Problem set for the course "The Physics of Disordered Systems", 2019

Rules: You are supposed to work alone as much as possible but you are allowed to consult other students and discuss with them. While discussions among students are encouraged, solving a problem together as a team work is NOT ALLOWED. Of course, also feel free to contact us and ask questions; We can help and give you further hints if you are stuck.

No more than 25 points can be obtained from one section.

Deadline: 20.01.2020. Delay penalty: 5points/day. (Days end at 4pm...)

Please scan the solutions and upload it to the moodle system: `http://newton.phy.bme.hu/moodle/`

Grading is as follows:

5: 55- points,
4: 45-54 points,
3: 35-44 points,
2: 25-34 points.

I. STRUCTURALLY DISORDERED SYSTEMS

1 (10 pts) Finite size scaling for percolation, scaling function.
(Recommended for those who have completed Phase transitions and critical phenomena)
Assume an intensive quantity X, scaling as:

$$X \propto |p - p_c|^{-\varrho}$$

in an infinitely large system. Derive the scaling function for $X(L, \xi)$ following the steps below.

(a) Using $\xi \propto |p - p_c|^{-\nu}$ express X as function of the correlation length.

(b) In case if $L \ll \xi$ the correlation length cannot be larger than the system size. Express $X(L, \xi)$ as function of the correlation length and a scaling function $x_1(L/\xi)$ which is constant for $L \ll \xi$.

(c) Express $X(L, p)$ in terms of a scaling function as:

$$X(L, p) = |p - p_c|^a x_2(L^b(p - p_c))$$

What are the exponents a and b.

[Hint: A good candidate for X is the average cluster size without the infinite cluster.]

2 (20 pts) Finite size scaling for percolation numerical simulation.

Simulate the two dimensional square lattice site percolation.

(a) (2 pts) Consider a periodic square lattice of size L = 20, 40, 80. Fill the lattice with occupied sites with probability p.

(b) (8 pts) You may use any of the following two algorithms to find the connected components:

- Hoshen-Kopelman, a pseudo code can be found in Wikipedia: `https://en.wikipedia.org/wiki/Hoshen-Kopelman_algorithm`
- Stack based method:
  1. Go through each occupied site. If the actual one is unlabelled, label it with a new label put it into a stack (list) and go to 2. otherwise go to the next occupied site.
  2. If the stack is empty go to 1.

3. Take a site from the stack
4. Check its four neighbors, and label all unlabelled occupied ones and put them into the stack.
5. Go back to 2.

(c) (5 pts) Calculate S, the mean cluster size without the largest cluster

(d) (5 pts) Detect the maximum of S as a function of p, and compare it with the "official" critical point of $p_c \simeq 0.593$. Do not to forget to use ensemble average of at least 100 independent systems. How does the maximum change as a function of L? Compare with the result of the previous problem.

3 (15 pts) Renormalization group of the 2D percolation model.
(Recommended for those who have completed Phase transitions and critical phenomena)

Consider the problem of two-dimensional site percolation. Let $R(p)$ be the renormalization function (i.e. the map $p \to \tilde{p} = R(p, b)$ generated by rescaling the lattice by a factor b). This can be estimated as:

$$R(p) = \sum_{n=1}^{N} \binom{N}{n} p^n (1-p)^{N-n} S(n) \ .$$

Here b is the renormalization factor, $N = b^2$ in two dimensions, and $S(n)$ is the probability of having a random $b \times b$ block with n occupied sites which percolates in the y direction. (One has to count all configurations and check percolation for both directions.)

(a) (3 pts) Show that for $b = 2$, $S(1) = 0$, $S(2) = 1/3$, $S(3) = 1$, $S(4) = 1$

(b) (5 pts) Create a code which calculates the coefficients for $b = 3, 4$. Either you can use the same algorithm as in the previous exercise part (b) or more easily,– since in 4×4 systems only directed paths are possible and we are only interested in the question whether it percolates or no,– you can go row by row and check if you can continue or not.

