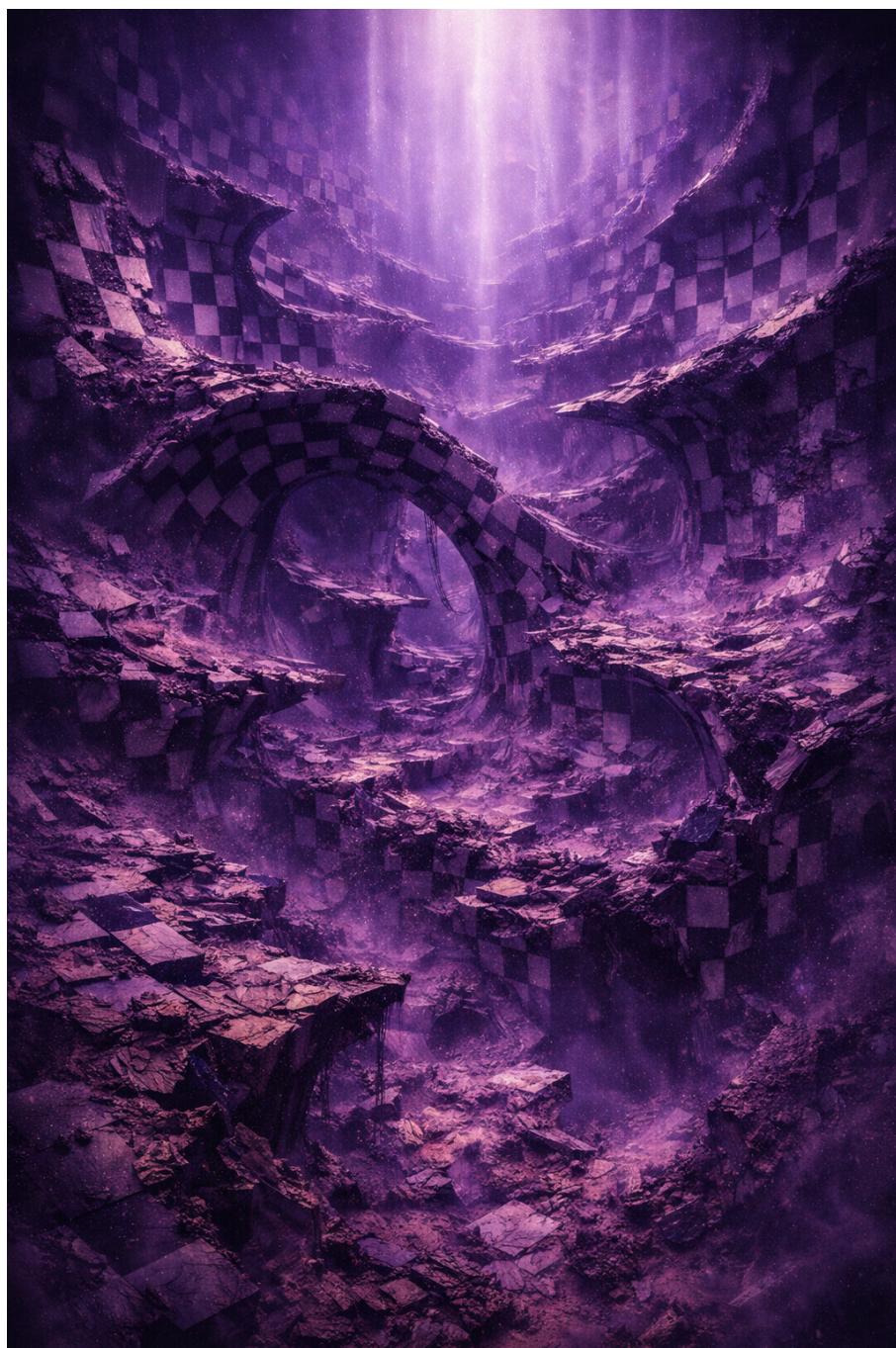


Fermi-Hubbard Model

Tristan.W

December 30, 2025



Contents

1 Fermi–Hubbard Model and Its Symmetries	3
1.1 Hamiltonian, conventions, and the shifted interaction form	3
1.2 Canonical ensemble description: conserved charges and constraints	3
1.3 Spin rotational symmetry	4
2 Particle–Hole Transformation	7
2.1 Why introduce a particle–hole transformation?	7
2.2 Naive PH transformation on one spin component	7
2.3 Bipartite lattices and the momentum-space form	8
2.4 Parameter mapping between repulsive and attractive models	9
3 Pairing and Antiferromagnetism: an exact correspondence	10
3.1 Attractive FHM with balanced spins: pairing order and competing CDW	10
3.2 Mapping to repulsive half-filled FHM: SDW/AFM order parameter	11
3.3 $U(1)$ degeneracy: pairing phase vs spin azimuth	12
3.4 Why infinitesimal interaction can order in weak coupling	12
4 Transition-temperature scales and strong-coupling effective models	13
4.1 Weak-coupling estimates	13
4.2 Strong coupling on the repulsive side: superexchange and Heisenberg limit . . .	13
4.3 Strong coupling on the attractive side: pair formation vs pair condensation . .	15
5 $SO(4)$ Symmetry at $\mu = h = 0$ and its consequences	16
5.1 Two commuting $SU(2)$ ’s and the $SU(2) \times SU(2)/\mathbb{Z}_2$ structure	16
5.2 Two-dimensional consequence: order-parameter manifold and KT transition . .	16
5.3 Experimental signatures under the mapping	17
6 Open problems and physical pictures	17
6.1 Near half-filling in 2D: d -wave superconductivity?	17
6.2 Low density: itinerant ferromagnetism vs strong-correlation alternatives . . .	18
A Ensemble theory primer: microcanonical, canonical, and grand-canonical	18
A.1 Why ensembles at all?	18
A.2 Microcanonical ensemble: fixed (E, N, S^z)	19
A.3 Canonical ensemble: fixed (N, S^z) , fluctuating E	19
