Transfer Matrix:

Connection Between QFT and Classical Statistical Mechanics

In the past lectures we have shown that there is a connection between ~~classical~~ quantum field theory (in D space-time dims, at $T=0$) and classical statistical mechanics in D Euclidean dimensions. We will now explore this issue further.

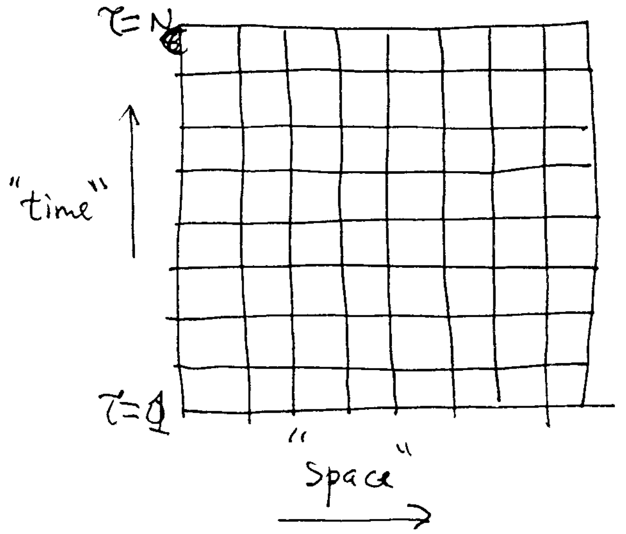
Let us consider a typical problem in equilibrium statistical mechanics. For the sake of simplicity, we will consider the Ising model in D dimensions. The arguments which we will give below are straightforward to generalize to other cases. Let us consider a D-dimensional hypercubic lattice of unit spacing. At each site $\vec{r}$ there is an Ising variable $\sigma(\vec{r})$. We will refer to the state of this lattice (or configuration $[\sigma]$) to a particular set of values of this collection of variables. Let $H[\sigma]$ be the classical energy ($j=1,\dots,D$)

$$H[\sigma] = -\underbrace{J}_{\text{exchange constant}} \sum_{\vec{r},j} \sigma(\vec{r})\,\sigma(\vec{r}+\hat{e}_j) - \underbrace{h}_{\text{magnetic field}} \sum_{\vec{r}} \sigma(\vec{r})$$

The partition function is ($k_B=1$, $J>0$ (for simplicity)).

$$Z = \sum_{[\sigma]} e^{-H[\sigma]/T}$$

(with periodic boundary conditions).



Let us regard one of the D spacial dimensions as "time" (or rather imaginary time). Let us say that we pick the dimension D as the "time dimension". Then we have D-1 "space dimensions" and one "time dimension". This is clearly an arbitrary choice given the symmetries of this problem. Thus we can view each configuration $[\sigma]$ as the evolution of an initial configuration at $\tau=0$ (i.e. the configuration on the first "row" (or hyperplane)) in time τ, i.e. as we go from row to row. The P.F. is thus a sum over histories of these configurations.

Let us now show that the partition function can be written in the form of a trace of a matrix, known as the Transfer Matrix.

$$Z = \sum_{[\sigma]} e^{-H[\sigma]/T} \equiv \operatorname{tr} \hat{T}^{N}$$

when N is the # of rows (or hyperplanes). To this end we define a complete set of states $\{|\sigma\rangle_\tau\}$ on each row τ ($\tau=1,\ldots,N$). If each row contains N^{D-1} sites the number of states in this basis is $2^{N^{D-1}}$. Let us find the matrix $\hat{T}$. In particular, we will look for a $\hat{T}$ with the factorized form

$$\hat{T} = \hat{T}_1^{1/2} \, \hat{T}_2 \, \hat{T}_1^{1/2}$$

It turns out that there exists a large number of interesting problems in ~~sta~~ equilibrium classical statistical mechanics (CSM) for which the matrix $\hat{T}$ can be chosen to be a hermitean matrix. From the point of view of CSM, this follows (in part) from the fact that the Boltzmann weights are positive real numbers. This condition is however not sufficient. The ~~cond~~ sufficient condition is known as reflection positivity (we will come back to this issue shortly). For the particular case of the Ising model it is possible to write the matrices $\hat{T}_1$ and $\hat{T}_2$ in terms of a set of real Pauli matrices $\hat{\sigma}_1(r)$ and $\hat{\sigma}_2(r)$ ~~defin~~ which act on the the states defined on each row. For the case at hand we ~~have~~ find, after some algebra,

