

QARS - Impurity solver

Plan

- Fermionic Gaussian States
- Wick's theorem
- ~~Stabilizers (the parallel with)~~
- ~~Impurity models Resource theory~~
- Impurity models

Fermionic Gaussian states

Dirac Fermions

(1) $|\vec{x}\rangle = (a_1^\dagger)^{x_1} (a_2^\dagger)^{x_2} \dots (a_n^\dagger)^{x_n} |\text{vacuum}\rangle$ $\vec{x} \in \{0,1\}^n = \mathbb{F}_2^n$

where

(2) $\{a_i, a_j\} = a_i a_j + a_j a_i = 0$

(3) $\{a_i^\dagger, a_j^\dagger\} = a_i^\dagger a_j^\dagger + a_j^\dagger a_i^\dagger = 0$

(4) $\{a_i^\dagger, a_j\} = a_i^\dagger a_j + a_j a_i^\dagger = \delta_{ij}$

Majorana fermions

(5) $c_{2j-1} = a_j + a_j^\dagger$

(6) $c_{2j} = -i(a_j - a_j^\dagger)$

(7) $\{c_i, c_j\} = c_i c_j + c_j c_i = 2\delta_{ij}$ and $c_i^2 = 1$

As Pauli strings:

(8) $c_{2j-1} = \underbrace{X \otimes \dots \otimes Z}_{j-1} \otimes X$ \leftrightarrow $\underbrace{Z \otimes \dots \otimes Z}_{j-1} \otimes X \otimes \underbrace{I \dots I}_{n-j}$

(9) $c_{2j} = \underbrace{Y \otimes \dots \otimes Z}_{j-1} \otimes Y$ \leftrightarrow $\underbrace{Z \otimes \dots \otimes Z}_{j-1} \otimes Y \otimes \underbrace{I \dots I}_{n-j}$

Gaussian state

(19) $|\varphi\rangle = U|\tilde{g}\rangle$

has covariance matrix

(20) $M_\varphi = R M_{\tilde{g}} R^T$ where $R \in O(2n)$

defined by

(21) $U c_p U^\dagger = \sum_{q=1}^{2n} R_{pq} c_q$

Valid covariance matrices satisfy

(22) $M^2 = -I$

Any real antisymmetric satisfying this encodes some gaussian fermionic state.

Expectation values

consider observables ~~etc~~ in the basis of Majorana monomials (Majorana strings)

(23) $c(\vec{x}) = c_1^{x_1} c_2^{x_2} \dots c_{2n}^{x_{2n}}$ $\vec{x} \in \{0,1\}^{2n} \cong \mathbb{F}_2^{2n}$

expectation value is computable from covariance matrix only (Wick's theorem)

(24) $\langle \varphi | c(\vec{x}) | \varphi \rangle = \text{Pf}(i M_\varphi[\vec{x}])$

Pfaffian $\in \mathbb{C}$
(to be defined)

submatrix where ~~we~~ we use only rows and column j if $x_j \neq 0$

(25) ex: $\langle c_1 c_2 c_3 c_4 \rangle = \langle c_1 c_2 \rangle \langle c_3 c_4 \rangle - \langle c_1 c_3 \rangle \langle c_2 c_4 \rangle - \langle c_1 c_4 \rangle \langle c_2 c_3 \rangle$

Pfaffian is analogous to the determinant, in fact but for $2k \times 2k$ skew-symmetric matrices,

$$(26) \quad A = \begin{pmatrix} 0 & a_{12} & a_{13} & \dots \\ -a_{12} & 0 & a_{23} & \dots \\ -a_{13} & -a_{23} & 0 & \ddots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \left. \vphantom{\begin{pmatrix} 0 & a_{12} & a_{13} & \dots \\ -a_{12} & 0 & a_{23} & \dots \\ -a_{13} & -a_{23} & 0 & \ddots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}} \right\} 2k = n$$

