Frustrierter Magnetismus: Von exakten Lösungen zu realen Materialien

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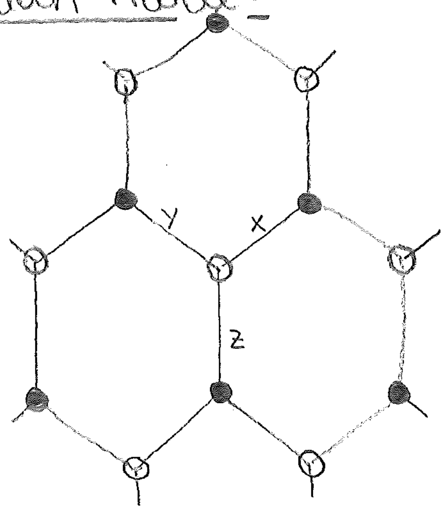
1. Kitaevs Honigwaben-Modell:

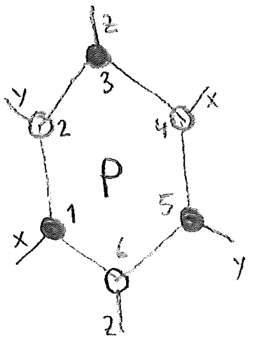
[Kitaev '06]



$$H = -J_x \sum_{x\text{-Links}} \sigma_j^x \sigma_k^x - J_y \sum_{y\text{-Links}} \sigma_j^y \sigma_k^y - J_z \sum_{z\text{-Links}} \sigma_j^z \sigma_k^z$$

$$= -\sum_{\alpha=x,y,z} \sum_{\alpha\text{-Links}} J_\alpha K_{jk} \quad , \quad K_{jk} = \begin{cases} \sigma_j^x \sigma_k^x & \text{falls } (j,k)\ x\text{-Link} \\ \sigma_j^y \sigma_k^y & \text{falls } (j,k)\ y\text{-Link} \\ \sigma_j^z \sigma_k^z & \text{falls } (j,k)\ z\text{-Link} \end{cases}$$

Plakettenoperator:



$$W_p = \underbrace{\sigma_1^x}_{-i\sigma_1^y \sigma_1^z} \sigma_2^y \sigma_3^z \sigma_4^x \sigma_5^y \sigma_6^z$$

$$= (-i)^6 \sigma_1^y \underbrace{\sigma_1^z \sigma_2^z}_{K_{12}} \sigma_2^x \sigma_3^x \sigma_3^y \sigma_4^y \sigma_4^z \sigma_5^z \underbrace{\sigma_5^x \sigma_6^x}_{K_{56}} \sigma_6^y$$

$$= K_{12} K_{23} K_{34} K_{56} K_{61}$$

Erhaltungsgröße:

$$[H, W_p] = [W_p, W_{p'}] = 0 \qquad \forall\, p, p' = 1, \dots, \overset{\substack{\text{Anzahl Plaketten} \\ \downarrow}}{m} = \underset{\text{Anzahl Spins}}{\frac{n}{2}}$$

z.B.

$$[K_{1j}, W_p] \overset{j \notin p}{=} [\sigma_1^x \sigma_j^x, W_p] = 0$$

$$[K_{12}, W_p] = [\sigma_1^z \sigma_2^z, W_p] = 0$$

Gleichzeitige Diagonalisierung:

$$\underset{\substack{\uparrow \\ d = 2^n}}{\mathcal{H}} = \bigoplus_{w_1, \dots, w_m} \underset{\substack{\uparrow \\ d = 2^n / 2^m = 2^{n/2}}}{\mathcal{H}_{w_1, \dots, w_m}} \quad , \quad w_p = \pm 1 \text{ Eigenwerte von } W_p$$

2. Majorana-Darstellung von Spins

A) Einzelner Spin

Majorana-Fermionen:

$$c_1 = a + a^\dagger \quad , \quad c_2 = \frac{a - a^\dagger}{i}$$

$$c_1^2 = c_2^2 = \{a, a^\dagger\} = \mathbb{1} \, ,$$

$$c_1 c_2 = -c_2 c_1 \quad , \quad c_1^\dagger = c_1 \, , \; c_2^\dagger = c_2$$

Darstellung eines Spins:

$$\underset{\in \mathcal{L}(\mathcal{H})}{\sigma^x} \mapsto \tilde{\sigma}^x = i b^x c \in \mathcal{L}(\tilde{\mathcal{H}})$$

$$\sigma^y \mapsto \tilde{\sigma}^y = i b^y c$$

$$\sigma^z \mapsto \tilde{\sigma}^z = i b^z c$$

b^x, b^y, b^z, c Majorana , $\dim \mathcal{H} = 2$, $\dim \tilde{\mathcal{H}} = 4$