$$\hat{T}_2 = \exp\left\{ \sum_{\vec{r}, j=1,\ldots,D-1} \frac{J_s}{T} \hat{\sigma}_3(\vec{r}) \hat{\sigma}_3(\vec{r}+\hat{e}_j) + \frac{h}{T} \sum_{\vec{r}} \hat{\sigma}_3(\vec{r}) \right\}$$

$$\hat{T}_1 = \left[\frac{1}{2}\sinh\left(\frac{2J_t}{T}\right)\right]^{N_s/2} \exp\left\{ b \sum_{\vec{r}} \hat{\sigma}_1(\vec{r}) \right\}$$

where

$$e^{-2b} = \tanh(J_t/T)$$

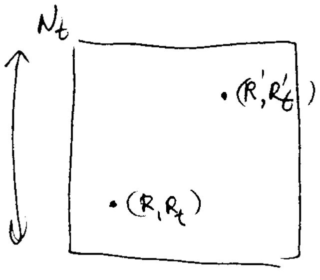
and N_s is the # of sites in each hyperplane (row). Here we have assumed that J_s and J_t, the coupling constants along the "space" and time directions are not necessarily equal to each other.

The correlation functions

$$\langle \sigma(R)\, \sigma(R') \rangle = \frac{1}{Z} \sum_{[\sigma]} \sigma(R)\, \sigma(R')\, e^{-H[\sigma]}$$

can be expressed in terms of $\hat{T}$ in the suggestive form

$$\langle \sigma(R)\, \sigma(R') \rangle = \frac{1}{Z} \operatorname{tr} \hat{T}^{R_t}\, \hat{\sigma}_3(R)\, \hat{T}^{R'_t - R_t}\, \hat{\sigma}_3(R'_t)\, \hat{T}^{N_t - R'_t}$$



$$\equiv \langle\langle T[\hat{\sigma}_3(R, R_t)\; \hat{\sigma}_3(R', R'_t)] \rangle\rangle$$

"time ordered product"

$$\hat{\sigma}_3(R, R_t) \equiv \hat{T}^{R_t}\, \hat{\sigma}_3(R)\, \hat{T}^{-R_t}$$

"Heisenberg" representation.

If λ_n are the eigenvalues of the ~~state~~ eigenstates $|n\rangle$

$$\Rightarrow \langle \sigma(R)\,\sigma(R')\rangle = \lim_{N_t\to\infty} \frac{\mathrm{tr}\; T\left[\hat{\sigma}_3(R,R_t)\,\hat{\sigma}_3(R',R'_t)\right]}{Z} =$$

$$= \sum_n \left|\langle G|\,\hat{\sigma}_3\,|n\rangle\right|^2 \left(\frac{\lambda_n}{\lambda_{Max}}\right)^{R'_t - R_t} \qquad (R=R')$$

If the matrix $\hat{T}$ is hermitean $\Rightarrow$ all correlation functions are positive. In this case there is a natural interpretation in terms of a Hilbert space. These are the cases in which there is a connection between CSM and QFT.

The positivity requirement can be relaxed down to the condition of <u>reflection positivity</u> which states the following. Let $A_r(\sigma)$ be some arbitrary local operator localized near r and let us define the operation of <u>reflection</u> across a hyperplane $\mathbb{P}$. Let $A_{\mathbb{P}_r}(\sigma)$ be the same operator after reflection. Then the positivity requirement

$$\langle A_r(\sigma) \quad A_{\mathbb{P}_r}(\sigma)\rangle \geq 0 \qquad \text{(reflection positivity)}$$

implies that the transfer matrix $\hat{T}$, defined on a direction <u>normal</u> to $\mathbb{P}$, must be a hermitean operator for all its eigenstates to have <u>positive norm</u>. This is the analog of unitarity in QFT. It is clearly obeyed in the Ising model and in a large number of cases of interest. There are, however, many interesting problems in CSM which do not satisfy this condition.

