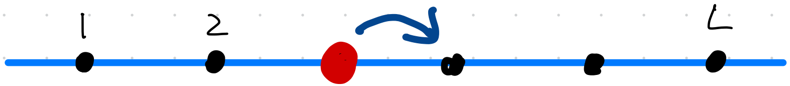
Integrable and non-integrable quantum spin chains

part Ia free fermions on the chain

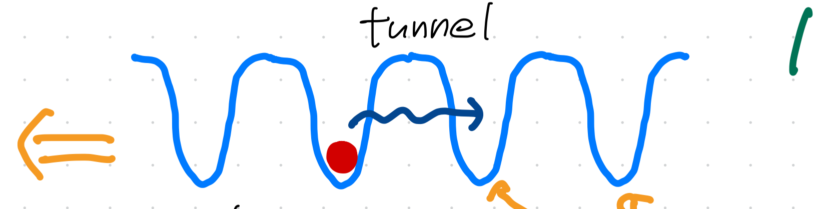
Advanced Topics in Statistical Physics
by Hal Tasaki

§ single particle on $\Lambda = \{1, \dots, L\}$



tight-binding description

$\Longleftarrow$



a particle in a periodic potential

atomic sites

state (wave function)

$$\varphi_u \in \mathbb{C}, \quad u = 1, \dots, L \qquad (1)$$

column vector $$\varphi = \begin{pmatrix} \varphi_1 \\ \varphi_2 \\ \vdots \\ \varphi_L \end{pmatrix} \in \mathbb{C}^L \qquad (2)$$

tight-binding Schrödinger equation

$$-t(\varphi_{u+1} + \varphi_{u-1}) = \epsilon \varphi_u \qquad (3) \quad (u = 1, \dots, L) \qquad \varphi_0 = \varphi_L, \ \varphi_{L+1} = \varphi_1$$

periodic b.c.

$t \in \mathbb{R}$ hopping amplitude

energy eigenvalue

vector form

hopping matrix T

$$(T)_{uv} = \begin{cases} -t, & |u - v| = 1 \\ 0, & \text{otherwise} \end{cases} \qquad (4)$$

$$(3) \Leftrightarrow \sum_{v \in \Lambda} (T)_{uv} \varphi_v = \epsilon \varphi_u \quad (u = 1, \dots, L) \qquad (5)$$

$$T \varphi = \epsilon \varphi \qquad (6)$$

energy eigenstates

$$\psi_u^{(k)} = \frac{1}{\sqrt{L}} e^{iku} \quad (1)$$

wave number $k \in (0, 2\pi]$

$$k \in K = \left\{ \frac{2\pi n}{L} \;\middle|\; n = 1, \cdots, L \right\} \quad (2)$$

$(e^{ikL} = 1 \text{ for } k \in K)$

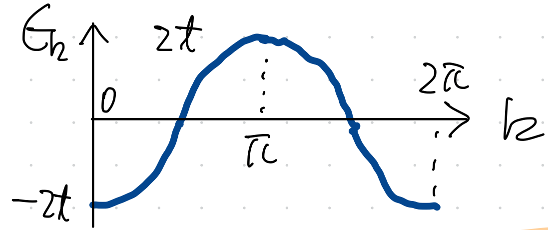
substituting into p1-(3)

$$-t(\psi_{u+1}^{(k)} + \psi_{u-1}^{(k)}) = -t \frac{1}{\sqrt{L}} (e^{ik(u+1)} + e^{ik(u-1)}) = \underbrace{-t(e^{ik} + e^{-ik})}_{= \epsilon_k} \underbrace{\frac{1}{\sqrt{L}} e^{iku}}_{= \psi_u^{(k)}} \quad (3)$$

energy eigenvalues

$$\epsilon_k = -2t \cos k \quad (4)$$

$$(k \in K)$$



cosine band

vector form

$$T \psi^{(k)} = \epsilon_k \psi^{(k)} \quad (5)$$

$$\langle \psi^{(k)}, \psi^{(k')} \rangle = \delta_{k,k'} \quad (6) \quad (k, k' \in K)$$

