Quantum Phase Transition in Transverse Ising Models

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February 15, 2011
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Cooperative interactions between spin-like degrees of freedom can describe the order-disorder transition in many systems.

Transverse Ising Model (TIM) successfully describes a class of such systems.

A specific example being the ferro-electric ordering in Potassium Dihydrogen Phosphate (KDP).

TIM is essentially a quantum model; it incorporates zero temperature fluctuations.

TIM in $d$-dimension corresponds to Ising model in $(d + 1)$ dimension.
In KDP, in each site the oxygen atom creates a double well and the proton resides in one of them.

$\sigma_i^z = +1$  $\sigma_i^z = -1$  $\sigma_j^z = +1$  $\sigma_j^z = -1$

In Pseudo-spin picture, the proton residing in left or right well can be represented by the states $|\uparrow>$ and $|\downarrow>$ respectively.

Dipolar interactions between nearest neighbor sites form the cooperative (exchange-interaction) term.

Proton being a quantum object, a tunneling term is required to study the system’s behavior.
In formulating the tunneling term, note that
\[ \sigma^x | \uparrow \rangle = | \downarrow \rangle \quad \text{and} \quad \sigma^x | \downarrow \rangle = | \uparrow \rangle, \]

A transverse field will correctly represent the tunneling term.

Therefore, the Hamiltonian of the system can be written as
\[ \mathcal{H} = - \sum_{\langle i,j \rangle} J_{ij} \sigma_i^z \sigma_j^z - \Gamma \sum_i \sigma_i^x, \]

where, \( \sigma^\alpha \)'s \( \rightarrow \) Pauli spin matrices,

\( J_{ij} \rightarrow \) cooperative interactions and

\( \Gamma \rightarrow \) tunneling integral, which depends on width and height of the barrier, particle mass etc.
Spin 1/2 case: $\sigma^z$ has two eigen values $\pm 1$, which corresponds to a spin being parallel on anti-parallel with $z-$ axis.

If we take

$$|↑\rangle \Leftrightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

and

$$|↓\rangle \Leftrightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

then taking these two eigen-vectors as basis, the Pauli matrices have the following representation

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$
One can make the non-commuting parts of the Hamiltonian commuting, by assuming

\[ \sigma_i^z = |\vec{\sigma}| \cos \theta, \quad \text{and} \quad \sigma_i^x = |\vec{\sigma}| \sin \theta, \]

The energy of the semi-classical system reduces to

\[ E = -\sigma \Gamma \sin \theta - \frac{1}{2} \sigma^2 J(0) \cos^2 \theta, \]

\[ J(0) = J_i(0) = \sum_{ij} J_{ij}, \text{ where } j \text{ denotes the } j-\text{th nearest neighbor.} \]

Average values of the spin components are \( \langle \sigma^x \rangle = \cos \theta \) and \( \langle \sigma^z \rangle = \sin \theta. \)
Minimisation of the energy function gives \( \sin \theta = \frac{\Gamma}{J(0)} \) or, \( \cos \theta = 0 \).

Thus following cases may occur

- For \( \Gamma = 0 \), \( \langle \sigma^x \rangle = 0 \) and order parameter \( \langle \sigma^z \rangle = 1 \)
- If \( \Gamma < J(0) \), then both \( \langle \sigma^x \rangle \neq 0 \) and \( \langle \sigma^z \rangle \neq 0 \).
- When \( \Gamma \leq J(0) \), then we must have \( \cos \theta = 0 \), implying \( \langle \sigma^z \rangle = 0 \) i.e., full disorder.