<u>The Ising Model in the limit of extreme special anisotropy:</u>

Let us now go back to the Ising Model (IM). Consider the limit $J_t \to \infty$ and ($J_s \to 0$, $h \to 0$)

such that

$$\hat{T}_1^{1/2} \; \hat{T}_2 \; \hat{T}_1^{1/2} \approx e^{-\epsilon \hat{H} + O(\epsilon^2)}$$

where $\hat{H}$ is a hermitean operator and ϵ is a suitably ~~for a~~ chosen <u>small</u> parameter. For this limit to work, we must demand $J_s \approx h$. Also since $\tanh b = e^{-2J_t/T}$ the limit of b <u>small</u> is the limit of $\frac{J_t}{T}$ <u>large</u>.

Thus we write

$$\frac{J_s}{T} = \lambda \, e^{-2J_t/T} \qquad\qquad \frac{h}{T} = \bar{h} \, e^{-2J_t/T}$$

and

$$\epsilon = e^{-2J_t/T}$$

for $\hat{H}$ given by

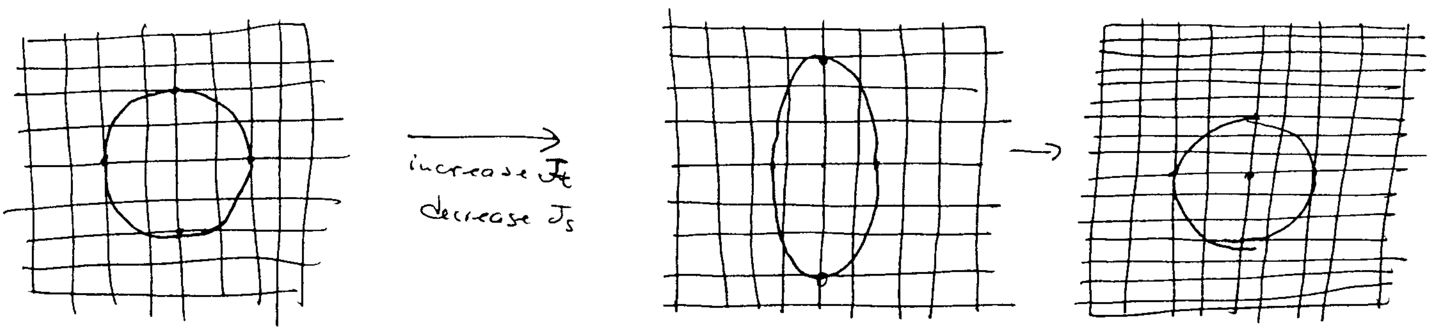
$$\hat{H} = -\sum_{\vec{r}} \hat{\sigma}_1(\vec{r}) - \lambda \sum_{r_{ij}} \hat{\sigma}_3(\vec{r})\, \hat{\sigma}_3(\vec{r}+\hat{e}_j) - \bar{h} \sum_{\vec{r}} \hat{\sigma}_3(\vec{r})$$

Thus λ large is the low-temperature limit whereas λ small is the high temperature case.

Since we want to demand that the anisotropic limit should have the <u>same</u> properties as the isotropic case we proceed as follows. Suppose we begin with a situation which is completely isotropic (for simplicity) and $J_s = J_t$ with lattice spacing 1. In this case the ~~correl~~ curves of equal correlation, i.e.

$$C(r,r') = \langle \sigma(r)\,\sigma(r')\rangle = \text{const}$$

are (approximately for $|r-r'| \gg 1$) ~~circles~~ circumferences of radius $R = |r-r'|$. If we increase J_t and decrease J_s



the curves are (approximately) ellipses. ~~If~~ We can now <u>increase</u> the # of vertical rows so as to reduce the size of the ellipse along the "time" direction back what it was originally, thus restoring isotropy. We can repeat this procedure indefinitely and get a system with a <u>dense set of rows</u>. In this limit "time" is continuous. The equivalence holds provided that we require that

