Aula IV

- Função de Partição:

$$Z = \sum_{\alpha}' \exp(-\beta E_\alpha) \qquad \beta = 1/k_B T.$$

conexão com a termodinâmica:

$$F = -\frac{1}{\beta} \ln Z \quad \text{energia livre de Helmholtz}$$

$$Z = \sum_{\alpha}' \langle \alpha | \exp(-\beta H) | \alpha \rangle$$

$$= \mathrm{Tr}(\exp(-\beta H))$$ traço é independente da base com que é calculado.

$$= \int dx \langle x | \exp(-\beta H) | x \rangle$$

$$= \int dx\, \hbar\, G(x, x; \tau = \hbar\beta)$$

Exemplo: Oscilador Harmônico:

$$Z = \sum_n' \exp(-\beta\hbar\omega(n + 1/2))$$

$$= \exp(-\beta\hbar\omega/2) \sum_{n=0}^{\infty} \exp(-\beta\hbar\omega n)$$

$$= \exp(-\beta\hbar\omega/2) \cdot \frac{1}{1 - \exp(-\beta\omega\hbar)}$$

$$= \left(2\sinh(\beta\hbar\omega/2)\right)^{-1}$$

Agora utilizando o propagador:

$$\hbar G(x,x;\tau=\beta\hbar)$$

$$= \left(\frac{m\omega}{2\pi\hbar\sinh(\beta\hbar\omega)}\right)^{1/2} \exp\left(\frac{-m\omega\, x^2}{\hbar\sinh(\beta\hbar\omega)}\left(\cosh(\beta\hbar\omega)-1\right)\right)$$

$$Z = \int dx\, \hbar\, G(x,x;\tau=\beta\hbar)$$

$$= \left(\frac{\cancel{m\omega}}{\cancel{2\pi\hbar\sinh}(\beta\hbar\omega)}\right)^{1/2}\left(\frac{\cancel{\pi\hbar\sinh(\beta\omega\hbar)}}{\cancel{m\omega}(\cosh(\beta\hbar\omega)-1)}\right)^{1/2}$$

$$= \frac{1}{(2\sinh(\beta\hbar\omega))}$$

→ Mapa clássico - quântico:

sistema quântico em n-dimensões é equivalente a um sistema clássico em $(n+1)$-dimensões. Com a dimensão adicional sendo o tempo.

Quântico: Um spin localizado.

B ↑ $s = 1/2$, $H = -B\sigma_z - h\sigma_x$

→ h $\quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

campo B quebra a degenerescência dos estados de spin para cima e para baixo.

o campo h induz transições $|\uparrow\rangle \to |\downarrow\rangle$

$\sigma_z |\uparrow\rangle = |\uparrow\rangle$, $\sigma_z|\downarrow\rangle = -|\downarrow\rangle$

$\sigma_x |\uparrow\rangle = |\downarrow\rangle$, $\sigma_x |\downarrow\rangle = |\uparrow\rangle$

autovalores de H : $\pm h_{tot} = \pm\sqrt{h^2 + B^2}$.

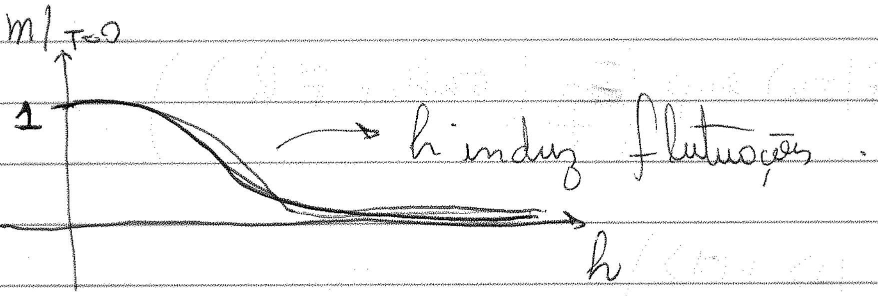
$Z = \exp(-\beta h_{tot}) + \exp(\beta h_{tot})$

$= 2\cosh(\beta h_{tot})$.

$F = -\frac{1}{\beta} \ln Z = -\frac{1}{2}\left[\ln \cosh(\beta h_{tot}) + \ln 2\right]$

$m \to$ magnetização ao longo de B.

$m\Big|_{T=0} = -\frac{\partial F}{\partial B}\Big|_{T=0} = \frac{B}{h_{tot}}$



$$Z = \sum_{\sigma=\uparrow\downarrow} \langle \sigma | \exp(-\beta H) | \sigma \rangle$$

$$= \sum_{\sigma_0, \dots, \sigma_N}^{\sigma_0 = \sigma_N} \langle \sigma_0 | \exp(-\beta H/N) | \sigma_1 \rangle \langle \sigma_1 | \dots | \sigma_{N-1} \rangle \langle \sigma_{N-1} | \exp(-\beta H/N) | \sigma_N \rangle$$

mas: $\exp(-\beta H/N) = \exp\left(-\frac{\beta B \sigma_z}{N}\right) \exp\left(-\frac{\beta h \sigma_x}{N}\right) + \mathcal{O}(N^{-2})$