(c) (7 pts) Determine numerically the critical point for two dimensional site percolation using the values of $b = 2, 3, 4$, and also the critical exponent ν, characterizing the divergence of the correlation length, $\xi \sim |p - p_c|^{-\nu}$. [Remember that critical point is the nontrivial unstable fix point of the equation: $R(p_c) = p_c$, and ν is related to the slope.]

4 (15 pts) Edwards ensemble.
Consider a binary mixture of hard sphere particles (A, B). We assume that if particles of the same size are next to each other then less volume is wasted on average compared to the case when grains next to each other differ in size. Let us define the average wasted volume as $v^{\alpha,\beta}$, where $\alpha, \beta \in \{A, B\}$ ($\alpha \neq \beta$, $v^{\alpha,\beta} > v^{\alpha,\alpha} = v^{\beta,\beta}$).

(a) (5 pts) Use the mean field approach to derive the average volume function, W as function of the n_A, n_B fractions of particles A, B.

(b) (5 pts) Show that the volume can, in general, be converted to an Ising Hamiltonian with $\sigma = \{0, 1\}$ for grain A and B respectively and J a combination of $v^{\alpha,\beta}$.

(c) (5 pts) Use the mean field solution of the Ising model and determine those values of the compactivity (X), for which we have mixed or segregated phases.

II. DISORDERED SPINS AND SPIN GLASSES

5 (20 pts)Avalanche distribution in the 3D random field Ising model.
Consider the random field Ising model in $D = 3$ dimension,

$$H = -J \sum_{(i,j)} \sigma_i \sigma_j - \sum_i (f_i + H) \sigma_i,$$

with $J = 1$ taken as the energy unit, and the f_i random Gaussian variables, $\rho(f) \sim \exp(-f^2/(2R^2))$. Make sweeps with the external field from $H = -\infty \to \infty$, and compute numerically the avalanche distribution as a function of R, and show that there is a critical value, $R_c \approx 2.23$, below which an avalanche of the order of the system size occurs. Use the work of Sethna et al, as a reference (https://arxiv.org/abs/cond-mat/9210018), and reproduce Fig.2 and its inset, and estimate the critical exponent σ, $s_{\max} \sim (R - R_c)^{-1/\sigma}$.

Some hints: You will have to take large systems of linear size $L \approx 50 \times 50 \times 50$ to get decent statistics. In course of an avalanche, the field increases at neighboring spins, which can then flip, and increase the field at neighboring spins etc. Using this structure, you can look for the field value H, at which the first spin becomes unstable, change H to that value, and start an avalanche by flipping this spin. Then keep track of spins which become unstable, until you reach a stable configuration.

6 (20 pts) Mean field theory of avalanche distribution in the random field Ising model.
Consider the random field Ising model in $D = \infty$ dimension,

$$H = -\frac{J}{N} \sum_{(i,j)} \sigma_i \sigma_j - \sum_i (f_i + H) \sigma_i,$$

with $N \to \infty$, and the f_i independent random Gaussian variables of distribution $\rho(f) \sim \exp(-f^2/(2R^2))$. Here each lattice site is connected to all other sites. Follow Sethna et al (https://arxiv.org/abs/cond-mat/9210018), as a reference in the following.

a. (5pts) As a warm-up, derive the mean field equation (Eq. (3) of Sethna), also discussed at class,

$$M = 1 - 2 \int_{-\infty}^{-JM-H} \rho(f)\, \mathrm{d}f, \tag{1}$$

and prove that the magnetization obeys the scaling form, $M(h, r) \sim |r|^\beta \mathcal{M}_\pm(h/|r|^{\beta\delta})$ with $\delta = 3$ and $\beta = 1/2$, and the scaling variables defined as $r = (R - R_C)/R_C$ and $h = H - H_C$. [Hint: First perform a graphical analysis to show that the critical point corresponds to a disorder value, R_c, where $2J\rho(0) = 1$, and is at $H_c = 0$. Then assume that $r \approx 0$ and $H \approx 0$, and expand (1) to third order in M and to first order in H.]