$$N_t \, e^{-2 J_t / T} = \text{fixed} = \bar{\beta}$$

Thus, as $\frac{J_t}{T} \to \infty$ we should ~~get~~ let $N_t \to \infty$. The fixed number $\bar{\beta}$ should be infinite ~~for~~ if the original system is thermodynamically large along that direction. Thus

$$Z = \operatorname{tr} \hat{T}^{N_t} \underset{\substack{N_t \to \infty \\ \frac{J_t}{T} \to \infty}}{\approx} \operatorname{tr} e^{-\bar{\beta} \hat{H}} \xrightarrow[\bar{\beta} \to \infty]{} e^{-\bar{\beta} E_0}$$

where E_0 is the lowest eigenvalue of $\hat{H}$, i.e. its ground state. Therefore if we know the ground state energy of $\hat{H}$, or equivalently the largest eigenvalue of $\hat{T}$, we know the partition function Z. This observation is the key to (one of the very many methods) to solve the IM in $D=2$.

Solution of the $D=2$ dimensional Ising Model

The arguments given above tell us that the Ising Model on a square lattice is equivalent to the one-dimensional quantum system with Hamiltonian

$$H = -\lambda \sum_{n=-\frac{L}{2}+1}^{L/2} \hat{\sigma}_3(n)\hat{\sigma}_3(n) - \bar{h}\sum_{n=-\frac{L}{2}+1}^{\frac{L}{2}} \hat{\sigma}_3(n) - \sum_{n=-\frac{L}{2}+1}^{\frac{L}{2}} \hat{\sigma}_1(($$

We will consider the case $\bar{h}=0$.

Before plunging into the actual solution ~~of this system~~, it is worthwhile to discuss the symmetries of this system. The classical Ising model has (if $h=0$) the global spin-flip symmetry $[\sigma] \to [-\sigma]$. Thus, $H[\sigma]$ is invariant under the operations $I:[\sigma]\to[\sigma]$ (the identity) and $R:[\sigma]\to[-\sigma]$ (global spin reversal). These operations form a group since $I \circledast I = I \qquad I\circledast R = R\circledast I = R$

$$R\circledast R = I$$

where $\circledast$ means composition of the two operations.

This is the group $\mathbb{Z}_2$ (permutations of two elements).

The equivalent quantum problem has exactly the same symmetries. The operators $\hat{I}$ and $\hat{R}$ act on the quantum states defined on the ~~rows~~ rows (or hyperplanes) precisely in the same way, i.e.

$$\hat{I}\,|[\sigma]\rangle = |[\sigma]\rangle \qquad \text{(Identity)}$$

$$\hat{R}\,|[\sigma]\rangle = |[-\sigma]\rangle \qquad \text{(Spin flip)}$$

We can construct these operators quite explicitely. Let $\hat{I}(\vec{r})$ and $\hat{R}(\vec{r}) \equiv \hat{\sigma}_1(\vec{r})$ be the identity and the σ_1-Pauli matrices acting on the spin state at $\vec{r}$. Then we can write for $\hat{I}$ and $\hat{R}$ the expressions

$$\hat{I} = \prod_{\vec{r}} \otimes\, \hat{I}(\vec{r})$$

tensor product

$$\hat{R} = \prod_{\vec{r}} \otimes\, \hat{\sigma}_1(\vec{r})$$

These operators have the obvious properties

$$\hat{I}^{-1} = \hat{I} \qquad \hat{R}^{-1} = \hat{R}$$

$$\hat{I}\;\hat{\sigma}_1(\vec{r})\;\hat{I}^{-1} = \hat{\sigma}_1(\vec{r})$$

$$\hat{I}\;\hat{\sigma}_3(\vec{r})\;\hat{I}^{-1} = \hat{\sigma}_3(\vec{r})$$

$$\hat{R}\;\hat{\sigma}_1(\vec{r})\;\hat{R}^{-1} = \hat{\sigma}_1(\vec{r})$$

$$\hat{R}\;\hat{\sigma}_3(\vec{r})\;R^{-1} = -\hat{\sigma}_3(\vec{r})$$

From these properties it follows that, at $h=0$, the Hamiltonian is <u>invariant</u> under the $\mathbb{Z}_2$ symmetry