The pfaffian is

$$(27) \quad \text{Pf}(A) = \frac{1}{2^k k!} \sum_{\sigma \in S_n} (-1)^\sigma a_{\sigma(1)\sigma(2)} a_{\sigma(3)\sigma(4)} \dots a_{\sigma(2k-1)\sigma(2k)}$$

ex: $\dim = 2 \rightarrow \text{Pf}(A) = a_{12}$
 $\dim = 3 \rightarrow \text{Pf}(A) = 0$
 $\dim = 4 \rightarrow \text{Pf}(A) = a_{12}a_{34} - a_{13}a_{24} + a_{14}a_{23}$

$$\begin{aligned} \dim = 6 \rightarrow \text{Pf}(A) = & a_{12}a_{34}a_{56} - a_{12}a_{35}a_{46} + a_{12}a_{36}a_{45} \\ & - a_{13}a_{24}a_{56} + a_{13}a_{25}a_{46} - a_{13}a_{26}a_{45} \\ & + a_{14}a_{23}a_{56} - a_{14}a_{25}a_{36} + a_{14}a_{26}a_{35} \\ & - a_{15}a_{23}a_{46} + a_{15}a_{24}a_{36} - a_{15}a_{26}a_{34} \\ & + a_{16}a_{23}a_{45} - a_{16}a_{24}a_{35} + a_{16}a_{25}a_{34} \end{aligned}$$

we see a recursive pattern

$$(28) \quad \text{Pf}(A) = \sum_{j=2}^{2k} (-1)^j a_{1j} \text{Pf}(A_{\hat{1}\hat{j}})$$

matrix with row and columns 1 and j removed

note that $\text{Pf}(A)^2 = \det(A)$.

Note also that when the matrix is the covariance of some free ferm gaussian state terms simplify,

$$(29) \quad \begin{aligned} M_{pq} M_{rs} &= \frac{1}{4} (\langle c_p c_q \rangle - \langle c_q c_p \rangle) (\langle c_r c_s \rangle - \langle c_s c_r \rangle) \\ &= \frac{1}{4} (\langle c_p c_q \rangle \langle c_r c_s \rangle - \langle c_p c_q \rangle \langle c_s c_r \rangle) \end{aligned}$$

$$(30) \quad M_{pq} = -\frac{i}{2} \langle \phi | (c_p c_q - c_q c_p) | \phi \rangle = -\frac{i}{2} (\langle \phi | c_p c_q | \phi \rangle - \delta_{pq})$$

the key is a change of variable under the integral, which constitute one of a few important Gaussian integral of field theory

$$(10) \quad Z[b] = \int d^n x \exp\left(-\frac{1}{2} \bar{x}^T \Sigma^{-1} \bar{x} + b^T \bar{x}\right) \quad \left. \begin{array}{l} \\ \end{array} \right\} \bar{x} \rightarrow \bar{x} + \Sigma b$$

$$(11) \quad = \int d^n x \exp\left(-\frac{1}{2} (\bar{x} + \Sigma b)^T \Sigma^{-1} (\bar{x} + \Sigma b) + b^T \bar{x}\right)$$

$$(12) \quad = \int d^n x \exp\left(-\frac{1}{2} \bar{x}^T \Sigma^{-1} \bar{x} + \frac{1}{2} b^T \bar{x} + \frac{1}{2} \bar{x}^T b - \frac{1}{2} b^T \Sigma b + b^T \bar{x}\right)$$

$$(13) \quad = Z[0] \exp\left(-\frac{1}{2} b^T \Sigma b\right)$$

As a result, we have (9), and with (8), it implies

$$\langle x_i x_j \dots x_k \rangle = \frac{1}{Z} \frac{\partial^m}{\partial b_i \partial b_j \dots \partial b_k}$$

$$(14) \quad \langle x_i x_j \dots x_k \rangle = \frac{\partial^m}{\partial b_i \partial b_j \dots \partial b_k} \exp\left(-\frac{1}{2} b^T \Sigma b\right)$$

$$(15) \quad = \frac{\partial^m}{\partial b_i \partial b_j \dots \partial b_k} \left(1 - \frac{1}{2} b^T \Sigma b + \frac{1}{2! 2} (b^T \Sigma b)^2 + \dots \right) \Big|_{b=0}$$

