Title: Statistical Physics Lecture - 121123

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Quantum Statistics and Quantum Phase transitions

Back to the millions of equations...

- $\mathcal{N}$ identical systems $\mathcal{N} >> 1$
- defined by Hamiltonian $\hat{H}$

systems will have wavefunctions $|\Psi^k(\vec{r},t)\rangle$

kth system of the $\mathcal{N}$ systems

Schrödinger Equations:

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

New basis:

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

complete set of orthonormal functions

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

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 propability 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 <u>density matrix</u>:

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

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

- double averaging
  - ↳ statistical — from the ensemble ↖ prob. of being in state $|\psi\rangle$
  - ↳ probabilistic from wavefunction ↖ given state $|\psi\rangle$, prob. of being in state $|\phi\rangle$ ↑ quantum fluctuation

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

of ... space

Now we define a density matrix:

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

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

- double averaging

↳ statistical – from the ensemble — prob. of being in state $|\psi\rangle$

↳ probabilistic from wavefunction — given state $|\psi\rangle$, prob. of being in state $|\phi\rangle$ — quantum fluctuation

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

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

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

Density matrix in operator form

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

Now:

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

$=$

$=$

$=$

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

$\Rightarrow$ probabilistic from wavefunction being in sta

Now:

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

Schrödinger $\rightarrow$ Ha

matrix in ...tor form

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

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

$$= \sum_{\ell}\left[H_{m\ell}\,\rho_{\ell n}(t) - \rho_{m\ell}(t)\,H_{n\ell}^*\right]$$

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

$$\boxed{i\hbar\dot{\hat{\rho}} = [\hat{H}, \hat{\rho}]}$$ $\leftarrow$ von Neumann 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 ge

$\hat{H}$.

$\hat{H}$, then

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

some basis

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

Detailed Balance:

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

Expectation values:

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

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

unnormalized

unnormalized:

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

Ensembles:

Microcanonical: N, V, fixed $\quad E$ within $E-\frac{1}{2}\Delta, E+\frac{1}{2}\Delta$

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

$$\rho_{mn} = \rho_n \delta_{mn}$$

$$\rho_n = \begin{cases} \frac{1}{\Gamma} & \text{for relevant states} \\ 0 & \text{for all others} \end{cases}$$

$\boxed{\Gamma = 1}$ pure state

$\therefore \rho^2 = \rho$ because $1^2 = 1,\ 0^2 = 0$

$Tr(\rho^2) = Tr(\rho) = 1$ for normalized ρ

$\boxed{\Gamma > 1}$ 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 probabilites

$$= c\langle e^{i(\theta_m^k - \theta_n^k)} \rangle$$

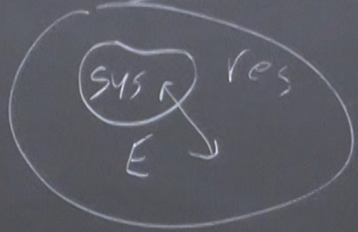
$$= c\,\delta_{mn}$$

Second Assumption

- random a priori phases for a_n^k

$a_m^* G_{nm} \Big]$

Canonical Ensemble



N, V, T define macrostate

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

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

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

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

$\rho c_n|$

some basis

te $|n\rangle$

equilibrium.

Grand Canonical Ensemble

N and E can vary.

