Phys 511: HOMEWORK ASSIGNMENT No (3)

March 11th 2007

DUE DATE: Monday April 2nd 2007.

(Please note that late assignments may not receive a full mark.)

QUESTION (1): INSTANTON FOR SPIN TUNNELING

A spin tunneling in a biaxial potential with Hamiltonian $\mathcal{H} = -D\hat{S}_z^2 + E\hat{S}_x^2$, with $D, E > 0$. The semiclassical instanton paths for tunneling are along the 2 lines defined by $0 \leq \theta \leq \pi$, and $\phi = 0, \pi$.

(i) Show that the instanton solutions are given, after eliminating the dependence on ϕ from the imaginary equations of motion, by

$$\sin\theta(\tau) \; = \; \frac{1}{\cosh(\omega_o \tau)} \; ; \qquad \textit{where} \qquad \omega_o = 2S\sqrt{D(D+E)} \tag{1}$$

(ii) Then show that the semiclassical instanton action along these paths is given by the expression

$$\mathcal{S}_o^{(\eta)} \; = \; 2S\hbar \ln\left[\left(\frac{D+E}{E}\right)^{1/2} + \left(\frac{D}{E}\right)^{1/2}\right] \; + \; i\pi\eta S \tag{2}$$

where $\eta = \pm 1$ labels the paths.

(iii) Now show that if we add a very small extra field $\mathbf{b}$ to the problem, oriented in the xy-plane, then there will be a small extra term in the action given by

$$\delta\mathcal{S}_b^{(\eta)} \; = \; \frac{\pi\eta}{\omega_o}[b_x + if(D/E)b_y] \tag{3}$$

and find an expression for $f(D/E)$.

QUESTION (2): QUANTUM REGISTER WITH DIAGONAL COUPLINGS

A well-known model for a 'quantum memory' device has the simple Hamiltonian given by

$$\mathcal{H} \; = \; \sum_{j=1}^{M} \epsilon_j \hat{\tau}_j^z \; + \; \frac{1}{2}\sum_{i \neq j} K_{ij}^{zzz} \hat{\tau}_i^z \hat{\tau}_j^z \; + \; \sum_q \sum_j v_j(q) x_q \hat{\tau}_j^z \; + \; \frac{1}{2}\sum_q \left(\frac{p_q^2}{m_q} + m_q \omega_q^2 x_q^2\right) \tag{4}$$

where $v_j(q)$ couples the j-th 'qubit', modeled by a Pauli spin $\hat{\tau}_j$, to a set of oscillators with coordinates $\{x_q\}$ and momenta $\{p_q\}$. Note that both the couplings and the fields ϵ_j acting on the qubits are diagonal. This model is also a useful 'zero-th order' starting point for the discussion of not only errors in quantum computation, but also for quantum spin glasses.

(i) Consider first a single qubit alone, so that the effective Hamiltonian is

$$\mathcal{H} \; = \; \epsilon\hat{\tau}^z \; + \; \sum_q v(q) x_q \hat{\tau}^z \; + \; \frac{1}{2}\sum_q \left(\frac{p_q^2}{m_q} + m_q \omega_q^2 x_q^2\right) \tag{5}$$

and find a canonical transformation of this Hamiltonian which allows a decoupling of the qubit from the oscillators. You should also explain the reasoning which leads you to this transformation.

(ii) Now give an analogous transformation for the entire register. Then assume a more specific form for the couplings in this problem, in which $v_j(q) = v_o(q)e^{iqR_j}$, where $R_j = ja_o$ is the distance along the line of qubits (assumed to be a 1-dimensional structure); write down the final form of the transformed Hamiltonian for this case.

QUESTION (3): INTEGRATING OUT THE OSCILLATORS

Consider a system described by a Lagrangian which couples a set $\{X_q\}$ of oscillators to a particle with coordinate Q, according to the effective Lagrangian

$$\begin{aligned} L &= \frac{1}{2}M\dot{Q}^2 - U(Q) - \sum_q c_q X_q Q \;+\; \frac{1}{2}\sum_q m_q(\dot{X}_q^2 - \omega_q^2 X_q^2) \\ U(Q) &= V_o(Q) - \sum_q \frac{c_q^2 Q^2}{2m_q\omega_q^2} \qquad (6) \\ & \qquad (7) \end{aligned}$$

in which the extra term in the renormalised potential U is there to cancel the shift in the original potential V_o caused by the oscillators.