So, even in the absence of thermal fluctuation, only quantum fluctuation can lead to an order-disorder phase transition of the system as \( \Gamma \) increases from 0 to \( J(0) \).
One can write the Hamiltonian as

\[ \mathcal{H} = - \sum_i \vec{h}_i \cdot \vec{\sigma}_i. \]

where, \( \vec{h}_i = \Gamma \hat{x} + \left( \frac{1}{2} \sum_j J_{ij} \langle \sigma_j^z \rangle \right) \hat{z} \), and \( \vec{\sigma}_i = \sigma_i^x \hat{x} + \sigma_i^z \hat{z} \),

Under MF approximation one can replace \( \vec{h}_i \) by \( \vec{h} = \Gamma \hat{x} + \langle \sigma^z \rangle J(0) \hat{z} \).

Implying \( \vec{\sigma} = \tanh(\beta |\vec{h}|) \cdot \frac{\vec{h}}{|\vec{h}|} \) and \( |\vec{h}| = \sqrt{\Gamma^2 + (J(0) \langle \sigma^z \rangle)^2} \).

Therefore, \( \langle \sigma^z \rangle = \left[ \tanh(\beta |\vec{h}|) \right] \left( \frac{J(0) \langle \sigma^z \rangle}{|\vec{h}|} \right), \) and \( \langle \sigma^x \rangle = \left[ \tanh(\beta |\vec{h}|) \right] \frac{\Gamma}{|\vec{h}|}. \)
MFT for TIM

\[ \Gamma = 0 \]

- Here, \( \langle \sigma^z \rangle = \tanh \left( \frac{J(0) \langle \sigma^z \rangle}{k_B T} \right) \) and \( \langle \sigma^x \rangle = 0 \).

- Graphical solution gives \( \langle \sigma^z \rangle \neq 0 \) for \( k_B T < J(0) \)
  \( \langle \sigma^z \rangle = 0 \) for \( k_B T > J(0) \).

- It shows that without quantum fluctuation, thermal fluctuation can drive the system to complete disorder beyond \( T_c = J(0) \).

\[ k_B T = 0 \]

- Here, \( \langle \sigma^z \rangle = \frac{J(0) \langle \sigma^z \rangle}{\sqrt{(\Gamma)^2 + (J(0) \langle \sigma^z \rangle)^2}} \)

- Phase boundary: \( \langle \sigma^z \rangle \rightarrow 0 \ 1 = \frac{J(0)}{\Gamma_c} \Rightarrow \Gamma_c = J(0) \) as obtained earlier.

\[ k_B T \text{ finite} \]

- Phase boundary: \( \langle \sigma^z \rangle \rightarrow 0 \).
  \[ \langle \sigma^z \rangle = \tanh \left( \frac{\Gamma_c}{k_B T} \right) \frac{J(0) \langle \sigma^z \rangle}{\Gamma} \text{ or, } \tanh \left( \frac{\Gamma_c}{k_B T} \right) = \frac{\Gamma_c}{J(0)} \].
The phase boundary is as follows

\[ \langle \sigma^z \rangle = 0 \]

\[ \langle \sigma^z \rangle \neq 0 \]
The cooperative Hamiltonian in the BCS theory of superconductivity has the following form
\[ \mathcal{H} = \sum_k \epsilon_k^0 (c_k^\dagger c_k + c_{-k}^\dagger c_{-k}) - V \sum_{kk'} c_{k'}^\dagger c_{-k}^\dagger c_{-k} c_k \]

In terms of the number operator \( \hat{n}_k = c_k^\dagger c_k \), the above Hamiltonian reduces to (\( \sum_k \epsilon_k = 0 \))
\[ \mathcal{H} = - \sum_k \epsilon_k^0 (1 - \hat{n}_k - \hat{n}_{-k}) - V \sum_{kk'} c_{k'}^\dagger c_{-k}^\dagger c_{-k} c_k. \]

Considering the low-lying spectra containing the pair of electrons in state \((k, -k)\), the relevant states are pair occupied (denoted by \(|1_k1_{-k}\rangle\)) or pair unoccupied (denoted by \(|0_k0_{-k}\rangle\)).