Projektion:

$$|\xi\rangle \in \mathcal{H} \subset \mathcal{H}' \quad \Leftrightarrow \quad D|\xi\rangle = |\xi\rangle \quad , \quad D = b^x b^y b^z c$$

"$\mathbb{Z}_2$-Eichtrafo"

Spin-Algebra:

$$(\tilde{\sigma}^\alpha)^\dagger = (i b^\alpha c)^\dagger = \tilde{\sigma}^\alpha$$

$$(\tilde{\sigma}^\alpha)^2 = i^2 b^\alpha c b^\alpha c = \mathbb{1}$$

$$\tilde{\sigma}^x \tilde{\sigma}^y \tilde{\sigma}^z = i^3 b^x c b^y c b^z c = i b^x b^y b^z c = i D$$

und $[\tilde{\sigma}^\alpha, D] = 0$ ($\mathcal{H}$ erhalten).

B) Anwendung auf Honigwabenmodell

Multi-Spinsystem:

$$\tilde{\sigma}_j^\alpha = i b_j^\alpha c_j \qquad D_j = b_j^x b_j^y b_j^z c_j$$

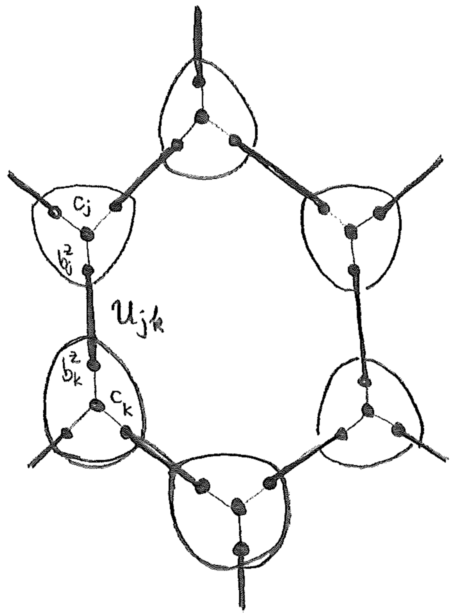
$$|\xi\rangle \in \mathcal{H} \Leftrightarrow D_j |\xi\rangle = |\xi\rangle \quad \forall j = 1, \dots, n$$

Hamiltonian:

$$\tilde{K}_{jk} = (i b_j^\alpha c_j)(i b_k^\alpha c_k) = -i \underbrace{(i b_j^\alpha b_k^\alpha)}_{\equiv \hat{u}_{jk} = \hat{u}_{jk}^\dagger} c_j c_k$$

$$\tilde{H} = \frac{i}{4} \sum_{j,k} \hat{A}_{jk} c_j c_k \quad , \quad \hat{A}_{jk} = \begin{cases} 2 J_\alpha \hat{u}_{jk}, & \text{falls } (j,k) \text{ verbunden} \\ 0, & \text{sonst} \end{cases}$$

"$\mathbb{Z}_2$-Eichtheorie mit Majorana-Fermionen"



$\mathbb{Z}_2$-Eichfeld $\hat{u}_{jk}$: $\quad u_{jk} = \pm 1$ Eigenwerte

$$[\hat{u}_{jk}, \hat{u}_{j'k'}] = [i b_j^\alpha b_k^\alpha, i b_{j'}^\beta b_{k'}^\beta] = 0$$

$$[\hat{u}_{jk}, \tilde{H}] = [\hat{u}_{jk}, \frac{i}{4} \sum_{j'k'} \hat{A}_{j'k'} c_j c_k] = 0$$

$\Rightarrow$ Eichfeld "statisch"

Gleichzeitige Diagonalisierung:

$$\tilde{\mathcal{H}} = \bigoplus_{u} \tilde{\mathcal{H}}_u$$

$\uparrow$ alle u_{jk}

Hamiltonian in $\tilde{\mathcal{H}}_u$:

$$\tilde{H}_u = \frac{i}{4} \sum_{j,k} A_{jk} c_j c_k \quad \text{mit } (A_{jk}) \in \mathbb{R}^{n \times n} \text{ schiefsymmetrisch}$$

Bem.: $\tilde{\mathcal{H}}_u$ nicht eichinvariant

$$D_j \hat{u}_{jk} = (i b_j^x b_j^y b_j^z)(i b_j^\alpha b_k^\alpha) = -\hat{u}_{jk} D_j$$