Termo genérico:

$$\langle \sigma_{k-1} | \exp\left(-\frac{\beta B \sigma_z}{N}\right) \exp\left(-\frac{\beta h \sigma_x}{N}\right) | \sigma_k \rangle$$

$$= \langle \sigma_{k-1} | \exp\left(-\frac{\beta h \sigma_x}{N}\right) | \sigma_k \rangle \exp\left(-\frac{\beta B \sigma_k}{N}\right)$$

$$= \langle \sigma_{k-1} | \exp\left(-\frac{\beta h \sigma_x}{N}\right) \sum_{\tilde{\sigma}} |\tilde{\sigma}\rangle \langle \tilde{\sigma} | \sigma_k \rangle \exp\left(-\frac{\beta B \sigma_k}{N}\right)$$

$|\tilde{\sigma}\rangle$ = autoestado de σ_x.

$$= \langle \sigma_{k-1} | \sum_{\tilde{\sigma}} |\tilde{\sigma}\rangle \langle \tilde{\sigma} | \sigma_k \rangle \exp\left(-\frac{\beta}{N} \sigma_k B - \frac{\beta h \tilde{\sigma}}{N}\right)$$

$$= \sum_{\tilde{\sigma}} \langle \sigma_{k-1} | \tilde{\sigma} \rangle \langle \tilde{\sigma} | \sigma_k \rangle \exp\left(-\frac{\beta}{N} (\sigma_k B + \tilde{\sigma} h)\right)$$

$$|\tilde{1}\rangle = \frac{1}{\sqrt{2}} \left(|1\rangle + |-1\rangle \right)$$

$$|\tilde{-1}\rangle = \frac{1}{\sqrt{2}} \left(|1\rangle - |-1\rangle \right)$$

$$= \langle \sigma_{k-1} | \left(\frac{1}{\sqrt{2}} \left(|1\rangle + |-1\rangle \right) \right) \left(\frac{1}{\sqrt{2}} \left(\langle 1| + \langle -1| \right) \right) |\sigma_k\rangle \; \exp(\ldots)$$

$$+ \ \ldots$$

$$= \frac{\langle \sigma_{k-1} |}{2} \left(|1\rangle\langle 1| + |1\rangle\langle -1| + |-1\rangle\langle 1| + |-1\rangle\langle -1| \right) |\sigma_k\rangle \exp\left(\frac{-\beta \sigma_k B}{N} - \frac{\beta h}{N} \right)$$

$$+ \frac{\langle \sigma_{k-1} |}{2} \left(|1\rangle\langle 1| - |1\rangle\langle -1| - |-1\rangle\langle 1| + |-1\rangle\langle -1| \right) |\sigma_k\rangle \exp\left(-\frac{\beta \sigma_k B}{N} + \frac{\beta h}{N} \right)$$

$$= \frac{1}{2} \exp\left(-\frac{\beta \sigma_k B}{N} - \frac{\beta h}{N} \right)$$

$$+ \frac{(\sigma_{k-1})(\sigma_k)}{2} \exp\left(-\frac{\beta \sigma_k B}{N} + \frac{\beta h}{N} \right)$$

$$= \frac{\exp}{2}\left(-\frac{\beta B \sigma_k}{N} \right) \left(\exp\left(-\frac{\beta h}{N} \right) + \sigma_{k-1} \sigma_k \exp\left(\frac{\beta h}{N} \right) \right)$$

$$= \exp\left(- f(\sigma_{k-1}, \sigma_k) \right)$$

$$f(\sigma_{k-1}, \sigma_k) = -\frac{1}{2} \ln\left(\coth\left(\beta h / N \right) \right) \sigma_{k-1} \sigma_k$$

$$-\frac{1}{2} \ln\left(\sinh\left(\frac{2\beta h}{N} \right) \right)$$ ← vérifier !

$$\Rightarrow \langle \sigma_{k-1} | \exp\left(-\frac{\beta h \sigma_x}{N}\right) \exp\left(-\frac{\beta B \sigma_z^z}{N}\right) | \sigma_k \rangle$$

$$= \sqrt{\sinh\left(\frac{2\beta h}{N}\right)} \exp\left(\tilde{B}\,\sigma_k\right) \exp\left(\tilde{J}\,\sigma_{k-1}\sigma_k\right)$$

$$\tilde{B} = \frac{B}{N}\beta \,, \quad \tilde{J} = \frac{1}{2}\ln\left(\coth\left(\frac{\beta h}{N}\right)\right)$$

$$Z = \lim_{N\to\infty} \left(\sinh\left(\frac{2\beta h}{N}\right)\right)^{N/2}$$

$$\sum_{\sigma_1 \ldots \sigma_N} \exp\left(-S_E\right)$$

$$S_E = \sum_{k=1}^{N}\left(-\tilde{B}\sigma_k - \tilde{J}\sigma_{k-1}\sigma_k\right)$$

pode ser pensado como hamiltoniano de uma teoria clássica em $n+1=1$ dimensão

modelo quântico em 0-dimensão tornou-se um modelo clássico em 1-dimensão.

o modelo de ising encontrado pode ser pensado como uma direção temporal.

Quanticamente: $\uparrow$ a partícula está parada e varia spin

Classicamente: o spin varia junto com outra dimensão temporal $\uparrow \downarrow \uparrow \downarrow \uparrow \ldots$

função de correlação:

$$\langle 0 | \sigma_z(\tau) \sigma_z(\tau) | 0 \rangle \sim G(\tau)$$

$$\xrightarrow[\tau \to \infty]{} \exp\left(-\frac{\Delta}{\hbar}\tau\right), \quad \Delta = 2 h_{tot}$$

comprimento de correlação:

$$\xi \propto = 1/\Delta$$