Then
\[
(1 - \hat{n}_k - \hat{n}_{-k})|1_k1_{-k}\rangle = (1 - 1 - 1)|1_k1_{-k}\rangle = -|1_k1_{-k}\rangle, \text{ and } \\
(1 - \hat{n}_k - \hat{n}_{-k})|0_k0_{-k}\rangle = (1 - 0 - 0)|0_k0_{-k}\rangle = |0_k0_{-k}\rangle
\]
The correspondence to the pseudo-spin picture can be made by noting

\[ |1_k 1_{-k}\rangle \Leftrightarrow |\downarrow\rangle_k, \quad |0_k 0_{-k}\rangle \Leftrightarrow |\uparrow\rangle_k, \quad \text{and} (1 - n_k - n_{-k}) \Leftrightarrow \sigma_k^z. \]

Since \( c_k^\dagger c_{-k}^\dagger |\uparrow\rangle_k = |\downarrow\rangle_k \), \( c_k^\dagger c_{-k}^\dagger |\downarrow\rangle_k = 0 \)

\& \( c_{-k} c_k |\downarrow\rangle_k = |\uparrow\rangle_k \), \( c_{-k} c_k |\uparrow\rangle_k = 0 \), and:

\[
\sigma^- = \sigma^x - i\sigma^y = \begin{pmatrix} 0 & 0 \\ 2 & 0 \end{pmatrix}; \quad \sigma^+ = \begin{pmatrix} 0 & 2 \\ 0 & 0 \end{pmatrix}.
\]

One can identify

\[
c_k^\dagger c_{-k}^\dagger = \frac{1}{2} \sigma_k^-, \quad c_{-k} c_k = \frac{1}{2} \sigma_k^+. \]
With the above identifications, the Hamiltonian can be written as 
\[ \mathcal{H} = -\sum_k \epsilon_k^0 \sigma_k^z - \frac{1}{4} V \sum_{kk'} \sigma_{k'}^- \sigma_k^+. \]

Further, the term \( \sum_{kk'} (\sigma_{k'}^x \sigma_k^y - \sigma_{k'}^y \sigma_k^x) \) vanishes due to symmetric summing done over \( k \) and \( k' \).

Hence the pseudo-spin BCS Hamiltonian reads
\[ \mathcal{H} = -\sum_k \epsilon_k^0 \sigma_k^z - \frac{1}{4} V \sum_{kk'} (\sigma_{k'}^x \sigma_k^x + \sigma_{k'}^y \sigma_k^y). \]

As before, the Hamiltonian can be written as
\[ \mathcal{H} = -\sum_k \vec{h}_k \cdot \vec{\sigma}_k, \text{ with } \vec{h}_k = \epsilon_k^0 \hat{z} + \frac{1}{2} V \sum_{k'} (\langle \sigma_{k'}^x \rangle \hat{x} + \langle \sigma_{k'}^y \rangle \hat{y}) \]

Using \( \langle \sigma_k^x \rangle = \langle \sigma_k^y \rangle \),
\[ \vec{h}_k = \epsilon_k^0 \hat{z} + \frac{1}{2} V \sum_{k'} \langle \sigma_{k'}^x \rangle \hat{x} \]

If
\[ \tan \theta_k = \frac{h_k^x}{h_k^z} = \frac{1}{2} V \sum_{k'} \langle \sigma_{k'}^x \rangle \langle \sigma_{k'}^0 \rangle \equiv \frac{\Delta}{\epsilon_k^0} \]

then \( \sin \theta_k = \frac{\Delta}{\sqrt{\Delta^2 + \epsilon_k^0}} \) and \( \cos \theta_k = \frac{\epsilon_k^0}{\sqrt{\Delta^2 + \epsilon_k^0}}. \)
BCS theory: Excitation spectra at $T = 0$

- $\Delta = \frac{1}{2} V \sum_{k'} \langle \sigma^x_{k'} \rangle = \frac{1}{2} V \sum_{k'} \sin \theta_{k'} = \frac{1}{2} \sum_{k'} \frac{\Delta}{\sqrt{\Delta^2 + \epsilon^2_{k'}}}$.