$$\hat{I}\,\hat{H}\,\hat{I}^{-1} = \hat{H}$$

$$\hat{R}\,\hat{H}\,R^{-1} = \hat{H}$$

Qualitative Behavior of the Ground State

(a) Let us consider first the limit $\lambda \ll 1$ (i.e. high temperature). Clearly we can write $\hat{H}$ as a sum of two terms

$$\hat{H} = \hat{H}_0 + \hat{V}$$

with

$$\hat{H}_0 = -\sum_{\vec{r}} \hat{\sigma}_1(\vec{r})$$

$$\hat{V} = -\lambda \sum_{\vec{r},j} \hat{\sigma}_3(\vec{r})\,\hat{\sigma}_3(\vec{r}+\hat{e}_j)$$

If $\lambda \ll 1$ we can ~~discuss~~ study the properties of the ground state in perturbation theory in ~~powers~~ λ. The (unperturbed) ground state $|\Psi_0\rangle_0$ is

$$|\Psi_0\rangle_0 = \prod_{\vec{r}} \otimes |+,\vec{r}\rangle \equiv |+\rangle \quad ; \quad \hat{R}\,|+\rangle = |+\rangle$$

which is <u>unique</u>.

Here $|+,\vec{r}\rangle$ is the eigenstate of $\hat{\sigma}_1(\vec{r})$ with eigenvalue $+1$. Notice that, in this state,

$$_0\langle \Psi_0|\,\hat{\sigma}_3(\vec{R})\,|\Psi_0\rangle_0 = 0$$

since $\hat{\sigma}_3(R)$ is off-diagonal in the basis of eigenvectors of $\hat{\sigma}_3$. Similarly the equal-time correlation function (equivalent to the correlation function on a fixed row in the D-dimensional theory) is

$$ {}_0\langle \Psi_0 | \; \hat{\sigma}_3(\vec{R}) \;\; \hat{\sigma}_3(\vec{R}') \, | \Psi_0 \rangle_0 = 0 $$

In perturbation theory the ground state gets corrected by virtual processes which include σ_1 spin flips.

$$ |\Psi_0\rangle \simeq |\Psi_0\rangle_0 + \frac{\hat{P}\,\hat{V}}{E_0 - \hat{H}_0} |\Psi_0\rangle + \cdots $$

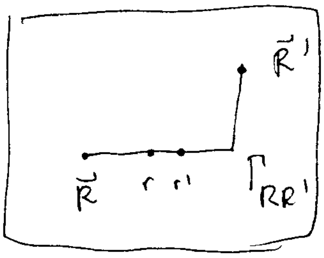
where $\hat{P}$ projects the state $|\Psi_0\rangle$ out of the sum (Brillouin-Wigner pert. theory, see Baym's Quantum Mechanics). For instance, for $D=2$, the state $|++\cdots\cdots+\rangle$ gets perturbed in such a way that a pair of σ_1 spinors are flipped

$$ \hat{V} \; | \Psi_0 \rangle = -\lambda \sum_R \# \, | ++\cdots+\overset{R}{\underline{--}}+\cdots+\rangle $$

where R is the location of the flipped pair. ~~The~~

To higher orders, we will get more pairs in flipped states. What does this observation say about the correlation function? Since $\sigma_3^2 = I$, ~~Clearly~~ we can write

$$\hat\sigma_3(\vec R)\,\hat\sigma_3(\vec R') = \prod_{(\vec r,\vec r')\in\Gamma_{RR'}} \hat\sigma_3(\vec r)\,\hat\sigma_3(\vec r')$$



where $\vec r$ and $\vec r'$ are pairs of neighboring sites on the (arbitrary) path $\Gamma_{RR'}$ which goes from $\vec R$ to $\vec R'$

Thus

$$C(\vec R,\vec R') = \frac{\langle \Psi_0 |\, \hat\sigma_3(\vec R)\,\hat\sigma_3(\vec R')\, | \Psi_0\rangle}{\langle \Psi_0 | \Psi_0\rangle} \simeq \text{const}\,\lambda^{|\vec R-\vec R'|} + \cdots$$

only picks up a leading non-zero contribution in perturbation theory in λ if we go to an order n sufficiently high so that $n \geq |\vec R-\vec R'|$ (where $|R-R'|$ is the # of bonds on $\Gamma_{RR'}$. This argument shows that the correlation function decays exponentially fast

$$C(\vec R,\vec R') \approx \text{const}\; e^{-|\vec R-\vec R'|(\ln\lambda + \cdots)}$$

(It is possible to prove that this approximation is a strict lower bound for $C(R,R')$).

