

Title: Statistical Physics Lecture - 121123

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Quantum Statistics and Quantum Phase transitions

Back to the millions of equations...

- N identical systems $N \rightarrow \infty$

- defined by Hamiltonian \hat{H}

systems will have wavefunctions

$$|\psi_{\vec{r}_i}^k\rangle$$

k th system
of the N systems

Schrödinger Equations:

$$\hat{H} |\Psi^k(\vec{r}, t)\rangle = i\hbar \frac{d}{dt} |\Psi^k(\vec{r}, t)\rangle$$

New basis:

$$|\Psi^k(\vec{r}, t)\rangle = \sum_n a_n^k(t) |\phi_n^k(\vec{r})\rangle$$

$$a_n^k(t) = \int \langle \phi_n^k | \Psi^k(\vec{r}, t) \rangle d\tau$$

complete set
of orthonormal
functions

volume
element
of coord
space

$a_n^k(t)$ can fully describe
the system state

From here we can get: (see notes)

$$i\hbar \dot{a}_n^k(t) = \sum_m H_{nm} a_m^k(t)$$

with $H_{nm} = \int \langle \phi_n | \hat{H} | \phi_m \rangle d\tau$

$a_n^k(t)$ are the probability amplitudes for states $|\phi_n^k(t)\rangle$. prob: $|a_n^k(t)|^2$

$$\sum_n |a_n^k(t)|^2 = 1$$

Now we define a density matrix:

$$\rho_{mn}(t) = \frac{1}{N} \sum_{k=1}^N \{ a_m^k(t) a_n^k(t) \}$$

$\rho_{nn}(t)$ is the ensemble average of the probability $|a_n^k(t)|^2$

- double averaging

↳ statistical - from the ensemble

↳ probabilistic from wavefunction

prob. of being in state $|Y\rangle$

given state $|Y\rangle$, prob. of
being in state $|\phi\rangle$

↑ quantum
fluctuation

$a_n(t)$ can fully describe the system state of config space

Now we define a density matrix:

$$\rho_{mn}(t) = \frac{1}{N} \sum_{k=1}^N \{ a_m^k(t) a_n^{k*}(t) \}$$

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- $\rho_{nn}^{(t)}$ is the probability that a system, chosen at random from an ensemble at time t , is found in state ϕ_n .

$$\sum_n \rho_{nn} = 1 \quad [\text{Tr}(\rho) = 1]$$

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$$\sum_n \rho_{nn} = 1 \quad [\text{Tr}(\rho) = 1]$$

Now
 $i\hbar \dot{\rho}_{mn}(t)$

Density matrix in operator form

$$\hat{\rho} = \sum_{m,n} \rho_{mn} |\phi_m\rangle\langle\phi_n|$$

$$i\hbar \dot{\hat{\rho}} =$$

probabilistic from wavefunction

being in state

Now

$$i\hbar \dot{\rho}_{mn}(t) = \frac{1}{N} \sum_{k=1}^N \left[i\hbar \left(\dot{a}_m^k(t) a_n^{k*}(t) + a_m^k(t) \dot{a}_n^{k*}(t) \right) \right]$$

Schrödinger $\rightarrow H a$

matrix in
1st form

$$= \frac{1}{N} \sum_{k=1}^N \sum_{\ell} \left[H_{m\ell} a_{\ell}^k(t) a_n^{k*}(t) - a_m^k(t) H_{n\ell}^* a_{\ell}^{k*}(t) \right]$$

$$\sum_{m,n} \rho_{mn} |\phi_m\rangle\langle\phi_n| = \sum_{\ell} \left[H_{m\ell} \rho_{\ell n}(t) - \rho_{m\ell}(t) H_{n\ell}^* \right]$$

$$= (\hat{H}\hat{\rho} - \hat{\rho}\hat{H})_{mn}$$

$i\hbar \dot{\hat{\rho}} = [\hat{H}, \hat{\rho}]$

\leftarrow von Heisenberg equation

For equilibrium, $\dot{\rho}_{mn} = 0$

$$i\hbar \dot{\hat{\rho}} = [\hat{H}, \hat{\rho}]$$

$\therefore \hat{\rho}$ must be a function of \hat{H}

$$\hat{\rho} = f(\hat{H})$$

Now if ϕ_n are eigenfunctions of \hat{H} , then

$$H_{mn} = E_n \delta_{mn}, \quad \rho_{mn} = \rho_n \delta_{mn}$$

$$\hat{\rho} = \sum_n \rho_n |\phi_n\rangle \langle \phi_n|$$

In general $\hat{\rho} = \sum_{m,n} \rho_{mn} |m\rangle \langle n|$

ρ_{mn} is the transition probability from state $|n\rangle$ to state $|m\rangle$ in equilibrium.