b. (5pts) Now consider avalanches. Follow again the work of Sethna. Assume that you create an avalanche by flipping one spin having a local random magnetic field value, $f_0 = -JM - H$. Flipping this spin increases the exchange field on all other spins by $2J/N$. It will flip a spin if it has a random field value, $f_1 = f_0 + x_1 \in [f_0, f_0 + 2J/N]$, i.e., if the separation x_1 between f_0 and f_1 is $0 \le x_1 \le 2J/N$. Argue that the distribution of x_1 is Poissonian of the form $p(x)\mathrm{d}x = e^{-x/\langle x \rangle}\mathrm{d}x/\langle x \rangle$. Determine $\langle x \rangle$, and compute the probability $D(2)$ of having an avalanche of length 2. Show that it is given by

$$D(2) = 2J\rho\, e^{-4J\rho}\ .$$

[Hint: The next unstable spin has a field $f_2 = f_1 + x_2$. To have an avalanche of length 2 one must have $0 < x_1 < 2J/N$ but $x_1 + x_2 > 4J/N$, since the next spin is not destabilized by flipping the first two spins. Furthermore, x_1 and x_2 are independent Poissonian variables.]

c. (5pts) Extend the previous calculation, and compute $D(3)$.

d. (5pts) According to Sethna et al,

$$D(s) = \frac{s^{s-2}}{(s-1)!}\, (2J\rho)^{s-1}\, e^{-s\, 2J\rho}$$

Verify that this formula describes $D(2)$ and $D(3)$ as computed above. The critical point is where $2\rho J = 1$. Assume that $2\rho J = 1 - t$, and verify using the Stirling formula that the scaling form given by Sethna indeed applies [Hint: you will need the subleading correction in the Stirling formula.]

7 (20 pts) Replica symmetrical solution of the Sherrington-Kirkpatrick model.

At class, we have shown that the average partition function of the SK model reads

$$\overline{\ln Z} = \lim_{n \to 0} \frac{1}{n} \big(\overline{Z^n} - 1\big), \tag{2}$$

with the replicated action expressed in the large N limit as

$$\overline{Z^n} = \int \mathcal{D}Q \exp\Big\{\frac{\beta^2}{4}nN - \frac{1}{2}N\beta^2\sum_{a<b} Q_{ab}^2 + N\,\ln \mathcal{Z}(Q)\Big\}.$$

Here $\mathcal{Z}(Q)$ denotes the partition function of a single (replicated) spin in the presence of the mean field Q_{ab}, generating correlations between the replicas,

$$\mathcal{Z}(Q) = \sum_{S^a} \exp\big[-\beta H(S,Q)\big], \tag{3}$$

$$H(S,Q) = -\beta\sum_{a<b} Q_{ab}S^aS^b - h\sum_a S^a\ . \tag{4}$$

a. (10pts) Assume that $Q_{a\neq b} = q$ while its diagonal is 0. Follow the steps at class and show that

$$\mathcal{Z}(Q) = e^{-n\,q\,\beta^2/2}\int \frac{\mathrm{d}y}{\sqrt{2\pi\,q}}\ e^{-y^2/(2\,q)}\ [\cosh(\beta(y+h))]^n. \tag{5}$$

Show also that in this limit,

$$\overline{Z^n} = \int \mathcal{D}Q \exp\Big\{-NA(q)\Big\},$$

with

$$A(q) = -n\frac{\beta^2}{4} + n(n-1)\frac{\beta^2}{4}q^2 + \frac{n}{2}\beta^2 q - \ln\Big[\int \frac{\mathrm{d}y}{\sqrt{2\pi\,q}}\ e^{-y^2/(2\,q)}\ [\cosh(\beta(y+h))]^n\Big].$$