The derivative only keep terms containing all relevant b_i and evaluation at $b=0$ remove all terms containing extra b_i 's. The remaining terms can only contain even powers of b_i and a pattern emerges:

$$\underbrace{\langle x_i x_j \dots x_k \rangle}_m = \sum_{\text{pairings } P} \prod \Sigma_p \quad \Sigma_{ij} \equiv \langle x_i x_j \rangle$$

$$= \Sigma_{ij} \Sigma_{kl} \Sigma_{mn} \dots + \Sigma_{ik} \Sigma_{jl} \dots + \dots$$

which is Wick's theorem! (Actually this is Isserlis theorem) The nuance with fermions is that since the fermionic field (which would take the place of the x_i here) anti-commute, the sign changes accordingly in the product of $\Sigma_{ij} \Sigma_{kl}$. Proving this follow the exact steps used above but requires to introduce grassman variables (anti-commuting scalars) for the source fields b .

QARS - Impurity model

Simon Verret 03/2026 ⑦

Impurity model: free fermion bath coupled to a small, strongly interacting impurity

$$H = H_0 + H_{\text{imp}}$$

\uparrow \uparrow
m fermionic modes with interaction
n ~~m~~ fermionic modes free
n modes total

History:

- Kondo⁶⁴ problem: resistivity upturn at low T (1933)
- Solved by Anderson '61, Wilson '75: localization, NRG numerical renormalization group (predecessor of TN)
- Used in DMFT to treat correlations in materials impurity model with bath fixed self-consistently with ~~that~~ lattice of such impurities
- Bauer 2015: could use a quantum computer to solve larger impurities in DMFT

Why care? Impurity models sit at the frontier between ~~exactly solvable~~ efficiently simulable free fermions systems and QMA-complete systems

Hubbard 2D: QMA-complete

Hubbard 1D: exact Bethe ansatz

Hubbard ∞ D: exact DMFT

Our best approximation to Hubbard 2D is DMFT and CDMFT (cluster impurity)

Today: Gosset & Bravyi 2017: complexity of Quantum impurity problems

Impurity models in the Majorana basis:

(1) $H_0 = \frac{i}{4} \sum_{ij=1}^{2n} h_{ij} c_i c_j$ energy scale s.t. $\|h\| \leq 1$

(2) $H_{\text{imp}} = \sum_{\substack{\vec{x} \in \{0,1\}^m \\ |\vec{x}| \text{ even}}} g_{\vec{x}} c_1^{x_1} c_2^{x_2} \dots c_m^{x_m}$ where $c_i c_j + c_j c_i = 2\delta_{ij}$
 $c_i^2 = 1$

The bath diagonalized by (Gaussian unitary)

(3) $H_0 = \sum_{j=1}^n \epsilon_j b_j^\dagger b_j + \underbrace{E_0}_{\text{ignore this}}$ where $b_j^2 = 0$
 $b_i b_j^\dagger + b_j^\dagger b_i = \delta_{ij}$

with $b_j = U a_j U^\dagger$

the spectrum is $\{\epsilon_j\}$ where $0 \leq \epsilon_j \leq 1$ because of the scale we chose. we identify

(4) $\epsilon_0 = 0$

(5) $\omega = \text{gap} = \min \epsilon_j \text{ s.t. } \epsilon_j \neq 0 \quad \epsilon_j \geq \omega > 0 \quad \forall j=1,2,\dots$

Define the covariance matrix

(6) $C_{pq} = \langle \psi | b_p^\dagger b_q | \psi \rangle$

where $|\psi\rangle$ is the ground state of the impurity then Gossel & Bravyi's main result is:

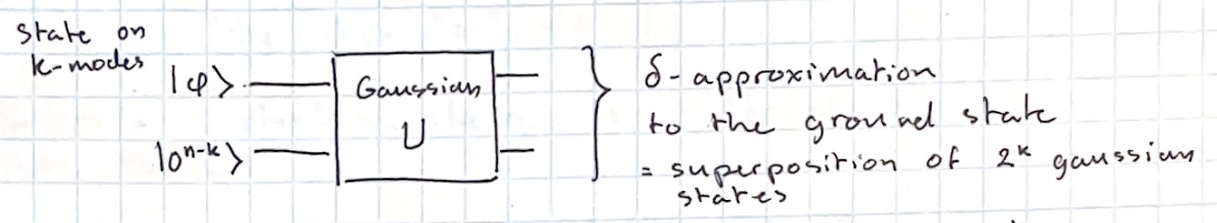
Theorem: eigenvalues σ_i of C decay exponentially

(7) $\sigma_j \leq \text{const.} \exp\left(-\frac{j}{4m \log(2\omega^{-1})}\right) \quad \sigma_1 \geq \sigma_2 \geq \dots$

7 in the paper, 14 in the talk

with no dependence on n .