(i) Find the coupled equations of motion for the classical paths $Q(t)$ and the $\{x_q(t)\}$, treating (7) as a classical Lagrangian.

(ii) Now go to imaginary time and also make the Fourier transform

$$Q(\tau) \;=\; \frac{1}{\hbar\beta}\sum_{m=-\infty}^{+\infty} Q_m e^{i\Omega_m \tau} \qquad (8)$$

with a similar transform for the $\{X_q(m)\}$. Then show that we can write the Euclidean (ie., imaginary time) action for the system as $\tilde{S}_o[Q] + \tilde{S}_R[Q, X_q]$, where the action for the 'rest' includes the interaction plus the bath, and can be written as

$$\tilde{S}_R[Q, X_q] \;=\; \frac{1}{\hbar\beta}\sum_m\sum_q \frac{m_q}{2}\left(\Omega_m^2|X_q(m)|^2 + \omega_q^2\left|X_q(m) - \frac{c_q}{m_q\omega_q^2}\right|^2\right) \qquad (9)$$

and show also the form for the Euclidean $\tilde{S}_o[Q]$. Show that the solution for the classical path of each oscillator is just

$$X_q(m) = \frac{c_q}{m_q(\Omega_m^2 + \omega_q^2)}Q_m \qquad (10)$$

(iii) Now to find the quantum behaviour write the Euclidean paths for the oscillators in the form $X_q(m) = \bar{X}_q(m) + x_q(m)$, where $x_q(m)$ is a small deviation from the classical path $\bar{X}_q(m)$ of minimum action, already discussed above. By expanding the action to quadratic order in the deviations around the classical paths, show that we can now write the Euclidean action in the form $\tilde{S}_R[Q, x_q] \;=\; \tilde{S}_E[x_q] + \tilde{S}_{int}[Q]$, where the self-interaction term $\tilde{S}_{int}[Q]$ has the form

$$\tilde{S}_{int}[Q] \;=\; \frac{M}{2}\frac{1}{\hbar\beta}\sum_m \int_0^\infty \frac{d\omega}{\pi}\frac{J(\omega)}{\omega}\frac{\Omega_m^2}{\omega^2 + \Omega_m^2} \qquad (11)$$

in which the spectral function is defined by

$$J(\omega) \;=\; \frac{\pi}{2}\sum_q \frac{c_q^2}{m_q\omega_q^2}\delta(\omega - \omega_q) \qquad (12)$$

You should also exhibit the form of $\tilde{S}_E[x_q]$, which describes fluctuations in the oscillator environment. Finally, Fourier transform $\tilde{S}_{int}[Q]$ to imaginary time τ, and show it is given as a convolution over paths $Q(\tau)$ and $Q(\tau')$, with a kernel whose form you should exhibit.

QUESTION (4): SHERRINGTON-KIRKPATRICK MODEL

When the replica trick is applied to the partition function for a simple infinite-range exchange spin glass, we define the average of n replicas of the original partition function, each one labelled by a 'replica index' α, as

$$Z_n \;=\; \prod_{\alpha=1}^{n} \equiv \langle \sum_{J_{ij}} P[J_{ij}] Z^n(J_{ij}) \rangle \tag{13}$$

where the 'sum' $\sum_{J_{ij}}$ is really a functional integral over the distribution of the random couplings $\{J_{ij}\}$, with a weighting function $P[J_{ij}]$, in a Hamiltonian whose form we assume to be

$$\mathcal{H}_J \;=\; -\frac{1}{2}\sum_{i\neq j}^{N} J_{ij} s_i s_j \;-\; h_o \sum_{j}^{N} s_j \tag{14}$$

To be specific here we will assume a set of random couplings satisfying the constraints $\langle J_{ij}\rangle = 0$, $\langle J_{ij}^2\rangle = J_o^2/N$; and we assume that the Ising spins take the values $s_j = \pm 1$.

(i) Show that after sample averaging, we can write this n replica average as

$$Z_n \;=\; \sum_s \exp\left[\frac{J_o^2}{2N(kT)^2}\sum_{i<j}\left(\sum_{\alpha=1}^{n} s_{i\alpha}s_{j\alpha}\right)^2 + \frac{h_o}{kT}\sum_j\sum_\alpha s_{j\alpha}\right] \tag{15}$$

where T is the temperature, and where the sum $\sum_s$ is a sum over the different configurations of the $\{s_{j\alpha}\}$, ie., over the 2^N spin configurations and over the 2^n replica configurations for each spin.