Find now the saddle point equation and show that $\partial_q A = 0$ implies in the $n\to 0$ limit the self-consistency condition for $q = q(T)$,

$$q = \langle \tanh^2(\beta(y+h))\rangle_y\ , \tag{6}$$

where averaging is with the random local field, y, having a distribution $\sim e^{-y^2/(2q)}$. [Hint: first find saddle point than take $n \to 0$.]

b. (5pts) Solve (6) numerically for $h = 0$ as well as for $h \neq 0$ and show that $q(T) \neq 0$ below a critical temperature. Plot $q(T)$ for some fixed values of h, and determine the phase diagram in the (T,h) plane. [$q(T) \neq 0$ means you have a spin glass.]

c. (5pts) Take the $n \to 0$ limit of the free energy and show that the average free energy per spin is:

$$f(T,h) = -\frac{\beta}{4}(1-q)^2 - \frac{1}{\beta}\int \frac{\mathrm{d}y}{\sqrt{2\pi\,q}}\ e^{-x^2/(2\,q)}\ \ln[\cosh(\beta(y+h))]. \tag{7}$$

Compute the entropy as a function of T (you can use numerical differentiation), and show that it becomes negative as $T \to 0$. Determine its value at $T = 0$.

III. DISORDERED QUANTUM-SYSTEMS

8 (20 pts) Numerical investigation of localization transition

Consider a three dimensional tight binding Hamiltonian with periodic boundary conditions on a simple cubic lattice,

$$H = -\sum_{(i,j)}(c_i^\dagger c_j + c_j^\dagger c_i) + \sum_i \xi_i\ c_i^\dagger c_i\ , \tag{8}$$

with the ξ_i's being random, uniformly distributed, and independent energy variables, $\xi_i \in [-W, W]$, and the $i \in L^3$ labeling the lattice sites.

a (5 pts) Consider a system of size $L = 9$, and compute its energy spectrum for $W = 8$. Average over disorder configurations, and determine the average density of states per lattice site, $\overline{\varrho(E)}$ as a function of energy. [Hint: Remember that $L^3 \varrho(E)\, \mathrm{d}E$ is the average number of states in a small energy window, $[E - \mathrm{d}E/2, E + \mathrm{d}E/2]$. Divide therefore the energy axis onto appropriately chosen energy windows. As a cross-check, you should verify that $\overline{\varrho(E)}$ integrates to 1.]

b (5 pts) Plot the unaveraged *local* density of states, $\varrho(E, \mathbf{r})$ at several lattice sites for a given disorder realization. [Hint: Be careful with the normalization of the wave functions.]

c (10 pts) Determine the IPR for each eigenstate, and determine the average IPR, IPR(E) as a function of energy. Determine the mobility edge (approximately) for $W = 8$ by comparing the IPR(E) curves computed for systems with $L = 9$, $L = 8$, and $L = 10$ sites. Plot (estimate) the localization length as a function of energy for these system sizes.

9 (10 pts) Variable range hopping

Generalize Mott's variable range hopping formula for the case of a Coulomb gap, by simply replacing the energies of the localized states in the non-interacting calculation by the Hartree energies, $\epsilon_i \to \tilde{\epsilon}_i$. [Hint: Use the asymptotic form of the distribution function, $p(\tilde{\epsilon}_i)$, obtained at class, and repeat the probabilistic arguments that lead to the variable range expression.] How does the result depend on dimensionality?

10 (20 pts) Weak localization corrections at low temperatures and universal scaling.

Consider a 3-dimensional system, described by a beta function, $\beta(g)$, asymptotically behaving as

$$\beta(g) \approx \begin{cases} 1 - \frac{\tilde{g}}{g}, & g \gtrsim 2\tilde{g} \,, \\ s\, \frac{g - g_c}{g_c}, & \text{for } g \approx g_c \text{ and } g < 2\tilde{g} \,. \end{cases}$$

Here we now included the first non-trivial $1/g$ correction (weak localization correction). Denote with l_0 the size of a microscopic cube of dimensionless conductance $g_0 > g_c$. (Remember that we typically tune g_0 by applying pressure, or changing the chemical potential by a back gate, and we assume that it varies continuously with the external parameters.)