Detailed Balance:

$$\rho_{mn} = \rho_{nm}$$

Expectation values:

$$\langle G \rangle = \frac{1}{N} \sum_{k=1}^N \int \psi^k \hat{G} \psi^k d\tau = \frac{1}{N} \sum_{k=1}^N \left[\sum_{m,n} a_n^{k*} a_m^k G_{nm} \right]$$

$$\rightarrow \langle G \rangle = \sum_{m,n} \rho_{mn} G_{nm} = \text{Tr}(\hat{\rho} \hat{G})$$

unnormalized:

$$\langle G \rangle = \frac{\text{Tr}(\hat{\rho} \hat{G})}{\text{Tr}(\hat{\rho})}$$

← unnormalized

Ensembles

Microcanonical: N, V , fixed

E within $E - \frac{1}{2}\Delta, E + \frac{1}{2}\Delta$

total # of microstates: $\Gamma(N, V, E, \Delta)$

$$P_{mn} = P_n \delta_{mn}$$

$$\left\{ \begin{array}{l} P_n = \frac{1}{\Gamma} \text{ for relevant states} \\ 0 \text{ for all others} \end{array} \right.$$

Δ $\boxed{\rho = 1}$ pure state
 $\therefore \rho^2 = \rho$ because $1^2 = 1, 0^2 = 0$
 $\text{Tr}(\rho^2) = \text{Tr}(\rho) = 1$ for normalized

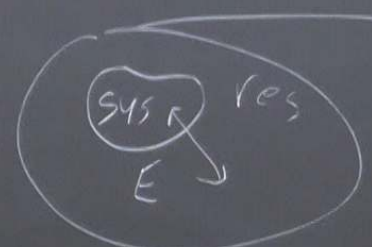
Second Assumption
 - random a priori phases
 for a_n^k

$\boxed{\rho \neq 1}$ we have a mixed state

$$\rho_{mn} = \frac{1}{N} \sum_{k=1}^N a_m^k a_n^k = \frac{1}{N} \sum_{k=1}^N |a|^2 e^{i(\theta_m^k - \theta_n^k)}$$
 equal a priori probabilities
 $= c \langle e^{i(\theta_m - \theta_n)} \rangle$
 $= c \delta_{mn}$

Canonical Ensemble

$\neq G_{nm}$



N, V, T define macrostate

$p_n = C e^{-\beta E_n}$, and $C = \frac{1}{\sum_n e^{-\beta E_n}}$

$$\hat{\rho} = \frac{e^{-\beta \hat{H}}}{\text{Tr}(e^{-\beta \hat{H}})}$$

$$\langle \hat{O} \rangle = \frac{\text{Tr}_N(\hat{O} e^{-\beta \hat{H}})}{\text{Tr}_N(e^{-\beta \hat{H}})}$$

$$e^{-\beta \hat{H}} = \sum_j (-1)^j \frac{(\beta \hat{H})^j}{j!}$$

Grand Canonical Ensemble

N and E can vary.

$$[\hat{H}, \hat{\rho}] = 0, [\hat{N}, \hat{\rho}] = 0$$

$$\langle \hat{O} \rangle = \frac{\text{Tr}(\hat{O} e^{-\beta \hat{H} + \beta \mu \hat{N}})}{\text{Tr}(e^{-\beta \hat{H} + \beta \mu \hat{N}})}$$

can/
↑ some
basis

te \ln
equilibrium.

Quantum Statistics and Quantum Phase transitions

- Occur at zero temperature
- their origin is due to quantum fluctuations

Consider

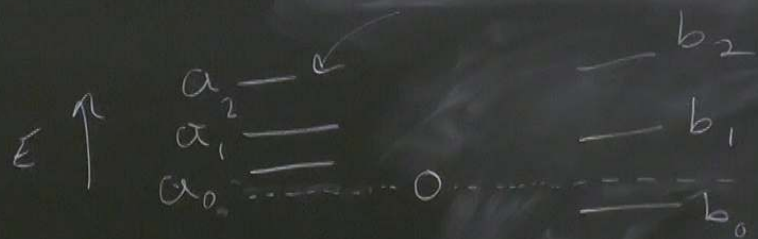
$$\hat{H}(g)$$

↑ coupling

- We can get a nonanalytic ground state energy in a simple way if

$$\hat{H}(g) = \hat{H}_0 + g\hat{H}_1 \quad \text{and} \quad [\hat{H}_0, \hat{H}_1] = 0$$

