, $J\Delta\tau$.

We can now infer the phase diagram of the quantum model in d dimensions from what is known concerning the classical model in $d+1$ dimensions. Consider, for example, the case of a one–dimensional Ising model in a transverse field. The mapping to the two–dimensional anisotropic classical model tells us there is a phase transition in the J–B plane whose boundary is given by Eq. 22, namely, $2\tanh[2J\Delta\tau]\tanh[2\lambda] = 1$. This curve separates a small B ferromagnetic phase, in which there is a symmetry–breaking spontaneous magnetization in the z direction, from a paramagnetic phase at larger B.

It is important to distinguish the role of β in the original quantum model and its classical analog. The classical model exhibits a phase transition *in the thermodynamic limit*, that is, when the size of the lattice is infinite, and when βJ_x and βJ_y satisfy Eq. 22. In the language of the one–dimensional Ising model in a transverse field, the condition that the classical lattice be infinite corresponds to taking $\beta \rightarrow \infty$, since β gives one of the classical linear dimensions. $N \rightarrow \infty$ is also required of the original linear lattice size. In other words, there is a "quantum phase transition" in the *ground state* of the one–dimensional Ising model in a transverse field as a function of the parameters J and B.

Besides predicting a phase transition and giving an analytic expression for the phase boundary, the mapping also tells us the dynamic critical exponent z, which defines the relationship between the correlation length in the spatial and imaginary time directions near the critical point. (See also section 7.) Since the mapping is to a classical model which, to within an anisotropy in coupling constants, looks the same in these directions, we infer that $z = 1$ for the Ising model in a transverse field (in any dimension). In the Hamiltonians to be discussed in the following sections, the structure of the action will be rather different in the space and imaginary time directions, so that one might expect $z \neq 1$. We will briefly discuss the implications of the value of z for finite size scaling in Section 7.

We conclude this section by noting that the problem of a one–dimensional Ising model in a *random* transverse magnetic field has recently revealed a number of fascinating features.[10, 11] None of the steps in the above discussion of the world–line formulation required that the field B is site independent, or that the coupling constant J not depend on the link **ij**. World–line simulations of the disordered model[13] are then a simple generalization of the clean case, again illustrating the powerful feature of these simulations that new Hamiltonians and their associated physics can often be explored with simple modifications of codes.

4. The Spin–1/2 XXZ Hamiltonian

In the preceding section we saw how a d–dimensional Ising model in a transverse magnetic field maps onto an anisotropic $d+1$–dimensional classical Ising model. The quantum mechanical Hamiltonian had a simple classical analog because the non–diagonal terms in the Hamiltonian appeared only as single site operators. We now turn to Hamiltonians where the non–diagonal terms appear in pairs. As we shall see, this results in more complicated effective actions and restrictions on the allowed spin patterns.