Grundzustand:

$$\underset{\substack{\uparrow \\ \text{Äquivalenzklasse} \\ \text{von } u \text{ unter Eich-Trafos}}}{|\Psi_w\rangle} = \prod_j \left(\frac{\mathbb{1} + D_j}{2}\right) \underset{\substack{\uparrow \\ \text{Grundzustand} \\ \text{in } \tilde{\mathcal{H}}}}{|\tilde{\Psi}_u\rangle} \in \mathcal{H}$$

Plakettenoperator:

$$\tilde{W}_p = \prod_{(j,k)\in p} \hat{u}_{jk} \qquad (j \text{ gerade, } k \text{ ungerade})$$

$$\text{Eigenwerte} \quad \underset{\substack{\uparrow \\ \text{„magn. Fluss"}}}{w_p} = \prod_{(j,k)\in p} u_{jk} = \overset{\substack{\text{„vortexfrei"} \\ \swarrow}}{+}\underset{\substack{\uparrow \\ \text{„Vortex"}}}{-} 1$$

Wegoperator:

$$\tilde{W}(j_0, \ldots, j_s) = \underbrace{\left(\prod_{\ell=1}^{s} (-i)\, \hat{u}_{j_\ell j_{\ell-1}}\right)}_{\text{„Paralleltransporter"}} c_s c_0 \qquad \text{eichinvariant}$$

$$= \tilde{K}_{j_s j_{s-1}} \cdots \tilde{K}_{j_1 j_0}$$

Wilson-Schleife: $j_s = j_0$

Plakettenoperator: $\tilde{W}(j_0, \ldots, j_6 = j_0) = \tilde{W}_p$

3. Fermionenspektrum und Phasendiagramm

Hamiltonian:

$$H_u = \frac{i}{4} \sum_{j,k} A_{jk}\, c_j c_k \quad , \quad A_{jk} = 2J_\alpha u_{jk} \quad , \; u_{jk} = \pm 1$$

Lieb-Theorem: [Lieb '94]

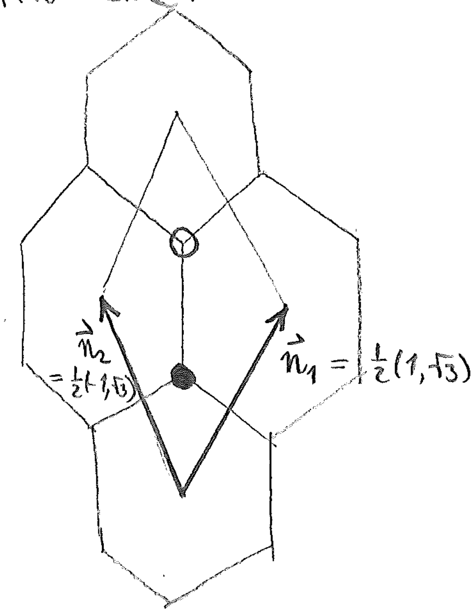
Grundzustand ist vortexfrei $\Rightarrow w_p = 1 \quad \forall p = 1, \dots, m$

Eichinvarianz:

o.B.d.A. $u_{jk} = 1 \quad \forall (j,k)$ (j gerade, k ungerade)

$\Rightarrow$ Translationsinvarianz

Elementarzelle:



atomare Position

$$j \mathrel{\hat{=}} (s, \lambda) \quad , \quad s = 1, \dots, N \qquad \lambda = 1, 2$$

Elementarzelle

$$H = \frac{i}{4} \sum_{s\lambda, t\mu} \underbrace{A_{s\lambda, t\mu}}_{= A_{0\lambda, t-s\mu}} c_{s\lambda} c_{t\mu} = \frac{1}{2} \sum_{\vec{q}, \lambda, \mu} i A_{\lambda\mu}(\vec{q})\, a_{-\vec{q},\lambda} a_{\vec{q},\lambda}$$

mit

Gittervektor

$$a_{\vec{q}\lambda} = \frac{1}{\sqrt{2N}} \sum_{s} e^{-i\vec{q}\cdot\vec{r}_s} c_{s\lambda} = a^{\dagger}_{-\vec{q}\lambda}$$

$$iA_{\lambda\mu}(\vec{q}) \equiv \sum_{t} e^{i\vec{q}\cdot\vec{r}_t}\, iA_{0\lambda,t\mu}$$

$$= \begin{pmatrix} 0 & i f(\vec{q}) \\ -i f^{*}(\vec{q}) & 0 \end{pmatrix}_{\lambda\mu}, \qquad f(\vec{q}) = 2\left(J_x e^{i\vec{q}\vec{n}_1} + J_y e^{i\vec{q}\vec{n}_2} + J_z\right)$$