(b) $\lambda \gg 1$ (i.e. low-temperature). In this limit the unperturbed and perturbation terms gets switched.

$$\hat{H}_0 = -\lambda \sum_{\vec{r},j} \hat{\sigma}_3(\vec{r})\, \hat{\sigma}_3(\vec{r}+\vec{e}_j)$$

$$\hat{V} = -\sum_{\vec{r}} \hat{\sigma}_1(\vec{r})$$

The unperturbed ground state must be an eigenstate of $\hat{\sigma}_3(\vec{r})$. The leading order ground state is <u>doubly degenerate</u>, i.e.

$|\Uparrow\rangle \equiv |\uparrow \cdots \uparrow\rangle$; $|\Downarrow\rangle \equiv |\downarrow \cdots \downarrow\rangle$

where

$$\hat{\sigma}_3 |\Uparrow\rangle = |\Uparrow\rangle \qquad \hat{R}\,|\Uparrow\rangle = |\Downarrow\rangle$$
$$\hat{\sigma}_3 |\Downarrow\rangle = -|\Downarrow\rangle \qquad \hat{R}\,|\Downarrow\rangle = |\Uparrow\rangle$$

If the system is <u>finite</u> these states will mix in perturbation theory. Indeed if the lattice has N_s spacial sites, the mixing will occur to order N_s in perturbation theory. But if $N_s \to \infty$ <u>first</u>, then is no mixing to <u>any order in perturbation theory</u>. The obvious exception is $D=1$ in which $N_s = 1$. Thus, for $D > 1$ (or $D \geq 2$)

these two states belong to two essentially decoupled pieces of the Hilbert space. In the classical system this property is known as broken ergodicity (in the sense that the system only explores 1/2 of the total possible configurations; This is an example of Spontaneous symmetry breaking: the Hamiltonian is invariant under $\mathbb{Z}_2$ transformations but the ground state is not (in the thermodynamic limit!). It is possible to prove rigorously that, for $D \geq 2$, the expansion in powers in $\frac{1}{\lambda}$ is convergent and that it has a finite radius of convergence (see, for example, Polyakov's book). In this state we have

$$|\Psi_\uparrow\rangle_0 = |\uparrow \cdots \uparrow\rangle$$

$${}_0\langle \Psi_\uparrow | \hat{\sigma}_3(r) | \Psi_\uparrow\rangle_0 = +1$$

$${}_0\langle \Psi_\downarrow | \hat{\sigma}_3(\vec{r}) | \Psi_\downarrow\rangle_0 = -1$$

In general $\langle \Psi_\uparrow | \hat{\sigma}_3(\vec{r}) | \Psi_\uparrow\rangle = m(\vec{r}) \equiv m$

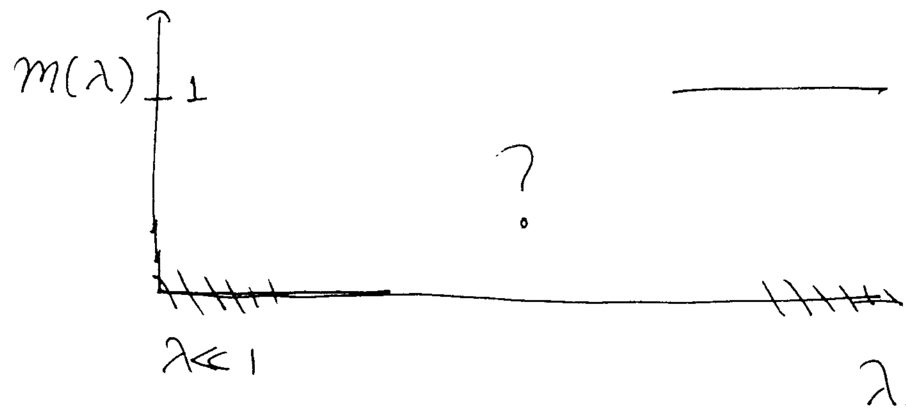
which is the spontaneous magnetization. Clearly $m = f(\lambda)$

