Computer modeling of physical phenomena: quantum Monte Carlo

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Plan

1. Quantum model of a magnet
2. Representation of spin models in imaginary time
3. Quantum phase transition (QPT)

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Quantum model of a magnet

- Spin operators
- Ising model in a transversal magnetic field (TFIM)
- Thermodynamic averages for a quantum system

Spin in quantum mechanics

Spin

hermitian operator ≡ observable

analogous to angular momentum:

$[\hat{S}_i, \hat{S}_j] = i\hbar \varepsilon_{ijk} S_k$ for $i, j, k = x, y, z$

... comm. relations enough to define

explicit matrix form for $s = \hbar/2$ spin

$\hat{S}_x = \frac{\hbar}{2}\sigma_x$, $\hat{S}_y = \frac{\hbar}{2}\sigma_y$, $\hat{S}_z = \frac{\hbar}{2}\sigma_z$

in $|\Uparrow\rangle$, $|\Downarrow\rangle$ – eigenbasis of $\hat{S}_z$

Spin in quantum mechanics

- matrix representation for spin $1/2$

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \; \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \; \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

- states as vectors

$$|+1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \; |-1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Transversal field Ising model

We consider a 1D chain of quantum spins

$$\mathcal{H} = H_0 + H_1, \quad H_0 = -J \sum_i \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z, \quad H_1 = -h \sum_i \hat{\sigma}_i^x.$$

- z axis determined e.g. by crystal anisotropy
- magnetic field acts to “flip” magnetization direction
- build-in competition (no common eigenbasis)
- parameters of the model: β, h, J

Thermodynamic averages for a quantum system

- how to sum over configurations?
- we use the energy eigenbasis

$$\langle Q\rangle = \frac{1}{Z}\sum_n \langle n|\hat{Q}|n\rangle e^{-\beta E_n} = \frac{1}{Z}\mathrm{Tr}\left(\hat{Q}e^{-\beta\mathcal{H}}\right)$$

- but well ... we do not (usually) know $E_n, |n\rangle$

Basis states

- basis state vector $|\uparrow,\uparrow,\downarrow,\uparrow,\ldots\rangle = |+1,+1,-1,+1,\ldots\rangle$
- configuration: $\{\sigma_i\}_{i=1,\ldots,N}$ for the state $|\{\sigma_i\}\rangle$
- $\sigma_i = \pm 1$ specifies $z-$axis eigenvalue for i spin in the chain

Limiting case $h = 0$ (diagonal in spin basis)

Limiting case $h=0$

$$Z = \mathrm{Tr}\, e^{-\beta \mathcal{H}(h=0)} = \sum_{\{\sigma_i\}} \left(\prod_{i=1}^{N} \langle \sigma_i |\right) e^{\beta J \sum_i \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z} \left(\prod_{i=1}^{N} |\sigma_i\rangle\right)$$

$\{\sigma_i\}_{i=1..N}$ means all configurations; σ_i eigenvalues of $\hat{\sigma}_i^z$

$$Z = \sum_{\{\sigma_i\}} \underbrace{\left(\prod_{i=1}^{N} \langle \sigma_i |\right)\left(\prod_{i=1}^{N} |\sigma_i\rangle\right)}_{\text{normalized}} e^{\beta J \sum_i \sigma_i \sigma_{i+1}}$$

$\hat{\sigma}_i^z$ acts in eigenbasis

so $Z = \sum_{\{\sigma_i\}} e^{\beta J \sum_i \sigma_i \sigma_{i+1}}$ is just partition function of the classical 1D Ising

Exact sum for x-axis states

Limiting case $J=0$

$$Z = \mathrm{Tr}\left[e^{\beta h \sum_i \hat{\sigma}_i^x}\right] = \mathrm{Tr}\left[e^{\beta h \hat{\sigma}_1^x} e^{\beta h \hat{\sigma}_2^x} \dots\right]$$

all σ_i^x commute

$$\sum_{\{\sigma_i\}} = \left(\prod_{i=1}^{N} \langle \sigma_i |\right) e^{\beta h \hat{\sigma}_1^x} e^{\beta h \hat{\sigma}_2^x} \dots \left(\prod_{i=1}^{N} |\sigma_i\rangle\right) = \left\{\begin{matrix}\text{just}\\ \text{think}\\ \text{carefully}\end{matrix}\right\}$$

$$= \prod_{i=1}^{N} \left[\sum_{\sigma_i = \pm 1} \langle \sigma_i | e^{\beta h \hat{\sigma}_i^x} | \sigma_i \rangle\right]$$

... just separates into indep. spins as there is no interaction; $\mathrm{tr}\left[e^{\beta h \sigma_x}\right] = \mathrm{tr}\left[e^{\beta h \sigma_z}\right]$

$$= 2 \operatorname{ch} \beta h$$

So called "quantum fluctuation"

so we get $Z = (2\,\mathrm{ch}\,\beta h)^N$

... a result of N independent spin $1/2$

in the external mag. field h

SIMPLIFICATION we found in TFIM:

both $J \to 0$ && $h \to 0$ correspond to classical, simple models;

note however that $[H_0, H_1] \neq 0$;

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Character of the ground state changes as a function of h/J!

