Problem Set 4
Quantum Field Theory and Many Body Physics (SoSe2015)

Due: Monday, May 11, 2015 before the beginning of the class

In this problem set, we continue our study of path integrals and consider path integrals for spin Hamiltonians. In two additional problems, we learn how to perform Matsubara sums, for both bosonic and fermionic Matsubara frequencies. These problems introduce a standard technique that one needs regularly.

Problem 1: Path integrals for spin (5+5+5+5+5 points)

In this problem we want to derive a path integral representation for a spin-$\frac{1}{2}$ Hamiltonian, e.g.,

$$H = -g\boldsymbol{\sigma} \cdot \mathbf{B}(t), \tag{1}$$

where the components σ_i of $\boldsymbol{\sigma}$ denote the Pauli matrices. Such path integrals are useful to study the quantum mechanics of spin models such as the Heisenberg model.

(a) Consider the unit vector $\hat{\mathbf{n}} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ in the radial direction in spherical coordinates. Now, consider the spin-up eigenvectors for a Zeeman field along $\hat{\mathbf{n}}$ as defined by the eigenvalue equation

$$\hat{\mathbf{n}} \cdot \boldsymbol{\sigma}|\hat{\mathbf{n}}\rangle = |\hat{\mathbf{n}}\rangle. \tag{2}$$

Show that when written in the usual spin basis with the quantization axis along the z axis, this is solved by the eigenvector

$$|\hat{\mathbf{n}}\rangle = \begin{pmatrix} e^{-i\phi}\cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix}. \tag{3}$$

Note also that the eigenvalue equation defines $|\hat{\mathbf{n}}\rangle$ only up to an overall phase.

(b) Show that the $|\hat{\mathbf{n}}\rangle$ define an overcomplete set of states, i.e., that

$$\mathbf{1} = \int \frac{d^2\hat{\mathbf{n}}}{2\pi}|\hat{\mathbf{n}}\rangle\langle\hat{\mathbf{n}}|, \tag{4}$$

where $d^2\hat{\mathbf{n}} = \sin\theta\, d\theta\, d\phi$ denotes the solid angle corresponding to the unit vector $\hat{\mathbf{n}}$. You can show this by evaluating the integrals explicitly for the individual matrix elements in the usual spin basis. The set of states $\hat{\mathbf{n}}$ is *over*complete because is contains more than the minimum number of required basis states (which would be two for a spin-$\frac{1}{2}$ problem).

(c) Consider the propagator for $H = 0$,

$$i\,G(\hat{\mathbf{n}}t, \hat{\mathbf{n}}'t') = \langle\hat{\mathbf{n}}|\mathcal{U}(t,t')|\hat{\mathbf{n}}'\rangle, \tag{5}$$

with $\mathcal{U}(t,t') = \mathbf{1}$. Following the derivation of the path integral, insert resolutions of the identity in terms of the overcomplete sets $|\hat{\mathbf{n}}(t_j)\rangle$ at the $N-1$ equally spaced intermediate times $t_1, \ldots, t_{N-1}$ (also define $t_0 = t'$ and $t_N = t$). Show that

$$i\,G(\hat{\mathbf{n}}t, \hat{\mathbf{n}}'t') = \int \left[\frac{d^2\hat{\mathbf{n}}(\tau)}{2\pi}\right] e^{i\int_{t'}^{t} d\tau\, i\langle\hat{\mathbf{n}}(\tau)|\frac{d}{d\tau}|\hat{\mathbf{n}}(\tau)\rangle}. \tag{6}$$