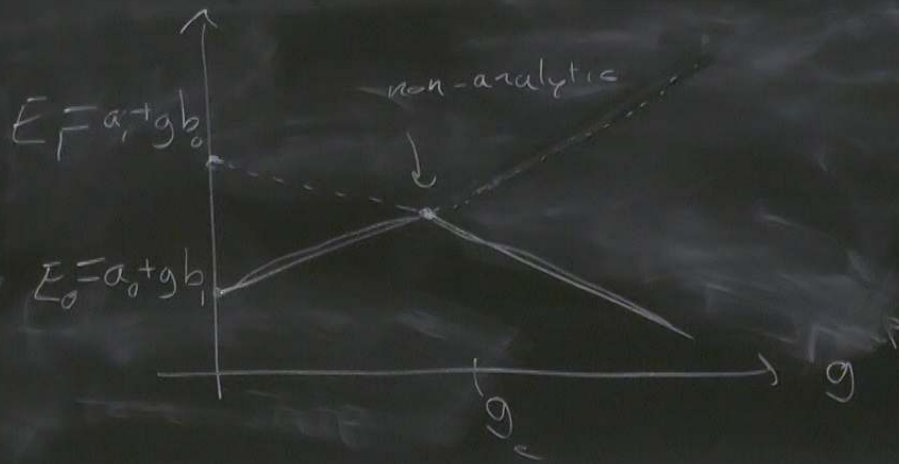
$$\hat{H} = \hat{H}_0 + g \hat{H}_1$$



Suppose we have $|\psi_0\rangle, |\psi_1\rangle$

such that $\hat{H}_0 |\psi_0\rangle = a_0 |\psi_0\rangle, \hat{H}_1 |\psi_0\rangle = b_1 |\psi_0\rangle$

$\hat{H}_0 |\psi_1\rangle = a_1 |\psi_1\rangle, \hat{H}_1 |\psi_1\rangle = b_0 |\psi_1\rangle$

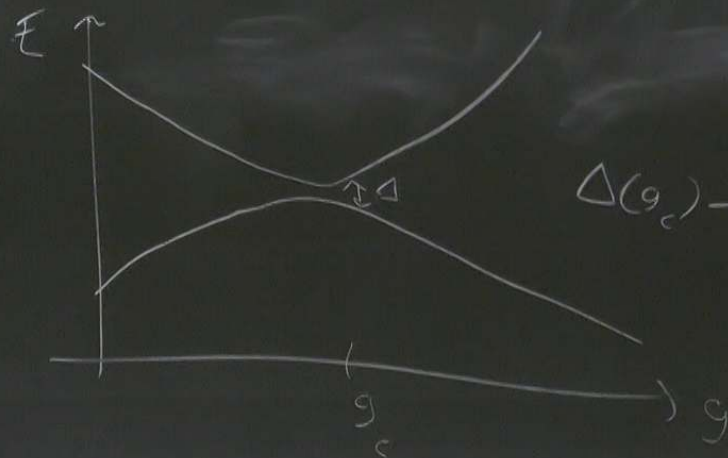


energy in a simple way if

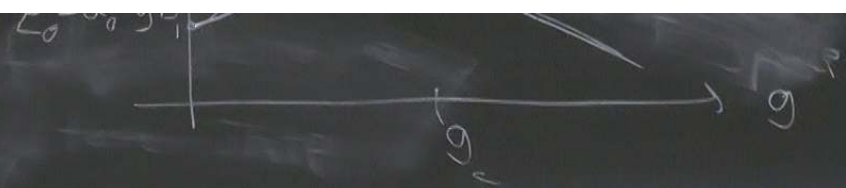
$$\hat{H}(g) = \hat{H}_0 + g\hat{H}_1 \quad \text{and} \quad [\hat{H}_0, \hat{H}_1] = 0$$

- This is a level crossing and
can happen for finite N sites

- We can also set an avoided level crossing.



$$\Delta(g_c) \rightarrow 0 \quad \text{as} \quad N \rightarrow \infty$$



In both cases we have

$$\Delta \sim |g - g_c|^{-z\nu}$$

dynamical critical exponent

(1 for relativistic phase transitions, $E \sim p$)

- The correlation length

$$\xi \sim |g - g_c|^{-\nu}$$

- other critical exponents:

replace t with $|g - g_c|$



Quantum - Classical Mapping

Transverse-field Ising Model:

