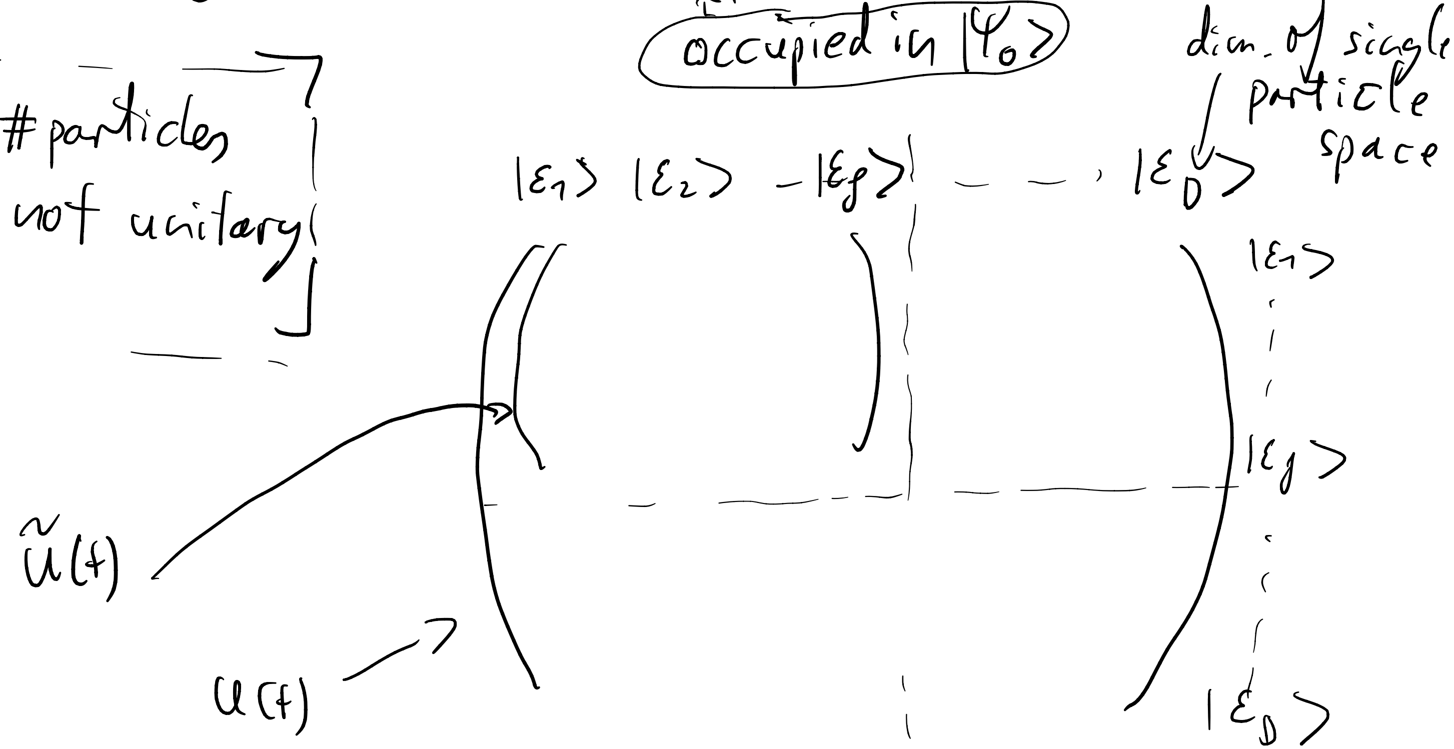
$\rightsquigarrow$ Recipe to compute $\langle \Psi_0 | \Psi(t) \rangle$:

(i) Compute $u(t) = e^{-iht}$ with h as in $H = \Psi^\dagger h \Psi$

(ii) Project $u(t)$ to initially occupied subspace:

$$\tilde{u}(t) = \Big(\langle \alpha | u(t) | \beta \rangle \Big)_{\underbrace{\alpha,\beta}_{\text{occupied in } |\Psi_0\rangle}}$$

particles × # particles matrix, not unitary



(iii) $\langle \Psi_0 | \Psi(t) \rangle = \det(\tilde{u}(t))$.