Plan

Mapping to imaginary time

- Suzuki-Trotter decomposition
- Resolution of unity
- Effective, classical model in D+1 dimensions
- Quantum phase transition

Suzuki-Trotter formula

We use $H_0 + H_1$ partition in the Suzuki – Trotter

$$e^{-\beta(H_0+H_1)} \cong \left(e^{-\beta/M\, H_0}\, e^{-\beta/M\, H_1}\right)^M$$

$\Delta\tau = \beta/M$ — imaginary time step.

$$Z_M = \mathrm{Tr}\left[e^{-\Delta\tau H_0}\, e^{-\Delta\tau H_1} \cdot \mathbb{1} \cdot e^{-\Delta\tau H_0}\, e^{-\Delta\tau H_1} \dots \right]$$

M times

we introduce $M-1$ unity resolutions:

$$\mathbb{1} = \sum_{\{\sigma_i\}} |\sigma_i\rangle\langle\sigma_i|$$

Extended configuration space

$$Z_M = \sum_{\{\sigma_i\}_1} \sum_{\{\sigma_i\}_2} \dots \sum_{\{\sigma_i\}_M}$$

← we label the config. $\{\}$ with time-step index $\ell = 1 \dots M$

$$\langle \{\sigma_i\}_1 | e^{-\Delta\tau H_0} e^{-\Delta\tau H_1} | \{\sigma_i\}_2 \rangle *$$

$$* \langle \{\sigma_i\}_2 | e^{-\Delta\tau H_0} e^{-\Delta\tau H_1} | \{\sigma_i\}_3 \rangle \dots$$

$$\dots \langle \{\sigma_i\}_M | e^{-\Delta\tau H_0} e^{-\Delta\tau H_1} | \{\sigma_i\}_1 \rangle$$

⊛ periodic b.c. in the imaginary time direction

⊛ extended configuration space $\{\sigma_{i\ell}\}$,

but with class. variables only, no operators!

Single matrix element

•)

$$\langle \{\sigma_i\}_\ell | e^{-\Delta\tau H_0} = e^{\Delta\tau J \sum_i \sigma_{i,\ell}\,\sigma_{i+1,\ell}} \langle \{\sigma_i\}_\ell |$$

H_0 eigenbasis

••)

$$\langle \{\sigma_i\}_\ell | e^{-\Delta\tau H_1} | \{\sigma_i\}_{\ell+1} \rangle = \left\{ \begin{array}{l} \text{separates with} \\ e^{h\Delta\tau \sum_i \hat{\sigma}_i^x} = \prod_i e^{h\Delta\tau \hat{\sigma}_i^x} \end{array} \right\}$$

$$= \prod_i \langle \sigma_{i,\ell} | e^{h\Delta\tau \hat{\sigma}^x} | \sigma_{i,\ell+1} \rangle$$

•••) matrix calculation

$$M_{\sigma\sigma'} = \langle \sigma | e^{h\Delta\tau \hat{\sigma}^x} | \sigma' \rangle \; ; \quad M = \begin{bmatrix} \mathrm{ch}(\Delta\tau h) & \mathrm{sh}(\Delta\tau h) \\ \mathrm{sh}(\Delta\tau h) & \mathrm{ch}(\Delta\tau h) \end{bmatrix}$$

in $\sigma, \sigma' = \pm 1$ basis.

Algebraic trick

algebraic trick $\Lambda e^{\gamma\sigma\sigma'} = \Lambda \begin{bmatrix} e^{\gamma} & e^{-\gamma} \\ e^{-\gamma} & e^{\gamma} \end{bmatrix}$ (5)

we can solve: $M_{\sigma\sigma'} = \Lambda e^{\gamma\sigma\sigma'}$

$$\Lambda e^{\gamma} = \mathrm{ch}(\Delta\tau h) \; ; \; \Lambda e^{-\gamma} = \mathrm{sh}(\Delta\tau \cdot h)$$

$$\rightarrow \Lambda^2 = \mathrm{ch}\Delta\tau h \, \mathrm{sh}\Delta\tau h \; , \; \gamma = -\tfrac{1}{2}\ln(\mathrm{th}\,\Delta\tau h)$$

with this trick we substitute $e^{h\Delta\tau\hat{\sigma}_x} \longrightarrow \Lambda e^{\gamma\hat{\sigma}_z\hat{\sigma}_z'}$

in all N factors, expression $\bullet\bullet$)