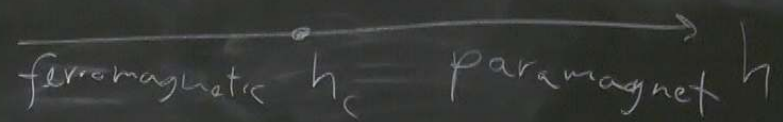
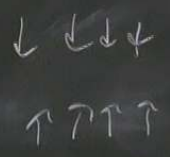
$$\hat{H} = -J \sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - h \sum_i \hat{\sigma}_i^x$$

↙ external magnetic field

$$H = \sum_i \hat{\sigma}_i^x$$

$$\prod_i (\hat{\sigma}_i^z - \hat{1})$$

T=0



replace t with $(g-g_c)$

$$Z = \text{Tr}(e^{-\beta \hat{H}}) \\ = \sum_{\sigma} \langle \sigma | e^{-\beta \hat{H}} | \sigma \rangle$$

$$\sigma = \{\sigma_1, \sigma_2, \dots, \sigma_N\}$$

measured in
the z -basis

$$\sigma_i = \pm 1$$

$$e^{-\beta \hat{H}} = (e^{-\varepsilon \hat{H}})^N$$

$$= \sum_{\{\sigma\}} \langle \sigma | e^{-\varepsilon \hat{H}} | \sigma_1 \rangle \langle \sigma_1 | e^{-\varepsilon \hat{H}} | \sigma_2 \rangle \langle \sigma_2 | \dots \langle \sigma_{N-1} | e^{-\varepsilon \hat{H}} | \sigma \rangle$$

$$\varepsilon N = \beta$$

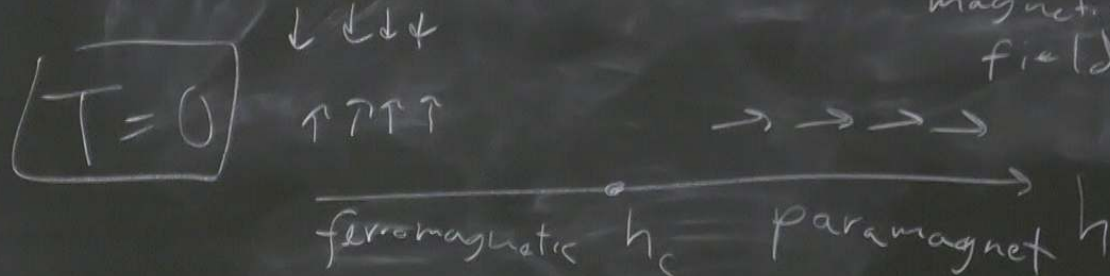
$$\langle \sigma_\tau | e^{-\varepsilon \hat{H}} | \sigma_{\tau+1} \rangle$$

Quantum - Classical Mapping

Transverse-field Ising Model:

$$\hat{H} = -J \sum_{\langle ij \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - h \sum_i \hat{\sigma}_i^x$$

← external magnetic field



$$\hat{H}' = \sum_i \hat{\sigma}_i^x$$

$$\hat{\sigma}_i^x = \frac{1}{2}(\hat{\sigma}_i^+ + \hat{\sigma}_i^-)$$

$$\hat{\sigma}_i^x = (\hat{\sigma}_i^+ + \hat{\sigma}_i^-) \frac{1}{2}$$

$$= \sum_{\sigma} \Lambda e^{\epsilon J \sum \sigma_{i,T} \sigma_{i+1,T} + \gamma (\sigma_{i,T} \sigma_{i,T} + \sigma_{i,T+1} \sigma_{i,T})}$$

$$\Lambda^2 = \sinh(\epsilon h) \cosh(\epsilon h)$$

$$\gamma = -\frac{1}{2} \ln[\tanh(\epsilon h)]$$

$$Z = \Lambda^N \sum_{\{\sigma(i,\tau)\}} e^{-\beta E(\{\sigma(i,\tau)\}, h)}$$

$$E(\sigma_{i,T}, \sigma_{i+1,T}) = -J \sum_{\langle i,j \rangle} \sigma_{i,T} \sigma_{j,T} - \gamma(h) \sum_i \sigma_{i,T} \sigma_{i,T+1}$$

$$E(\sigma_i, \sigma_{i+1}) = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j - \gamma(h) \sum_i \sigma_i \sigma_{i+1}$$

↑ anisotropic Ising model
 h plays the role of a
 new "temperature"

Consequences

- The quantum phase transition for transverse-field Ising model in D -dimensions is in the same universality class as the finite- T phase transition for the Ising model in $D+1$ dimensions!
- Mermin-Wagner says no long-range order for $D \leq 1$ for quantum systems with continuous symmetries.

↑ anisotropy
in plane