(ii) Now show, using the standard trick to deal with the Gaussian integrals above, that we can write (15) in the form

$$Z_n \;=\; \prod_{\alpha<\beta}\int dQ_{\alpha\beta}\left(\frac{N}{2\pi}\right)^{1/2} Z[Q]\exp\left[\frac{N}{4(kT)^2}\left(n - \sum_{\alpha\neq\beta} Q_{\alpha\beta}^2\right)\right] \tag{16}$$

$$Z[Q] \;=\; \sum_S \exp\left[\frac{1}{2(kT)^2}\sum_{\alpha\neq\beta} Q_{\alpha\beta}S_\alpha S_\beta + \frac{h_o}{kT}\sum_\alpha S_\alpha\right] \tag{17}$$

where we have now introduced a set of variables $S_\alpha = \pm 1$ which range over the 2^n replica spin configurations. Find an expression for $Q_{\alpha\beta}$ if we assume a Gaussian distribution for the probability distribution $P[J]$, of form

$$P[J_{ij}] \;=\; \frac{1}{(2\pi)^{1/2}J_o} e^{-\frac{1}{2}(J_{ij}/J_o)^2} \tag{18}$$

QUESTION (5): PHENOMENOLOGY OF DIPOLAR GLASSES

In a dipolar glass system (whether it be a spin dipole glass or an electric dipole glass), one begins with an effective Hamiltonian of form

$$\mathcal{H}_{eff} \;=\; \sum_j(\Delta_j \hat{\tau}_j^x + \epsilon_j \hat{\tau}_j^z + \frac{1}{2}\sum_{ij} V_{ij}^{zz}\hat{\tau}_i^z\hat{\tau}_j^z \tag{19}$$

in which distributions are assumed for the $\{\Delta_j, \epsilon_j\}$, and the bare interaction V_{ij}^{zz} is assumed, at least roughly, to have a dipolar form.

(i) Suppose the 2-level systems arise from a set of defects which move in a 2-well potential. Suppose that the particle which is tunneling has an effective mass of 50 atomic units (ie., the mass of 50 protons), and and it tunnels over a distance $d \sim 0.1$ Angstroms. Suppose also that the small oscillation frequency ω_o in the wells is ~ 400 GHz, and the barrier height V_o is roughly 200 K. What roughly is the tunnel splitting Δ_o?

(ii) Suppose now that both the barrier heights V and the barrier tunneling distances d are uniformly distributed between values 200-600K and $0.1 - 0.3$ Angstroms respectively, with $V \propto d$ always. Find now (a) the probability distribution $P(\Delta)$ of tunneling matrix elements, and (b) the probability distribution of tunneling splittings $P(E)$, where $E^2 = \Delta^2 + \epsilon^2$, and the bias energies ϵ have a Gaussian distribution $P(\epsilon)$, with a half-width W_o.

(iii) The low-T frequency-dependent ultrasonic attenuation $\alpha(\omega)$ of amorphous dielectrics rises steeply as one lowers T and then at a crossover temperature T_c is becomes T-independent. For a given TLS in this system, the crossover is defined by $\omega\tau_{min}^{-1} = 1$, where τ_{min} is the minimum relaxation rate when $E_o \sim kT$. The phonon relaxation rate for a single two-level system with tunneling matrix element Δ_o and splitting E_o has the form

$$\tau^{-1} \sim \frac{\gamma^2}{v^5}\left(\frac{\Delta_o}{E_o}\right)^2 \frac{E_o^3}{2\pi\hbar^4\rho} \coth\left(\frac{E_o}{2kT}\right) \tag{20}$$

where γ is the phonon-TLS coupling, v the sound velocity and ρ the density. Assuming the same probability distribution that you found above for the tunneling splittings and tunnel matrix elements (but now assuming that W_o is much larger than all energies of interest here, so $P(E)$ can be assumed flat) find (a) what is the probability distribution $P(\tau_{min})$ of minimum relaxation times in the system, and (b) for a given frequency ω, what will be the crossover temperature T_c.

END OF ASSIGNMENT (3)