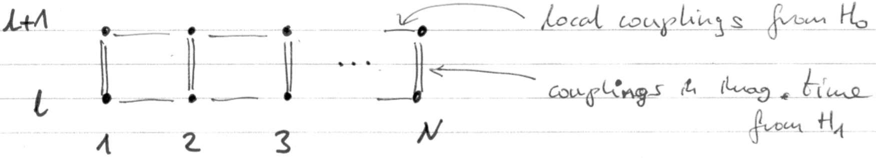
$$\langle \{\sigma_i\}_\ell | e^{-\Delta\tau H_1} | \{\sigma_i\}_{\ell+1} \rangle = \Lambda^N e^{\gamma \sum_{i=1}^{N} \sigma_{i,\ell}\, \sigma_{i,\ell+1}}$$

Effective (1+1)D model (Kogut '78)

Full partition function, which includes configurations in all imag. time slices $l = 1, \dots M$

$$Z_M = \Lambda^{NM} \sum_{\{\sigma_{il} = \pm 1\}} e^{\Delta\tau J \sum_{i,l} \sigma_{il}\sigma_{i+1\,l} + \gamma \sum_{il} \sigma_{il}\sigma_{il+1}}$$

(for all $i = 1 \dots N$, $l = 1 \dots M$)



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Critical coupling

Duality relation (known for Ising model)

$$\mathrm{sh}(2J_h\beta_a^*)\,\mathrm{sh}(2J_v\beta_a^*) = 1$$

in our effective (1+1)D model

$$\beta_a^* J_h = \Delta z\, J^* \;;\quad \beta_a^* J_v = \gamma^*$$

so $$\mathrm{sh}(2\Delta z J^*)\,\mathrm{sh}(2\gamma^*) = 1$$

with $$\gamma^* = -\tfrac{1}{2}\ln \mathrm{th}(h^*\Delta z)$$

eliminating γ^* (& some algebra) we get

$$1 = \mathrm{sh}(2\Delta z J^*)\,\frac{1}{\mathrm{sh}(2\Delta z h^*)}$$

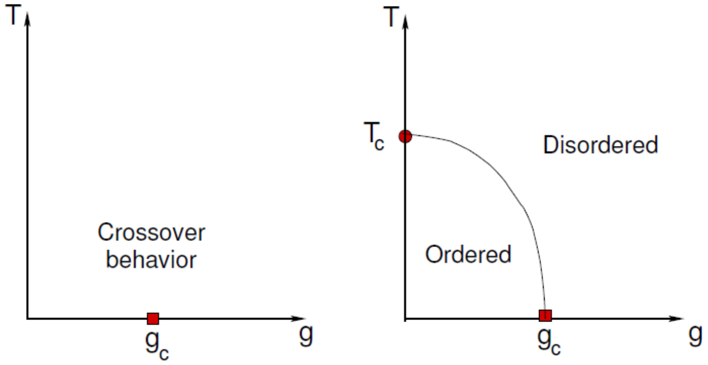
with $\Delta z \to 0$: $J^*/h^* = 1$ at criticality

Quantum phase transition

- as a function of the coupling constant $g = h/J$
- critical point $g^* = 1$
- transition at $T \to 0$

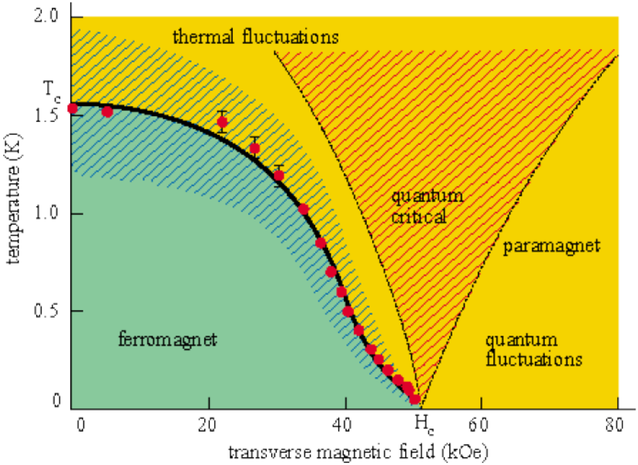
QPT diagrams: 1D and 2D TFIM

Diagrams in temperature – coupling coordinates.
The relative coupling is $g = h/J$.



QPT diagrams

Quantum criticality in a ferromagnet $LiHoF_4$ ('96 experiment)



QPT diagrams

Competing orders in superconductors (HTSC)