a. (5 pts) Assume you have a metallic sample. Show first that a length scale, the so-called coherence length exists, which diverges as $\xi = l_0\, (a/(g_0 - g_c))^{\nu}$ with $\nu = s$. For system sizes $L < \xi$, the conductance of a small cube scales as $g/g_c \approx 1 + a\ (L/\xi)^{1/s}$, while for $L \gg \xi$ one obtains a metallic behavior, $g \propto L/\xi$. [Hint: define the coherence length ξ as the length scale at which $g(L = \xi) = 2\tilde{g}$. Otherwise just assume a beta function of arbitrary form, approaching $\beta \to 1$ in the $g \to \infty$ limit, and having a logarithmic slope, s at $g = g_c$.].

b. (5 pts) At finite temperatures, inelastic scattering of the electrons in a metal (on phonons or on each other) leads to a loss of quantum coherence. Inelastic scattering processes occur at a rate $1/\tau_{\text{inel}} \sim T^p$, with the power p determined by the relevant process ($p = 2$ for electron-electron scattering, $p = 3$ for scattering on phonons etc.). Since electrons in a disordered metal move roughly diffusively, this introduces an inelastic scattering length, $L_{\text{inel}}(T) \sim \sqrt{D\tau_{\text{inel}}} \propto T^{-p/2}$. The resistivity can then be estimated as that of $(L/L_{\text{inel}})^3$ resistors, each of volume L_{inel}^3 , and each having a corresponding dimensionless conductance $g(L_{\text{inel}})$.

   Prove by integrating the single parameter scaling equation that the resistivity can be expressed as

$$\varrho(T) = \frac{h\,\xi}{e^2}\, F(L_{\text{in}}(T)/\xi)$$

   with $F(y)$ a universal function. [Here you need to use the general properties of the β function, just as in a.]

c. (5 pts) Determine this universal function F in the limit of $L_{\text{in}} \gg \xi$, relevant for low temperatures. (Now take into account the $1/g$ part of the β function, too.) Assume that the inelastic scattering length behaves as $L_{\text{in}}(T) \sim T^{-p/2}$, and sketch the corresponding behavior of $\varrho(T)$ as you tune the system closer and closer to the localization transition.

d. (5 pts) Determine the function $F(L_{\text{in}}(T)/\xi)$ also in the opposite limit, when $L_{\text{in}} \ll \xi$, and determine/plot the high temperature behavior of $\varrho(T)$ as you get close to the transition.

11 (15 pts) Estimation of localization length in a quantum wire.

In this problem, you need to estimate the localization length of a one-dimensional gold wire of 1μm diameter, and the temperature to which you need to cool down the wire to see that electrons are localized in it. Look for experimental data on Gold nanowires (see, e.g. Fig.6 in http://arxiv.org/pdf/0709.4663.pdf), as a starting point, and also search for typical bulk residual resistivity data for your estimate. Estimate the mean free path from that (use the Drude model and assume a single valence for Au). Alternatively, assuming very thin wires, you can assume that $l \sim W$, with W the width of the wire.

Then estimate the temperature to which you need to cool down the wire to be in the localized regime. For this, electrons must move coherently through the whole wire. You must therefore estimate the length to which electrons can propagate coherently, the so-called inelastic length, $L_{\mathrm{inel}} \sim \sqrt{D\tau_{\mathrm{inel}}}$, with D the diffusion constant and τ_{inel} the inelastic scattering time (dephasing time). Assume that the latter comes from phonons, i.e., $1/\tau_{\mathrm{inel}} \approx 1/\tau_{e-ph} \approx AT^3$. Extract the coefficient A from experimental data (see, e.g. Fig.6 in http://arxiv.org/pdf/0709.4663.pdf). To estimate $L_{\mathrm{inel}}(T)$, you will also need the diffusion constant, which you can try and estimate by assuming ballistic motion of the electrons with a velocity v_F and scattering at the surface of the wire at typical distances, $l \sim W$.