$\rightsquigarrow$ Analogous calculation for bosons in states $\langle \alpha | \beta \rangle = \delta_{\alpha\beta}$

$$\langle \Psi_0 | \Psi(t) \rangle = \mathrm{per}(\tilde{u}(t))$$

$\uparrow$ permanent

$\lightning$ permanent cannot be efficiently calculated for a generic matrix! (cf. Boson sampling problem).

$\rightsquigarrow$ Work around for Gaussian bosonic states:

Consider $\langle \Psi_0 | \Psi(t) \rangle = \lim_{\beta \to \infty} \mathrm{Tr}_{\mathcal{H}_F^+} \left(\frac{e^{-\beta \tilde{H}}}{\mathrm{Tr}_{\mathcal{H}_F^+}(e^{-\beta \tilde{H}})} e^{-iHt} \right) = \lim_{\beta \to \infty} \langle e^{-iHt} \rangle_{\tilde{H}, \beta}$

$$\boxed{\lim_{\beta \to \infty} \frac{e^{-\beta \tilde{H}}}{\mathrm{Tr}_{\mathcal{H}_F^+}(e^{-\beta \tilde{H}})} = |\Psi_0\rangle\langle\Psi_0| \quad \text{for some } \tilde{H} = \psi^\dagger \tilde{h} \psi}$$

and use $\mathrm{Tr}_{\mathcal{H}_F^+}\left(e^{O_1}e^{O_2}\right) = \det_h\left(1 - e^{o_1}e^{o_2}\right)^{-1}$ for $O_1 = -\beta\tilde{H}$ and $O_2 = -iHt$

Fock space

O_1, O_2 bilinear operators $\psi^\dagger o_i \psi = O_i$

single particle Hilbert space

[I. Klich (2002)]

- General (particle number conserving) n-body operators:

$$O = \sum_{\substack{\alpha_1,\dots,\alpha_n \\ \beta_1,\dots,\beta_n}} O_{\substack{\alpha_1\dots\alpha_n \\ \beta_1\dots\beta_n}}\, a^\dagger_{\alpha_1}\cdots a^\dagger_{\alpha_n} a_{\beta_n}\cdots a_{\beta_1}$$

$$\langle\psi|O|\psi\rangle = \sum_{\substack{\alpha_1,\dots,\alpha_n \\ \beta_1,\dots,\beta_n}} \underbrace{\langle\psi| a^\dagger_{\alpha_1}\cdots a^\dagger_{\alpha_n} a_{\beta_n}\cdots a_{\beta_1}|\psi\rangle}_{} O_{\substack{\alpha_1\dots\alpha_n \\ \beta_1\dots\beta_n}}$$

$$= \sum_{\substack{\text{all pairings} \\ P}} (\pm)^{|P|} \left(\langle\psi|a^\dagger_{\alpha_1} a_{\beta_{P(1)}}|\psi\rangle \cdots \langle\psi|a^\dagger_{\alpha_n} a_{\beta_{P(n)}}|\psi\rangle\right)$$

Gaussian state

Wick's theorem

A. 4 Mean Field Theory

- Basic idea: Reduce an <u>interacting</u> many-body problem to effective one-body problem by approximating the effect of all other particles with a mean field potential seen by the individual particles.

- Consider the paradigmatic example of a spin-$\frac{1}{2}$ Heisenberg model on a d-dimensional hypercubic lattice (with $z = 2d$ nearest neighbors for every site)

$$H = -J \sum_{\underset{\text{NN}}{\langle i,j \rangle}} \vec{S}_i \cdot \vec{S}_j$$

- Express $\vec{S}_i$ as a sum of its thermal expectation value

$\langle \vec{S}_i \rangle$ and the deviation from this average:

$$\vec{S}_i = \langle \vec{S}_i \rangle + \delta_{\vec{S}_i} \quad , \text{with } \delta_{\vec{S}_i} = \vec{S}_i - \langle \vec{S}_i \rangle .$$

- Neglecting quadratic terms in δ-fluctuations yields:

$$\vec{S}_i \cdot \vec{S}_j = \left(\langle \vec{S}_i \rangle + \delta_{\vec{S}_i}\right)\left(\langle \vec{S}_j \rangle + \delta_{\vec{S}_j}\right) \underset{+\mathcal{O}(\delta^2)}{\approx} \langle \vec{S}_i \rangle \delta_{\vec{S}_j} + \langle \vec{S}_j \rangle \delta_{\vec{S}_i} + \langle \vec{S}_i \rangle \langle \vec{S}_j \rangle$$

$$\underset{\text{Def. } \delta_{\vec{S}_i}}{=} \langle \vec{S}_i \rangle \vec{S}_j + \langle \vec{S}_j \rangle \vec{S}_i - \langle \vec{S}_i \rangle \langle \vec{S}_j \rangle .$$

$\rightsquigarrow$ Effective one-body problem with thermal expectation values $\langle \vec{S}_i \rangle$ to be determined <u>self-consistently</u>.