Implies that the ground state has a concise representation, namely



the $2k$ basis vectors on the left map to 2^k gaussian states: the gaussian rank, then because of the theorem, we can use

$$k = \mathcal{O}(1) \cdot m \log(2\omega^{-1}) \cdot [\log \delta^{-1} + \log m + \log \log 2\omega^{-1}]$$

independant of n . The proof is roughly that for each vanishing eigenvalue of C the eigenstate

$$C\vec{v} \approx 0$$

~~correspond~~ there correspond a Fermi mode

$$B = \sum_{j=1}^n v_j b_j$$

such that $\langle \psi | B^\dagger B | \psi \rangle = 0$. ~~with that concise representation comes~~ So a Gaussian unitary U^\dagger can represent the ground state in a basis where most B are unoccupied. ~~is~~

With that concise representation, we can devise an algorithm:

Theorem: there is a classical algorithm to compute the ground energy of a quantum impurity model within tolerance ϵ with runtime

$$\text{complexity} \sim n^3 \exp(\mathcal{O}(m \log^3(m\epsilon^{-1})))$$

the resulting ground state is a superposition of

$$\chi = \exp[\mathcal{O}(m \log^3(m\epsilon^{-1}))]$$

Gaussian states. Here is a sketch of the algorithm:

1. diagonalize bath $\mathcal{O}(n^2) \rightarrow H_0 = \sum_j \epsilon_j b_j^\dagger b_j$
2. discretize $H_0 \rightarrow \tilde{H}_0 = \sum_j^n \epsilon_j b_j^\dagger b_j$ with $\epsilon_j \leq \epsilon_j \leq \epsilon_j + \Delta$
 this modifies the hamiltonian and the GS up to error $\mathcal{O}(\epsilon)$ for spacing

$$\Delta = \frac{\epsilon}{m \log^2(m\epsilon^{-1})}$$

$\|H_0 - \tilde{H}_0\|$ can be large but we only care about the few excitations subspace

3. This equally spaced grid $\epsilon_j - \epsilon_i = \Delta$ introduce degeneracy in the bath, ~~in which case~~ at most $1/\Delta = m\epsilon^{-1} \log^2(m\epsilon^{-1})$. When the bath have such degeneracy we can decouple all except m/Δ modes = $m^2 \epsilon^{-1} \log(m\epsilon^{-1})$

moreover, the decoupling unitary commutes with number operator $b_j^\dagger b_j$ so we can further truncate $\leq m \log^2(m\epsilon^{-1})$

Computing the smallest eigenvalue in this subspace yield the desired ground state

Time evolution is harder: Bravyi & Childs show it can't be simulated unless BPP = BQP

Appendix

(11)

From fermionic hamiltonians to Majorana

$$(1) \quad H = \sum_{ij} (t_{ij} c_i^\dagger c_j + \Delta_{ij} c_i c_j + h.c.)$$

$$(2) \quad = \sum_{ij} (t_{ij} c_i^\dagger c_j + \Delta_{ij} c_i c_j + \Delta_{ij}^* c_j^\dagger c_i + t_{ij}^* c_j^\dagger c_i)$$

$$(3) \quad = \sum_{ij} (t_{ij} c_i^\dagger c_j + \Delta_{ij} c_i c_j + \Delta_{ij}^* c_i c_j^\dagger + t_{ij}^* (\delta_{ij} - c_i c_j^\dagger))$$

$$(4) \quad = \sum_{ij} (c_i^\dagger \ c_i) \begin{pmatrix} t_{ij} & -\Delta_{ij}^* \\ \Delta_{ij} & -t_{ij}^* \end{pmatrix} \begin{pmatrix} c_j \\ c_j^\dagger \end{pmatrix} + \sum_i t_{ii}$$