$$\left(\langle \varphi, \psi \rangle = \sum_{u \in \Lambda} \varphi_u^* \psi_u \quad (7) \right)$$

$$\sum_{u=1}^{L} \frac{1}{L} e^{i(k'-k)u} = \sum_{u=1}^{L} \frac{1}{L} e^{i \frac{2\pi(n'-n)}{L} u} = \begin{cases} 0, & n \neq n' \\ 1, & n = n' \end{cases}$$

§ many fermions on $\Lambda = \{1, \cdots, L\}$

two-particle wave function $\quad \Phi_{u,v} = -\Phi_{v,u} \in \mathbb{C} \quad (1)$

wave function changes its sign when the labels of two particles are exchanged

N-particle wave function $(1 \leq N \leq L)$

$$\Phi_{u_1, u_2, \cdots, u_N} = (-1)^P \, \Phi_{u_{P(1)}, u_{P(2)}, \cdots, u_{P(N)}} \quad (2)$$

P: permutation of $\{1, \cdots, N\}$, $(-1)^P$ parity

Schrödinger equation for free (non-interacting) fermions

$$-t \sum_{j=1}^{N} \left(\Phi_{u_1, \cdots, u_{j-1}, u_j+1, u_{j+1}, \cdots, u_N} + \Phi_{u_1, \cdots, u_{j-1}, u_j-1, u_{j+1}, \cdots, u_N} \right) = E \, \Phi_{u_1, \cdots, u_N} \quad (3)$$

energy eigenstates and eigenvalues $\quad k_1, \cdots, k_N \in K, \; 0 < k_1 < k_2 < \cdots < k_N \leq 2\pi$

$$\Psi^{(k_1, \cdots, k_N)}_{u_1, \cdots, u_N} = \frac{1}{\sqrt{N!}} \sum_P (-1)^P \psi^{(k_1)}_{u_{P(1)}} \psi^{(k_2)}_{u_{P(2)}} \cdots \psi^{(k_N)}_{u_{P(N)}} \quad (4)$$

Slater determinant

$$E_{k_1, \cdots, k_N} = \sum_{j=1}^{N} \epsilon_{k_j} \quad (5)$$

§ creation/annihilation operators and many-fermion states

$$\begin{cases} \hat{c}_u : \text{annihilates a particle at site } u \in \Lambda \\ \hat{c}_u^\dagger : \text{creates a particle at site } u \in \Lambda \end{cases}$$

$\hat{I}\,\delta_{u,v}$

canonical anticommutation relations (CAR)

$$\{\hat{c}_u, \hat{c}_v\} = \{\hat{c}_u^\dagger, \hat{c}_v^\dagger\} = 0 \quad (1) \qquad \{\hat{c}_u, \hat{c}_v^\dagger\} = \delta_{u,v} \quad (2)$$

$$\hat{c}_u^2 = \hat{c}_u^{\dagger 2} = 0, \quad \hat{c}_u\hat{c}_v = -\hat{c}_v\hat{c}_u \ (u \neq v), \quad \hat{c}_u\hat{c}_u^\dagger = 1 - \hat{c}_u^\dagger\hat{c}_u$$

$|\Phi_0\rangle$ state with no particles $\qquad \langle\Phi_0|\Phi_0\rangle = 1 \quad (3)$

$$\hat{c}_u|\Phi_0\rangle = 0 \text{ for } {}^\forall u \in \Lambda \quad (4)$$

1-particle states

$|u\rangle = \hat{c}_u^\dagger|\Phi_0\rangle \quad (5)$ state with a particle at u

$$\langle u|u\rangle = \langle\Phi_0|\hat{c}_u\hat{c}_u^\dagger|\Phi_0\rangle = \langle\Phi_0|(1-\hat{c}_u^\dagger\hat{c}_u)|\Phi_0\rangle = \langle\Phi_0|\Phi_0\rangle = 1 \quad (6)$$

$$u \neq v \quad \langle u|v\rangle = \langle\Phi_0|\hat{c}_u\hat{c}_v^\dagger|\Phi_0\rangle = -\langle\Phi_0|\hat{c}_v^\dagger\hat{c}_u|\Phi_0\rangle = 0 \quad (7)$$