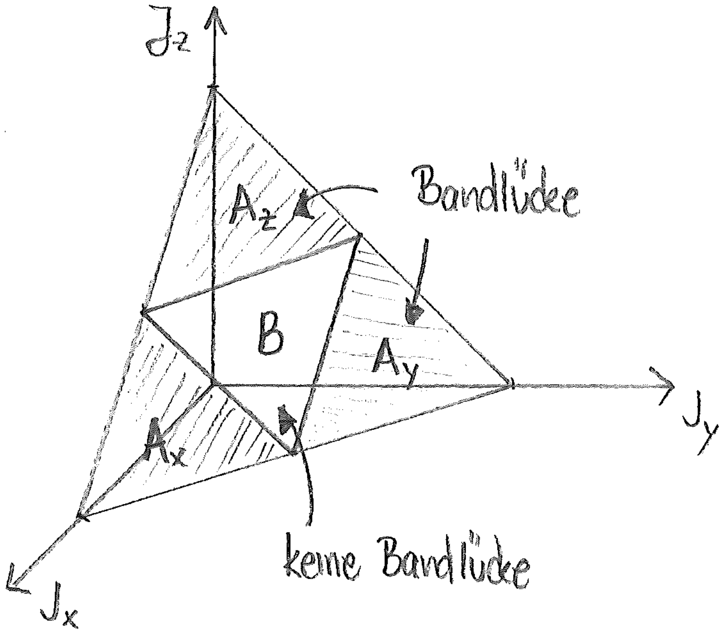
Majorana-Spektrum:

$$\varepsilon(\vec{q}) = +|f(\vec{q})|$$

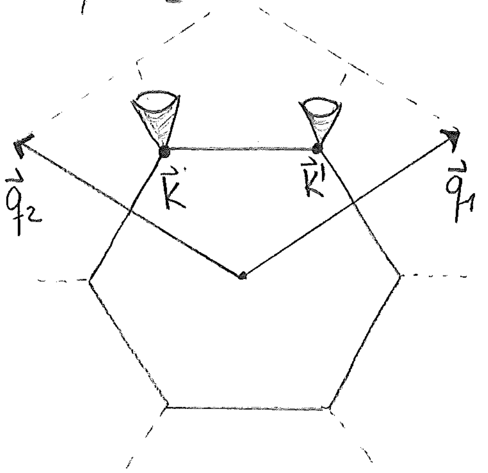
Bandlücke?

$$\exists\, \vec{q} \in BZ:\ \varepsilon(\vec{q}) = 0 \iff |J_x| \le |J_y| + |J_z|,\ |J_y| \le |J_x| + |J_z|,\ |J_z| \le |J_x| + |J_y|$$

Phasendiagramm ($J_x, J_y, J_z \geq 0$)



Beispiel $J_x = J_y = J_z = J$:



$$\varepsilon(\vec{q}) = \sqrt{3J^2|\delta\vec{q}|^2} + \mathcal{O}(\delta q^3)$$

$$\delta\vec{q} = \vec{q} - (\pm\vec{K})$$

"Dirac-Kegel"

Weitere Eigenschaften:

- A-Phasen $\hat{=}$ Toric-Code : Abelsche Anyonen $e, m, \varepsilon = e \times m$

- B-Phase im Magnetfeld:

$$\varepsilon(\vec{q}) \approx \sqrt{3J^2|\delta\vec{q}|^2 + \Delta^2}, \quad \Delta \propto \frac{h_x h_y h_z}{J^2} \text{ Bandlücke}$$

- Spektralprojektor $P(\vec{q}) = \frac{1}{2}[\mathbb{1} - \mathrm{sgn}(iA(\vec{q}))]$ definiert topologische Invariante

$$\nu = \begin{cases} 0 & \text{A-Phasen} \\ \pm 1 & \text{B-Phase (im Magnetfeld)} \end{cases} \qquad \text{"Chern-Zahl"}$$

$\Rightarrow$ topologische Randzustände

- <u>Halb-ganzzahliger</u> thermischer Quanten-Hall-Effekt:

$$\frac{\varkappa_{xy}}{T} = q\,\frac{\pi}{6}\,\frac{k_B^2}{\hbar} \quad \text{mit } q = \frac{1}{2} \quad (!)$$