- With $\rho_F$ as the density of states near the Fermi level, the above equation gives

$$1 = \frac{1}{2} V \rho_F \int_{-\omega_D}^{\omega_D} \frac{d\epsilon}{\sqrt{\Delta^2 + \epsilon^2}} = V \rho_F \sinh^{-1}(\omega_D/\Delta).$$

Here $\omega_D$ is Debye frequency.

- Thus $\Delta = \Delta(T = 0) = \frac{\omega_D}{\sinh(1/V \rho_F)} \approx 2 \omega_D e^{-1/V \rho_F}$, (if $\rho_F V << 1$)

- At first approximation, the excitation spectrum is obtained as the energy $\epsilon_k$ to reverse a pseudo-spin in the field $\tilde{h}_k$, i.e.,

$$\epsilon_k = 2 |\tilde{h}_k| = 2 (\epsilon^2_k + \Delta^2)^{1/2}.$$ Minimum excitation energy is $2\Delta$, i.e. $\Delta$ gives the energy gap in the excitation spectrum.
For $T = 0$, $\langle \sigma^z_k \rangle = \tanh \left( \beta |\vec{h}_k| \right)$.

Hence, $\tan \theta_k = \frac{h^x_k}{h^z_k} = \frac{V}{2\epsilon^0_k} \sum_k \langle \sigma^z_k \rangle$

$= \left( \frac{V}{2\epsilon^0_k} \right) \sum_{k'} \tanh \left( \beta |\vec{h}_{k'}| \right) \sin \theta_{k'} \equiv \frac{\Delta(T)}{\epsilon_k}$.

The superconducting transition is characterised by vanishing of the gap $\Delta$. Hence, as $T \to T_c$, $\Delta \to 0$.

Hence: $1 = \frac{V}{2} \sum_{k'} \frac{1}{\epsilon_{k'}} \tanh \left( \frac{\epsilon^0_{k'}}{T_c} \right)$ or,

$\frac{2}{V\rho_F} = \int_{-\omega_D}^{\omega_D} \frac{d\epsilon}{\epsilon} \tanh \left( \frac{\epsilon}{2T_c} \right) = 2 \int_0^{\omega_D/2T_c} \frac{\tanh x}{x} dx$.

Solution: $T_c = 1.14 \omega_D e^{-1/V\rho_F} \Rightarrow 2\Delta(T = 0) \approx 3.5 T_c$.

This is consistent with experimental results for a number of materials (ex: Al, Pb, Cd).
Real space block renormalization can be applied to transverse Ising chain.

Consider the 1D Hamiltonian

\[
\mathcal{H} = -\Gamma \sum_{i=1}^{N} \sigma_i^z - J \sum_{i=1}^{N-1} \sigma_i^x \sigma_{i+1}^x \\
= \mathcal{H}_B + \mathcal{H}_{IB} \quad \text{(say)}.
\]

Here

\[
\mathcal{H}_B = \sum_{p=1}^{N/b} \mathcal{H}_p \quad ; \quad \mathcal{H}_p = -\Gamma \sigma_{i,p}^z \sum_{i=1}^{b} \Gamma \sigma_{i,p}^z - \sum_{i=1}^{b-1} J \sigma_{i,p}^x \sigma_{i+1,p}^x
\]

and \( \mathcal{H}_{IB} = \sum_{p=1}^{N/(b-1)} \mathcal{H}_{p,p+1} \quad ; \quad \mathcal{H}_{p,p+1} = -J \sigma_{b,p}^x \sigma_{1,p+1}^x. \)
The above rearrangement of the Hamiltonian recasts the picture of $N$ spins with nearest-neighbour interaction into one in which there are $N/(b - 1)$ blocks, each consisting of $b$ number of spins.