2-particle states

$\hat{c}_u^\dagger \hat{c}_v^\dagger |\Phi_0\rangle$ (1) state with particles at $u, v \in \Lambda$

$\hat{c}_u^\dagger \hat{c}_u^\dagger |\Phi_0\rangle = 0$ (2) Pauli exclusion principle

$\hat{c}_u^\dagger \hat{c}_v^\dagger |\Phi_0\rangle = -\hat{c}_v^\dagger \hat{c}_u^\dagger |\Phi_0\rangle$ (3) symmetry of fermionic states

2-particle Hilbert space $\mathcal{H}_2$

spanned by $\hat{c}_u^\dagger \hat{c}_v^\dagger |\Phi_0\rangle$ with $1 \leq u < v \leq L$

N-particle Hilbert space $\mathcal{H}_N$ ($1 \leq N \leq L$)

spanned by $\hat{c}_{u_1}^\dagger \hat{c}_{u_2}^\dagger \cdots \hat{c}_{u_N}^\dagger |\Phi_0\rangle$ with $1 \leq u_1 < u_2 < \cdots < u_N \leq L$

$\longleftrightarrow$ orthonormal basis

(the inner product is defined by p4-(3) and p4-(2))

§ number operator

$$\hat{n}_u = \hat{c}^\dagger_u \hat{c}_u \quad (1)$$

$$\rightarrow \hat{n}_u^2 = \hat{c}^\dagger_u \overbrace{\hat{c}_u \hat{c}^\dagger_u}^{= 1 - \hat{c}^\dagger_u \hat{c}_u} \hat{c}_u = \hat{c}^\dagger_u \hat{c}_u = \hat{n}_u \quad (2)$$

$$\hat{n}_u^2 - \hat{n}_u = \hat{n}_u(\hat{n}_u - 1) = 0 \quad (3) \rightarrow \text{e.v. of } \hat{n}_u = 0 \text{ or } 1$$

$$[\hat{n}_u, \hat{c}^\dagger_u] = \underbrace{\hat{c}^\dagger_u \hat{c}_u}_{= 1 - \hat{c}_u \hat{c}^\dagger_u} \hat{c}^\dagger_u - \underbrace{\hat{c}^\dagger_u \hat{c}^\dagger_u}_{= 0} \hat{c}_u = \hat{c}^\dagger_u \quad (4) \qquad [\hat{n}_u, \hat{c}^\dagger_v] = 0 \quad (5) \quad u \neq v$$

$$[\hat{n}_u, \hat{c}^\dagger_v] = \delta_{u,v} \hat{c}^\dagger_u \quad (6) \qquad \hat{n}_u |\Phi_0\rangle = 0 \quad (7)$$

$\hat{n}_u$ counts the number of particles at site u

$$\hat{n}_u \hat{c}^\dagger_u |\Phi_0\rangle = (\hat{c}^\dagger_u + \hat{c}^\dagger_u \hat{n}_u)|\Phi_0\rangle = \hat{c}^\dagger_u |\Phi_0\rangle \quad (8)$$

$$\hat{n}_u \hat{c}^\dagger_v |\Phi_0\rangle = \hat{c}^\dagger_v \hat{n}_u |\Phi_0\rangle = 0 \quad (9) \qquad u \neq v$$

$$\hat{n}_u \hat{c}^\dagger_{u_1} \cdots \hat{c}^\dagger_{u_N} |\Phi_0\rangle = \begin{cases} 0, & u \notin \{u_1, \cdots, u_N\} \\ \hat{c}^\dagger_{u_1} \cdots \hat{c}^\dagger_{u_N} |\Phi_0\rangle, & u \in \{u_1, \cdots, u_N\} \end{cases} \quad (10)$$