Give explicit discrete versions of the action and the integration measure of this path integral. Note that remarkably, the action

$$S = i\int_{t'}^{t} d\tau\, \langle\hat{\mathbf{n}}(\tau)|\frac{d}{d\tau}|\hat{\mathbf{n}}(\tau)\rangle = \int_{t'}^{t} d\tau\, \frac{1}{2}\dot{\phi}(1+\cos\theta) \tag{7}$$

is non-zero even for a vanishing Hamiltonian! To arrive at this result, you may find the following little calculation for the overlap of the spin states at two neighboring times useful,

$$\begin{aligned}\langle\hat{\mathbf{n}}(t_j)|\hat{\mathbf{n}}(t_{j-1})\rangle &= 1-\langle\hat{\mathbf{n}}(t_j)(|\hat{\mathbf{n}}(t_j)\rangle-|\hat{\mathbf{n}}(t_{j-1})\rangle) \\ &= \exp\{-\langle\hat{\mathbf{n}}(t_j)(|\hat{\mathbf{n}}(t_j)\rangle-|\hat{\mathbf{n}}(t_{j-1})\rangle)\}.\end{aligned} \tag{8}$$

Explain in which sense the second equality is valid.

(d) Show that the action generalizes to

$$S=\int_{t'}^{t}d\tau\,\left(i\langle\hat{\mathbf{n}}(\tau)|\frac{d}{d\tau}|\hat{\mathbf{n}}(\tau)\rangle+g\hat{\mathbf{n}}(\tau)\cdot\mathbf{B}(\tau)\right) \tag{9}$$

for $H=-g\boldsymbol{\sigma}\cdot\mathbf{B}(\tau)$. To arrive at this result, write the time evolution operator for this Hamiltonian as a time-ordered exponential (as usual for time-dependent Hamiltonians – see the derivation of linear-response theory in the lecture). You may want to use the identity (prove!)

$$\langle\hat{\mathbf{n}}|\boldsymbol{\sigma}|\hat{\mathbf{n}}\rangle=\hat{\mathbf{n}}. \tag{10}$$

(e) Show that Hamilton's principle for the action (9) correctly reproduces the classical equation of motion of a spin

$$\dot{\hat{\mathbf{n}}}=2g\hat{\mathbf{n}}\times\mathbf{B}(t). \tag{11}$$

Note that this equation of motion is quite different from the usual equations of motion in classical mechanics. It is a first-order differential equation in time and the force involves a vector product. (The latter also appears for particles in a magnetic field whose path-integral description actually has some similarities with the present problem.)

Remark: To understand the physics of the action for spin more deeply, you may want to learn (or remember) the concept of a Berry phase in quantum mechanics and recognize that the first term of the action (9) is just such a Berry phase.

Problem 2: Bosonic Matsubara sums (5+10+5+5 points)

In evaluating the path integral for the harmonic chain, we encountered sums over bosonic Matsubara frequencies. They emerged because the fields we are integrating over are periodic in imaginary time with period $\hbar\beta$. It will turn out that this periodicity is a general feature of bosonic fields. In the class, we treated the two limiting cases of zero temperature (where the summation can be replaced by integration) and of $\hbar\to 0$ (where only one term of the sum survives). In this problem, we want to learn how to perform such sums in general by converting them into suitable contour integrals.

(a) Consider the Bose function

$$n_B(z)=\frac{1}{e^{\beta z}-1} \tag{12}$$

in the complex plane, i.e., z is a complex number. Show that it has poles for

$$z=i\hbar\Omega_n=\frac{2\pi i}{\beta}n \tag{13}$$

with n an integer and $\Omega_n=(2\pi/\hbar\beta)n$. Show also that the residues of these poles are all equal to $1/\beta$.

(b) Now consider the important Matsubara sum

$$I=\frac{1}{\beta}\sum_{\Omega_n}\frac{e^{-i\Omega_n\tau}}{i\hbar\Omega_n-x} \tag{14}$$

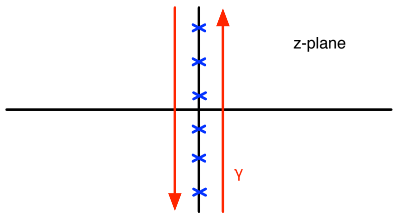
with $\tau \in [-\hbar\beta, \hbar\beta]$. Show that by Cauchy's theorem, this summation can be converted into the contour integral

$$I = \int_\gamma \frac{\mathrm{d}z}{2\pi i} \frac{e^{-z\tau/\hbar}}{z-x} \frac{-1}{e^{-\beta z}-1} \tag{15}$$