note: not exactly Nambu because spin is not there

Fermions de Majorana

$$(5) \quad \gamma_{2j-1} = \gamma_j^o = c_j + c_j^\dagger$$

$$(6) \quad \gamma_{2j} = \gamma_j^e = -i(c_j - c_j^\dagger)$$

$$\Rightarrow \begin{pmatrix} \gamma^o \\ \gamma^e \end{pmatrix} = \underbrace{\begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix}}_M \begin{pmatrix} c_j \\ c_j^\dagger \end{pmatrix}$$

inverse transform:

$$(7) \quad \underbrace{\begin{pmatrix} 1 & 1 \\ 1 & -i \end{pmatrix}}_{M^\dagger} \underbrace{\begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix}}_M = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix} \Rightarrow \begin{pmatrix} c_j \\ c_j^\dagger \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -i \end{pmatrix} \begin{pmatrix} \gamma^o \\ \gamma^e \end{pmatrix}$$

$$(8) \quad (c_i^\dagger \ c_i) = \frac{1}{2} (\gamma^o \ \gamma^e) \begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix}$$

Hamiltonian

$$(9) \quad H = \frac{1}{4} \sum_{ij} (\gamma_i^o \ \gamma_i^e) \begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix} \begin{pmatrix} t_{ij} & -\Delta_{ij}^* \\ \Delta_{ij} & -t_{ij}^* \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -i \end{pmatrix} \begin{pmatrix} \gamma_j^o \\ \gamma_j^e \end{pmatrix} + \sum_i t_{ii}$$

$$(10) \quad = \frac{1}{4} \sum_{ij} (\gamma_i^o \ \gamma_i^e) \begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix} \begin{pmatrix} t_{ij} - \Delta_{ij}^* & i t_{ij} + i \Delta_{ij}^* \\ \Delta_{ij} - t_{ij}^* & i \Delta_{ij} + i t_{ij}^* \end{pmatrix} \begin{pmatrix} \gamma_j^o \\ \gamma_j^e \end{pmatrix} + \sum_i t_{ii}$$

$$(11) \quad = \frac{1}{4} \sum_{ij} (\gamma_i^o \gamma_i^e) \begin{pmatrix} (t_{ij} - t_{ij}^*) + (\Delta_{ij} - \Delta_{ij}^*) & i(t_{ij} + t_{ij}^*) + i(\Delta_{ij} + \Delta_{ij}^*) \\ -i(t_{ij} + t_{ij}^*) + i(\Delta_{ij} + \Delta_{ij}^*) & (t_{ij} - t_{ij}^*) - (\Delta_{ij} - \Delta_{ij}^*) \end{pmatrix} \begin{pmatrix} \gamma_j^o \\ \gamma_j^e \end{pmatrix} + \sum_i t_{ii}$$

$$\left\{ \begin{array}{l} t = t' + it'' \\ \Delta = \Delta' + i\Delta'' \end{array} \right.$$

$$(12) \quad = \frac{1}{4} \sum_{ij} (\gamma_i^o \gamma_i^e) \begin{pmatrix} 2i(t_{ij}'' + \Delta_{ij}'') & 2i(\Delta_{ij}' + t_{ij}') \\ 2i(\Delta_{ij}' - t_{ij}') & 2i(t_{ij}'' - \Delta_{ij}'') \end{pmatrix} \begin{pmatrix} \gamma_j^o \\ \gamma_j^e \end{pmatrix} + \sum_i t_{ii}$$

$$(13) \quad = \frac{i}{2} \sum_{ij} (\gamma_i^o \gamma_i^e) \begin{pmatrix} \text{Im}(t + \Delta)_{ij} & \text{Re}(t + \Delta)_{ij} \\ -\text{Re}(t - \Delta)_{ij} & \text{Im}(t - \Delta)_{ij} \end{pmatrix} \begin{pmatrix} \gamma_j^o \\ \gamma_j^e \end{pmatrix} + \sum_i t_{ii}$$