§ fermion operators for general single-particle states

$$\hat{c}^\dagger(\varphi) = \sum_{u\in\Lambda} \varphi_u \hat{c}_u^\dagger \quad (1)$$

creates a particle in state $\varphi = \begin{pmatrix} \varphi_1 \\ \vdots \\ \varphi_L \end{pmatrix}$

$$\hat{c}^\dagger(\alpha\varphi + \beta\psi) = \alpha\,\hat{c}^\dagger(\varphi) + \beta\,\hat{c}^\dagger(\psi) \quad (2)$$

$$\{\hat{c}(\varphi), \hat{c}^\dagger(\psi)\} = \sum_{u,v\in\Lambda} \varphi_u^* \psi_v \{\hat{c}_u, \hat{c}_v^\dagger\} = \sum_{u\in\Lambda} \varphi_u^* \psi_u = \langle \varphi, \psi \rangle \quad (3)$$

§ operators corresponding to matrices

A $L\times L$ matrix with entries $(A)_{uv} \in \mathbb{C}$, $u,v\in\Lambda$

$$\hat{B}(A) = \sum_{u,v\in\Lambda} \hat{c}_u^\dagger (A)_{uv} \hat{c}_v \quad (4) \qquad \hat{B}(A)|\Phi_0\rangle = 0 \quad (5)$$

$$[\hat{B}(A), \hat{c}^\dagger(\varphi)] = \sum_{u,v,w\in\Lambda} (A)_{uv} \varphi_w [\hat{c}_u^\dagger \hat{c}_v, \hat{c}_w^\dagger]$$

$$[\hat{c}_u^\dagger \hat{c}_v, \hat{c}_w^\dagger] = \hat{c}_u^\dagger \underbrace{\hat{c}_v \hat{c}_w^\dagger}_{\delta_{v,w} - \hat{c}_w^\dagger \hat{c}_v} - \hat{c}_w^\dagger \hat{c}_u^\dagger \hat{c}_v = \delta_{v,w} \hat{c}_u^\dagger$$

$$= \sum_{u,v\in\Lambda} (A)_{uv} \varphi_v \hat{c}_u^\dagger = \sum_{u\in\Lambda} (A\varphi)_u \hat{c}_u^\dagger = \hat{c}^\dagger(A\varphi) \quad (6)$$

$$[\hat{B}(A), \hat{B}(A')] = \hat{B}([A, A']) \quad (7)$$

→ part Ib

§ many-body Hamiltonian and energy eigenstates

T : hopping matrix p1-(4)

$$\hat{H} = \hat{B}(T) = -t \sum_{u \in \Lambda} (\hat{c}_u^\dagger \hat{c}_{u+1} + \hat{c}_{u+1}^\dagger \hat{c}_u) \quad (1) \qquad \hat{H}|\Phi_0\rangle = 0 \quad (2)$$

$$\hat{H}\,\hat{c}^\dagger(\varphi)|\Phi_0\rangle = [\hat{B}(T), \hat{c}^\dagger(\varphi)]|\Phi_0\rangle = \hat{c}^\dagger(T\varphi)|\Phi_0\rangle \quad (3)$$

single-particle Schrödinger equation

p1-(6) $$T\varphi = \epsilon\varphi \quad (4)$$

$$\Updownarrow$$

$$\hat{H}\,\hat{c}^\dagger(\varphi)|\Phi_0\rangle = \epsilon\,\hat{c}^\dagger(\varphi)|\Phi_0\rangle \quad (5)$$

many-particle Schrödinger equation for free fermions (p3-(3))

$$\hat{H}|\Phi\rangle = E|\Phi\rangle \quad (6) \qquad |\Phi\rangle \in \mathcal{H}_N \quad (7)$$

creation operator for $\psi^{(k)}$ $(k\in K)$ p2-(1)

$$\hat{a}_k^\dagger = \hat{c}^\dagger(\psi^{(k)}) = \frac{1}{\sqrt{L}} \sum_{u\in\Lambda} e^{iku}\, \hat{c}_u^\dagger \qquad (1)$$