It is also clear that, for large λ,

$$C(\vec{R},\vec{R}') = \langle \Psi_T | \hat{\sigma}_3(R)\, \hat{\sigma}_3(R') | \Psi_T \rangle \approx m^2 + \cdots$$

which goes to a constant as $|R-R'| \to \infty$.

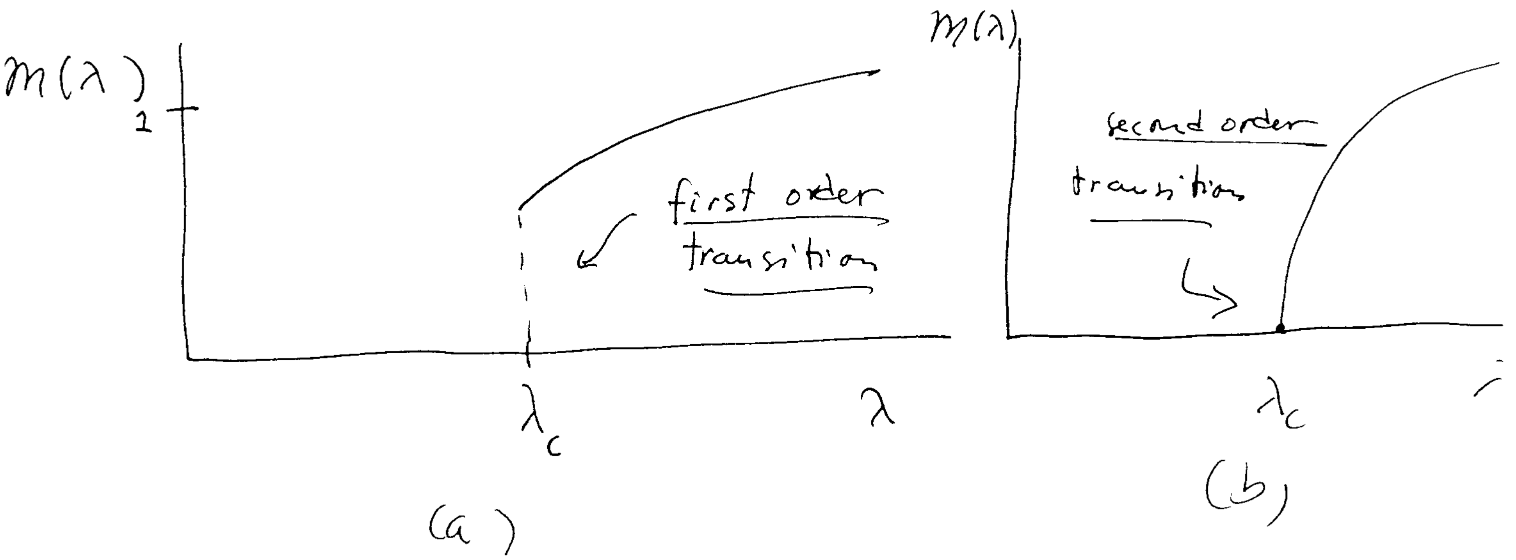
These arguments show that $m(\lambda) \neq 0$ only for λ sufficiently large but that it is zero if λ is very small.



What happens for intermediate values of λ?

At what value of λ does the ground state stop being two-fold (at least!) degenerate?

There are two clear possibilities



Which one is realized?

It is clear that, despite the (claimed but not shown!) convergence of perturbation theory on two disjoint ranges of λ, the answer to these issues lies beyond perturbation theory. For $D=2$ there is a non-perturbative solution for this problem (Onsager's solution) which answers many of this questions. ~~...~~ However the solution is very specific to $D=2$.