$$= \frac{i}{2} \sum_{pq} \gamma_p h_{pq} \gamma_q$$

example: Hubbard

$$H_U = U \sum_i a_{i\uparrow}^\dagger a_{i\uparrow} a_{i\downarrow}^\dagger a_{i\downarrow} = U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Majorana

$$c_{2j-1} = a_j + a_j^\dagger \quad \rightarrow \quad a_j = \frac{1}{2}(c_{2j-1} + i c_{2j})$$

$$c_{2j} = -i(a_j - a_j^\dagger) \quad a_j^\dagger = \frac{1}{2}(c_{2j-1} - i c_{2j})$$

done

$$H_U = \frac{U}{8} \sum_i \underbrace{(c_{2j-1} - i c_{2j})(c_{2j-1} + i c_{2j})(c_{2j-1} - i c_{2j})(c_{2j-1} + i c_{2j})}_{n_{i\uparrow} n_{i\downarrow}}$$

~~$$n_{i\uparrow} n_{i\downarrow} = c_{2j-1} c_{2j-1} - i c_{2j} c_{2j-1} + i c_{2j-1} c_{2j} + c_{2j} c_{2j}$$~~

$$= 2(1 + i c_{2j-1} c_{2j})$$

$$= \frac{4U}{8} \sum_i (1 + i c_{2j-1} c_{2j}) (1 + i c_{2j-1} c_{2j})$$

$$= \frac{U}{2} \sum_i (1 + i(c_{2j-1} c_{2j} + c_{2j} c_{2j-1}) + c_{2j-1} c_{2j} c_{2j-1} c_{2j})$$

$$H_U = \frac{U}{2} + \frac{U}{2} \sum_{i\sigma} c_{2j-1\sigma} c_{2j\sigma} + \frac{U}{2} \sum_{i\sigma} c_{2j-1\sigma} c_{2j-1\sigma} c_{2j\sigma} c_{2j\sigma}$$

$\underbrace{\hspace{1.5cm}}_{\text{constant}}$
 $\underbrace{\hspace{1.5cm}}_{\text{chemical potential term}}$

example: Hubbard

$$H_U = U \sum_i a_{i\uparrow}^\dagger a_{i\uparrow} a_{i\downarrow}^\dagger a_{i\downarrow} = U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Majorana

$$c_{2j-1} = a_j + a_j^\dagger \quad \rightarrow \quad a_j = \frac{1}{2}(c_{2j-1} + i c_{2j})$$

$$c_{2j} = -i(a_j - a_j^\dagger) \quad \rightarrow \quad a_j^\dagger = \frac{1}{2}(c_{2j-1} - i c_{2j})$$

done

$$H_U = \frac{U}{8} \sum_i \underbrace{(c_{2j-1} - i c_{2j})(c_{2j-1} + i c_{2j})(c_{2j-1} - i c_{2j})(c_{2j-1} + i c_{2j})}$$

~~$$= \frac{U}{8} \sum_i n_{i\uparrow} n_{i\downarrow}$$~~

$$n_{i\uparrow} n_{i\downarrow} = c_{2j-1} c_{2j-1} - i c_{2j} c_{2j-1} + i c_{2j-1} c_{2j} + c_{2j} c_{2j}$$

$$= 2(1 + i c_{2j-1} c_{2j})$$

$$= \frac{4U}{8} \sum_i (1 + i c_{2j-1} c_{2j}) (1 + i c_{2j-1} c_{2j})$$

$$= \frac{U}{2} \sum_i (1 + i(c_{2j-1\uparrow} c_{2j\uparrow} + c_{2j\downarrow} c_{2j-1\downarrow})) = c_{2j-1\uparrow} c_{2j\uparrow} + c_{2j-1\downarrow} c_{2j\downarrow}$$

$$H_U = \underbrace{\frac{U}{2}}_{\text{constant}} + \underbrace{\frac{U}{2} \sum_{i\sigma} c_{2j-1\sigma} c_{2j\sigma}}_{\text{chemical potential term}} + \frac{U}{2} \sum_{i\sigma} c_{2j-1\uparrow} c_{2j-1\downarrow} c_{2j\uparrow} c_{2j\downarrow}$$