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

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

Quantum Statistics and Quantum Phase transitions

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

Consider

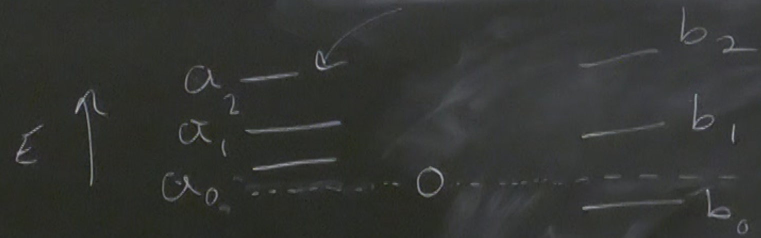
$$\hat{H}(g)$$

coupling

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

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

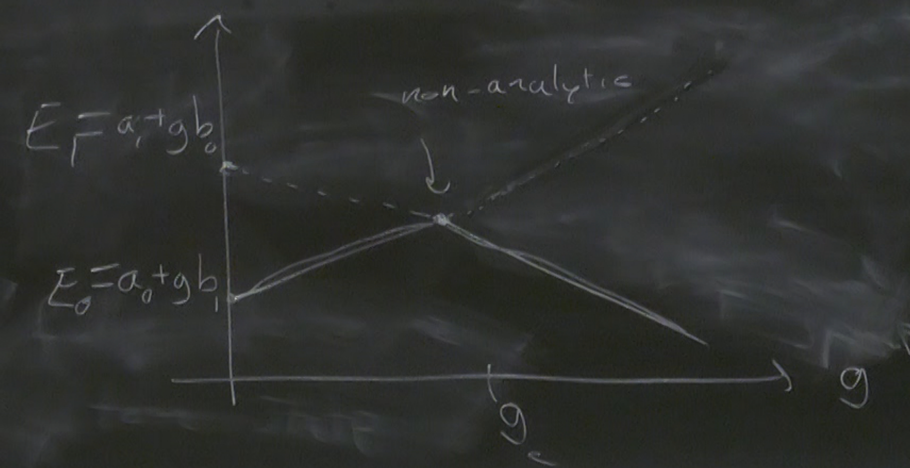
$$\hat{H} = \hat{H}_0 + g\hat{H}_1$$



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

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

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

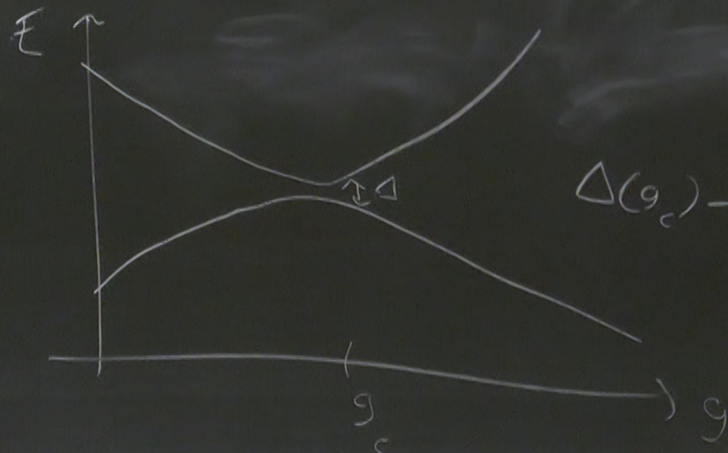


energy in a simple way if

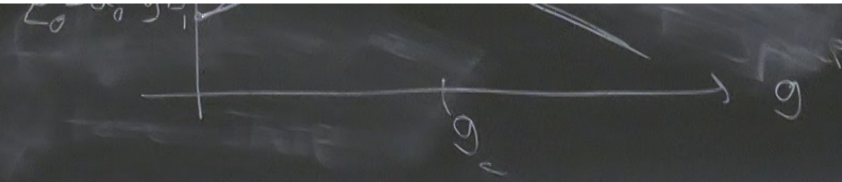
$$\hat{H}(g) = \hat{H}_0 + g\hat{H}_1 \quad \text{and} \quad [\hat{H}_0, \hat{H}_1] = 0$$

- This is a <u>level crossing</u> and can happen for finite N sites
- We can also get an <u>avoided level crossing</u>.

In



$\Delta(g_c) \to 0$ as $N \to \infty$



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 $|g-g_c|$

g_c g

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

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

$\prod_i (|\uparrow\rangle_i - |\downarrow\rangle_i)$

$\boxed{T=0}$

$\downarrow\downarrow\downarrow\downarrow$

$\uparrow\uparrow\uparrow\uparrow$ $\rightarrow\rightarrow\rightarrow\rightarrow$

ferromagnetic h_c paramagnet h

replace t with $|g-g_c|$

$$Z = \mathrm{Tr}\left(e^{-\beta \hat{H}}\right)$$

$$= \sum_{\sigma} \langle \sigma | e^{-\beta \hat{H}} | \sigma \rangle$$

$\sigma = \{\sigma_1, \sigma_2, \dots \sigma_N\}$ measured in the z-basis

$\sigma_i = \pm 1$

$$e^{-\beta \hat{H}} \simeq \left(e^{-\varepsilon \hat{H}}\right)^{N}$$

$\varepsilon N_\tau = \beta$

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

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

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

$$H' = \sum_i \sigma_i^x$$

$$\prod_i \left(|\uparrow\rangle_i - |\downarrow\rangle_i\right)$$

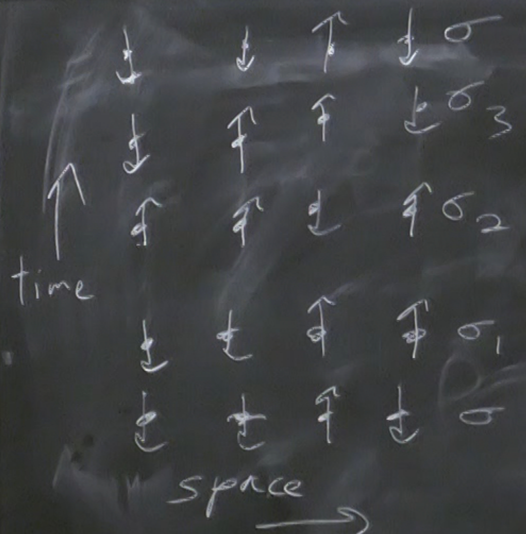
$\boxed{T=0}$

$\downarrow\downarrow\downarrow\downarrow$

$\uparrow\uparrow\uparrow\uparrow$ $\rightarrow\rightarrow\rightarrow\rightarrow$

ferromagnetic h_c paramagnet h

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

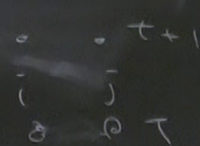


$$\langle \sigma_\tau | e^{-\varepsilon \hat{A}} | \sigma_{\tau+1} \rangle$$

$$\mathbb{1} - \varepsilon \hat{A}$$

— matrix elements connecting sites in time as well as space

$$\sum_{\substack{\sigma_{i,\tau},\sigma_{j,\tau} \\ \sigma_{i,\tau+1},\sigma_{j,\tau+1}}} \langle \sigma_{i,\tau}\sigma_{j,\tau} | e^{\varepsilon J \hat{\sigma}_i^z \hat{\sigma}_j^z + \varepsilon h(\hat{\sigma}_i^x + \hat{\sigma}_j^x)} | \sigma_{i,\tau+1}\sigma_{j,\tau+1} \rangle$$



$$= \sum_{\sigma} \Lambda e^{\varepsilon J \sigma_{i,\tau}\sigma_{j,\tau} + \gamma\left(\sigma_{i,\tau+1}\sigma_{i,\tau} + \sigma_{j,\tau+1}\sigma_{j,\tau}\right)}$$

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

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

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

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

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

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.

anisotro

h pla