- Replacing $\langle \vec{S}_i \rangle$ by free parameters $\vec{m}_i$ yields:

$$H_{MF}(\{\vec{m}_i\}) = -J \sum_{\langle i,j \rangle} \left(\vec{S}_i \cdot \vec{m}_j + \vec{S}_j \cdot \vec{m}_i - \vec{m}_i \cdot \vec{m}_j \right).$$

- With $Z = \mathrm{Tr}(e^{-\beta H_{MF}})$ and $F = -\frac{1}{\beta} \log Z$, we get

$$\nabla_{\vec{m}_i} F = \frac{1}{Z} \mathrm{Tr}\left(e^{-\beta H_{MF}} (\nabla_{\vec{m}_i} H_{MF}) \right) =: \langle \nabla_{\vec{m}_i} H_{MF} \rangle_{MF} =$$

$$= -J \left\langle \sum_{j \text{ NN of } i} (\vec{S}_j - \vec{m}_j) \right\rangle_{MF} =$$

Plug in H_{MF}

$$= -J \left(\sum_{j \text{ NN of } i} \left(\langle \vec{S}_j \rangle_{MF} - \vec{m}_j \right) \right).$$

$$\rightsquigarrow \nabla_{\vec{m}_i} F = 0 \iff \sum_{j \text{ NN of } i} \langle \vec{S}_j \rangle_{MF} = \sum_{j \text{ NN of } i} \vec{m}_j$$

satisfied for all j only if $\boxed{\langle \vec{S}_j \rangle_{MF} = \vec{m}_j}$

(self-consistency)

- Simplest practical implementation: Iterative solution of self-consistency equations.

(i) Start with randomly chosen parameters $\{\vec{m}_j\}_j$.

(ii) Compute $\langle \vec{S}_j \rangle_{MF(\{\vec{m}_j\})} =: \vec{M}_j \ \forall j$

(iii) Update $\vec{m}_j = \vec{M}_j \ \forall j$

repeat (ii), (iii) until $\langle \vec{S}_j \rangle_{MF(\{\vec{m}_j\})} = \vec{m}_j \ \forall j$ reached to satisfactory accuracy

— Two analytically solvable examples:

(a) $\vec{m}_j = \vec{m}$ (homogeneous ferromagnet)

$$H = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j \approx -J \Big(\sum_i \big[\underbrace{z}_{\#NN} \vec{S}_i \cdot \vec{m} - \frac{z}{2} \vec{m}^2 \big] \Big) \equiv \sum_i H^i_{MF}(\vec{m})$$

$$\rightsquigarrow F_i(\vec{m}) = -\frac{1}{\beta} \log\left(\mathrm{Tr}\left[e^{-\beta H_{MF}(\vec{m})} \right] \right) =$$

$$= -\frac{1}{\beta} \log\left(e^{-\beta J m^2 \frac{z}{2}} \, \mathrm{Tr} \begin{pmatrix} e^{\beta J m \frac{z}{2}} & 0 \\ 0 & e^{-\beta m J \frac{z}{2}} \end{pmatrix} \right)$$

$$\boxed{|\vec{m}| = m}$$

$$= \frac{J m^2 z}{2} - \frac{1}{\beta} \log\left(2 \cosh\left(\beta J m \frac{z}{2} \right) \right) =: F(m).$$

$$\Rightarrow \partial_m F(m) = 0 \iff J m z = \frac{1}{\beta} \frac{\beta J z}{2} \frac{\sinh\left(\frac{\beta J z m}{2} \right)}{\cosh\left(\frac{\beta J z m}{2} \right)}$$

$$\Leftrightarrow \quad m = \frac{1}{2}\tanh\left(\frac{\beta J z m}{2}\right).$$

$\rightsquigarrow$ Expand around $m = 0$ to find critical temperature T_c.

$$m \approx \frac{1}{4}\beta J z m \Rightarrow T_c = \frac{Jz}{4k_B} \quad \left(\beta = \frac{1}{k_B T}\right).$$