Canonical anticommutation relations!

p7-(3)

$$\{\hat{a}_k, \hat{a}_{k'}\} = \{\hat{a}_k^\dagger, \hat{a}_{k'}^\dagger\} = 0 \quad (2) \qquad \{\hat{a}_k, \hat{a}_{k'}^\dagger\} = \langle \psi^{(k)}, \psi^{(k')}\rangle = \delta_{k,k'} \quad (3)$$

$$[\hat{H}, \hat{a}_k^\dagger] = [\hat{B}(T), \hat{c}^\dagger(\psi^{(k)})] = \hat{c}^\dagger(T\psi^{(k)}) = \epsilon_k \hat{c}^\dagger(\psi_k) = \epsilon_k \hat{a}_k^\dagger \quad (4)$$

for given N, choose $k_1, \dots, k_N \in K$ s.t. $0 < k_1 < k_2 \cdots < k_N \leq 2\pi$

$$\hat{H}\, \boxed{\hat{a}_{k_1}^\dagger \cdots \hat{a}_{k_N}^\dagger |\Phi_0\rangle} = \epsilon_{k_1} \hat{a}_{k_1}^\dagger \cdots \hat{a}_{k_N}^\dagger |\Phi_0\rangle + \hat{a}_{k_1}^\dagger \hat{H} \hat{a}_{k_2}^\dagger \cdots \hat{a}_{k_N}^\dagger |\Phi_0\rangle$$

$$= (\epsilon_{k_1} + \epsilon_{k_2}) \hat{a}_{k_1}^\dagger \cdots \hat{a}_{k_N}^\dagger |\Phi_0\rangle + \hat{a}_{k_1}^\dagger \hat{a}_{k_2}^\dagger \hat{H} \hat{a}_{k_3}^\dagger \cdots \hat{a}_{k_N}^\dagger |\Phi_0\rangle$$

$\hat{H}|\Phi_0\rangle = 0$

$$= (\epsilon_{k_1} + \cdots + \epsilon_{k_N})\, \boxed{\hat{a}_{k_1}^\dagger \cdots \hat{a}_{k_N}^\dagger |\Phi_0\rangle} \qquad (5)$$

energy eigenvalue $E_{k_1,\dots,k_N}$

(we also have $\hat{H} = \sum_{k\in K} \epsilon_k \hat{a}_k^\dagger \hat{a}_k$ (6))

energy eigenvalues

$$E_{k_1,\cdots,k_N} = \sum_{j=1}^{N} \epsilon_{k_j} \quad (1)$$

the same as p3-(5)

energy eigenstates

$$|\Psi_{k_1,\cdots,k_N}\rangle = \hat{a}^{\dagger}_{k_1} \cdots \hat{a}^{\dagger}_{k_N} |\Phi_0\rangle$$

$$= \sum_{u_1,\cdots,u_N \in \Omega} \psi^{(k_1)}_{u_1} \cdots \psi^{(k_N)}_{u_N} \hat{c}^{\dagger}_{u_1} \hat{c}^{\dagger}_{u_2} \cdots \hat{c}^{\dagger}_{u_N} |\Phi_0\rangle \quad (2)$$

(equivalent to the Slater determinant expression p3-(4)

$$\Psi^{(k_1,\cdots,k_N)}_{u_1,\cdots,u_N} = \frac{1}{\sqrt{N!}} \sum_{P} (-1)^P \psi^{(k_1)}_{u_{P(1)}} \psi^{(k_2)}_{u_{P(2)}} \cdots \psi^{(k_N)}_{u_{P(N)}} \quad (3)$$