Consider $b = 2$:

The 4 eigen states of $\mathcal{H}_p$ can be expressed as the linear combinations of the eigen states of $\sigma^z_{1,p} \otimes \sigma^z_{2,p}$; namely, $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$, $|\uparrow\downarrow\rangle$, and $|\downarrow\uparrow\rangle$. 
The (orthonormal) eigen states of $\mathcal{H}_P$ are:

\begin{align*}
|0\rangle &= \frac{1}{\sqrt{1 + a^2}} (|\uparrow\uparrow\rangle + a|\downarrow\downarrow\rangle)
\quad |1\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)
\quad |2\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)
\quad |3\rangle = \frac{1}{\sqrt{1 + a^2}} (a|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle).
\end{align*}

Check: $\mathcal{H}_P |0\rangle = -(2\Gamma + Ja) \frac{1}{\sqrt{1 + a^2}} [ |\uparrow\uparrow\rangle + \left(-\frac{2\Gamma - J/a}{2\Gamma + Ja}\right) a|\downarrow\downarrow\rangle]$

$\Rightarrow \frac{2\Gamma - J/a}{2\Gamma + Ja} = -1 \Rightarrow a = \frac{\sqrt{4\Gamma^2 + J^2} - 2\Gamma}{J}.$
\[ \mathcal{H}_p |0\rangle = E_0 |0\rangle, \quad E_0 = -\sqrt{4\Gamma^2 + J^2} \]
\[ \mathcal{H}_p |1\rangle = E_1 |1\rangle, \quad E_1 = -J \]
\[ \mathcal{H}_p |2\rangle = E_2 |2\rangle, \quad E_2 = +J \]
\[ \mathcal{H}_p |3\rangle = E_3 |3\rangle, \quad E_3 = +\sqrt{4\Gamma^2 + J^2}. \]

We take \(|0\rangle\) and \(|1\rangle\) as the renormalized eigen states of the renormalized spins \(\sigma'\) where \(\langle 0 | \sigma'^x | 1 \rangle = \frac{1+a}{\sqrt{2(1+a^2)}}\), giving

\[ J' = J \frac{(1+a)^2}{2(1+a^2)}. \]

Since \(E_1 - E_0 = 2\Gamma'\) (was \(2\Gamma\) for unrenormalized state)
\[ \Gamma' = \frac{J}{2} [\sqrt{4\lambda^2 + 1} + 1] \]

The fixed points of the recurrence relations are \(\lambda^* = 0\)
\[ \lambda^* \rightarrow \infty \quad \text{and} \quad \lambda^* \simeq 1.277 \text{ with } \lambda = \frac{\Gamma}{J} \]
If correlation length $\xi \sim (\lambda - \lambda_c)^{-\nu}$, then in the renormalized system $\xi' \sim (\lambda' - \lambda_c)^{-\nu}$.

$$\frac{\xi'}{\xi} = b = \left( \frac{\lambda' - \lambda_c}{\lambda - \lambda_c} \right)^{-\nu} \Rightarrow \frac{d\lambda'}{d\lambda} \bigg|_{\lambda = \lambda_c \equiv \lambda^*} = b^{-1/\nu} \Rightarrow \nu \approx 1.47$$

(compare with 2d exact result $\nu = 1$).

Similarly, $z \approx 0.55$ (compare with $z = 1$ in 2d) and $s = \nu z \approx 0.81$ (compare with $s = 1$ for 2d).

Results improve rapidly for larger $b$ values.
Suzuki-Trotter formalism is essentially a method to transform a $d$-dimensional quantum Hamiltonian into a $(d+1)$-dimensional effective classical Hamiltonian giving the same canonical partition function.