for $\tau > 0$ and

$$I = \int_\gamma \frac{\mathrm{d}z}{2\pi i} \frac{e^{-z\tau/\hbar}}{z-x} \frac{1}{e^{\beta z}-1} \tag{16}$$

for $\tau < 0$. In both cases, the contour γ in the complex plane is given by



(c) Actually, so far both representations work independently of the sign of τ. The sign of τ becomes important only in the next step in which we deform the contour. Show that for both integrals with the specified sign of τ, the integrand vanishes exponentially for $|z| \to \infty$. (Remember that $|\tau| < \beta$.) Thus, we can add semicircles to the integration contour which go from $+i\infty$ to $-i\infty$ for $\mathrm{Re}z > 0$ and from $-i\infty$ to $+i\infty$ for $\mathrm{Re}z < 0$. These semicircles do not contribute to the integral. This yields two closed contours, one for $\mathrm{Re}z < 0$ and another for $\mathrm{Re}z > 0$. Use this to show that

$$I = -[n_B(x)+1]e^{-x\tau/\hbar} \tag{17}$$

for $\tau > 0$ and

$$I = -n_B(x)e^{-x\tau/\hbar} \tag{18}$$

for $\tau < 0$.

(d) Now return to the harmonic chain. As shown in class, the equal-time correlation function

$$C(\mathbf{R}) = \langle [\phi(\mathbf{R}+\mathbf{r}) - \phi(\mathbf{r})]^2 \rangle \tag{19}$$

can be computed from the path integral as

$$\mathbf{C}(\mathbf{R}) = \frac{1}{V}\sum_{\mathbf{q}} \frac{1}{\hbar\beta} \sum_{\Omega_n} \frac{\hbar \sin^2\left(\frac{\mathbf{q}\cdot\mathbf{R}}{2}\right)}{\rho\Omega_n^2 + \rho c^2 q^2} \tag{20}$$

where $\Omega_n = 2\pi n/(\hbar\beta)$ are the bosonic Matsubara frequencies. We had already computed this correlation function for all temperatures in a previous problem set (with the final result still written as a sum over momenta). Now reproduce this result by performing the Matsubara sum with the same technique that we just introduced. (In this case, the terms of the sum tend to 0 sufficiently fast that analogs of both integral expressions given above will work fine. Note that the sum in (b) above does not converge for $\tau = 0$.)

An alternative approach would be to note that

$$\sum_{\Omega_n} \frac{1}{\Omega_n^2 + c^2q^2} = \lim_{\eta\to 0^+} \sum_{\Omega_n} \frac{e^{i\Omega_n\eta}}{\Omega_n^2 + c^2q^2} = \lim_{\eta\to 0^+} \sum_{\Omega_n} \left[\frac{e^{i\Omega_n\eta}}{cq - i\Omega_n} - \frac{e^{i\Omega_n\eta}}{cq + i\Omega_n}\right] \tag{21}$$

and then to use the result of (c) above. Here, we introduced a convergence factor $e^{i\Omega_n\eta}$ into the sum which is entirely inconsequential as long as we consider the original sum which converges nicely. But it is important once we decompose the original expression into its partial fractions. Now, the individual sums diverge logarithmically without convergence factor. This convergence factor is thus needed to separate the terms and sum them independently.

Problem 3: Fermionic Matsubara sums (25 points)

As we will see later in the course, fermionic fields $\psi(\tau)$ are antiperiodic in imaginary time, i.e.,

$$f(0) = -f(\hbar\beta). \tag{22}$$

Explain that such functions can be written as Fourier series

$$f(\tau) = \sum_{\epsilon_n} f(i\epsilon_n) e^{-i\epsilon_n \tau} \tag{23}$$

with fermionic Matsubara freqencies

$$\epsilon_n = \frac{\pi}{\hbar\beta}(2n+1). \tag{24}$$

Now follow the blueprint of the bosonic Matsubara sums (replacing the Bose by the Fermi function) to perform the fermionic sum

$$I = \frac{1}{\beta} \sum_{\epsilon_n} \frac{e^{-i\epsilon_n \tau}}{i\hbar\epsilon_n - x}. \tag{25}$$