)

§ general free fermion system on lattice Λ

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Λ any finite set (lattice) wave function $\varphi = (\varphi_u)_{u\in\Lambda}$ (1)

single-particle Schrödinger equation $\mathsf{T}\varphi = \epsilon\varphi$ (2)

hopping matrix $\mathsf{T} = \mathsf{T}^\dagger$ (3) ($-(\mathsf{T})_{uv}$: hopping amplitude for $u \neq v$, $(\mathsf{T})_{uu}$: on-site potential)

single-particle energy e.s. $\mathsf{T}\psi^{(\alpha)} = \epsilon_\alpha \psi^{(\alpha)}$ ($\alpha = 1, \ldots, |\Lambda|$) (4)

the number of elements in Λ

many-body Hamiltonian and energy eigenstates

$$\hat{H} = \hat{B}(\mathsf{T}) = \sum_{u,v\in\Lambda} (\mathsf{T})_{uv}\, \hat{c}_u^\dagger \hat{c}_v \quad (5) \qquad \hat{a}_\alpha^\dagger = \hat{c}^\dagger(\psi^{(\alpha)}) \quad (6)$$

$$|\Psi_{\alpha_1,\ldots,\alpha_N}\rangle = \hat{a}_{\alpha_1}^\dagger \cdots \hat{a}_{\alpha_N}^\dagger |\Phi_0\rangle \quad (7)$$

$$\hat{H}|\Psi_{\alpha_1,\ldots,\alpha_N}\rangle = \Big(\sum_{j=1}^{N} \epsilon_{\alpha_j}\Big)|\Psi_{\alpha_1,\ldots,\alpha_N}\rangle \quad (8)$$

(also note $(\mathsf{T})_{uv} = \sum_{\alpha=1}^{|\Lambda|} \psi_u^{(\alpha)} \epsilon_\alpha \big(\psi_v^{(\alpha)}\big)^* \quad (9) \qquad \hat{H} = \hat{B}(\mathsf{T}) = \sum_{\alpha=1}^{|\Lambda|} \epsilon_\alpha\, \hat{a}_\alpha^\dagger \hat{a}_\alpha \quad (10)$)

§ notes

formalism based on the creation/annihilation operator (a.k.a. "second quantization")

- standard description of many-particle quantum mechanics
- equivalent to the wave function description

see, e.g., my lecture note:
H. Tasaki, arXiv:1812.10732

Hubbard model

tight-binding model of electrons with on-site interaction

$\hat{c}^\dagger_{u,\sigma}, \hat{c}_{u,\sigma}$: creation/annihilation operators of an electron at site $u \in \Lambda$ with spin $\sigma = \uparrow, \downarrow$

Λ any lattice

$$\hat{H} = \overbrace{-\sum_{\substack{u,v\in\Lambda \\ (u\neq v) \\ \sigma=\uparrow,\downarrow}} t_{uv}\,\hat{c}^\dagger_{u\sigma}\hat{c}_{v\sigma} + \sum_{\substack{u\in\Lambda \\ \sigma=\uparrow,\downarrow}} V_u\,\hat{n}_{u\sigma}}^{\hat{B}(T) \text{ with a suitabe matrix } T} + \underbrace{U\sum_{u\in\Lambda}\hat{n}_{u\uparrow}\,\hat{n}_{u\downarrow}}_{= \text{ on-site interaction}}$$

$t_{uv} = t_{vu}^* \in \mathbb{C}$, $V_u \in \mathbb{R}$ on-site potential

see, e.g., my review:
H. Tasaki, arXiv:cond-mat/9712219

ferro-, ferri-, antiferro-magnetism, metal/insulator trans., superconductivity ...

believed to describe various phenomena, but extremely difficult!