Consider the Hamiltonian

$$\mathcal{H} = -\Gamma \sum_{i=1}^{N} \sigma_i^x - \sum_{(i,j)} J_{ij} \sigma_i^z \sigma_j^z$$

$$\equiv \mathcal{H}_0 + \mathcal{V}$$

Trotter formula:

$$\exp (A_1 + A_2) = \lim_{M \to \infty} [\exp A_1 / M \exp A_2 / M]^M$$

Partition function $Z = \text{Tr} e^{-\beta \mathcal{H}}$

$$\lim_{M \to \infty} \text{Tr} \prod_{k=1}^{M} \langle \sigma_1,k ... \sigma_N,k | \exp \left( -\frac{\beta \mathcal{H}_0}{M} \right) \exp \left( -\frac{\beta \mathcal{V}}{M} \right) | \sigma_1,k ... \sigma_N,k \rangle.$$
Now \( \prod_{k=1}^{M} \langle \sigma_{1,k} \cdots \sigma_{N,k} | \exp \left( \frac{\beta}{M} \sum_{i,j} \sigma_i^z \sigma_j^z \right) | \sigma_{1,k+1} \cdots \sigma_{N,k+1} \rangle = \exp \left[ \sum_{i,j=1}^{N} \sum_{k=1}^{M} \frac{\beta J_{ij}}{M} \sigma_{i,k} \sigma_{j,k} \right] \)

Also,

\[
\prod_{k=1}^{M} \langle \sigma_{1,k} \cdots \sigma_{N,k} | \exp \left[ \frac{\beta M}{\sigma_i^x} \sum_{i} \sigma_i^x \right] | \sigma_{1,k+1} \cdots \sigma_{N,k+1} \rangle
\]

\[
= \left( \frac{1}{2} \sinh \left[ \frac{2 \beta M}{\sigma_i^x} \right] \right)^{\frac{NM}{2}} \exp \left[ \frac{1}{2} \ln \coth \left( \frac{\beta M}{\sigma_i^x} \right) \sum_{i=1}^{N} \sum_{k=1}^{M} \sigma_{i,k} \sigma_{i,k+1} \right].
\]

since: \( e^{a \sigma^x} = e^{-i(a \sigma^x)} = \cos (i a \sigma^x) - i \sin (i a \sigma^x) = \cosh (a) + \sigma^x \sinh (a) \), \( \Rightarrow \)

\[
\langle \sigma | e^{a \sigma^x} | \sigma' \rangle = \left( \frac{1}{2} \sinh (2a) \right)^{1/2} \exp \left[ (\sigma \sigma' / 2) \ln \coth (a) \right],
\]
since $\langle \uparrow | e^{a\sigma^x} | \uparrow \rangle = \langle \downarrow | e^{a\sigma^x} | \downarrow \rangle = \cosh (a) = \left[ \frac{1}{2} \sinh (2a) \cdot \coth (a) \right]^{1/2}$ and $\langle \uparrow | e^{a\sigma^x} | \downarrow \rangle = \langle \downarrow | e^{a\sigma^x} | \uparrow \rangle = \sinh (a) = \left[ \frac{1}{2} \sinh (2a) / \coth (a) \right]^{1/2}$.

Thus the partition function reads

$$Z = C \frac{N M}{2} \text{Tr}_\sigma (-\beta \mathcal{H}_{\text{eff}}[\sigma]) \quad ; \quad C = \frac{1}{2} \sinh \frac{2\beta \Gamma}{M}$$

Where the effective classical Hamiltonian is

$$\mathcal{H}_{\text{eff}}(\sigma) = \sum_{(i,j)}^{N} \sum_{k=1}^{M} \left[ - \frac{J_{ij}}{M} \sigma_{ik} \sigma_{jk} - \frac{\delta_{ij}}{2\beta} \ln \coth \left( \frac{\beta \Gamma}{M} \right) \sigma_{ik} \sigma_{ik+1} \right].$$
The Hamiltonian $\mathcal{H}_{\text{eff}}$ is a classical one, since the variables $\sigma_{i,k}$'s involved are merely the eigen-values of $\sigma^z$, and hence there is no non-commuting part in $\mathcal{H}_{\text{eff}}$.

$M$ should be at the order of $\hbar \beta$ (we have taken $\hbar = 1$ in the calculation) for a meaningful comparison of the interaction in the Trotter direction with that in the original Hamiltonian.
References

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