A.4 Grand-canonical ensemble: fixed (T, μ, h) , fluctuating (E, N, S^z)	20
A.5 Legendre transforms: switching the control variables	20
A.6 Hard constraint vs Lagrange multiplier (and why canonical is often natural for cold atoms)	21
A.7 When can ensembles differ? (phase separation and convexity)	21
B Pauli matrices, spinor bilinears, and $SU(2)$ generators	22
B.1 Pauli algebra and completeness (Fierz) identity	22
B.2 The generator \mathbf{S}	22
B.3 Useful operator identities on a single site	22

1 Fermi–Hubbard Model and Its Symmetries

1.1 Hamiltonian, conventions, and the shifted interaction form

Fermi–Hubbard Hamiltonian.

We consider spin-1/2 fermions on a lattice with annihilation operators $\hat{c}_{i\sigma}$ ($\sigma = \uparrow, \downarrow$). The local number operators are

$$\hat{n}_{i\sigma} \equiv \hat{c}_{i\sigma}^\dagger \hat{c}_{i\sigma}, \quad \hat{n}_i \equiv \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}, \quad \hat{S}_{zi} \equiv \frac{1}{2}(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}). \quad (1)$$

A convenient parametrization of the FHM is

$$\hat{H}_{\text{FH}} = -J \sum_{\langle ij \rangle, \sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{h.c.}) + U \sum_i \left(\hat{n}_{i\uparrow} - \frac{1}{2} \right) \left(\hat{n}_{i\downarrow} - \frac{1}{2} \right) - \mu \sum_i \hat{n}_i - 2h \sum_i \hat{S}_{zi}. \quad (2)$$

Here $J > 0$ is the nearest-neighbor hopping amplitude, U is the on-site interaction, μ is the chemical potential controlling the total density, and h is a Zeeman field coupling to the spin polarization.

Note that (??) is written in the grand-canonical form, which allows particle-number fluctuations.

Why write $U(\hat{n}_{i\uparrow} - \frac{1}{2})(\hat{n}_{i\downarrow} - \frac{1}{2})$?

A pure reparametrization (plus a constant). Expand the shifted interaction:

$$U \left(\hat{n}_{i\uparrow} - \frac{1}{2} \right) \left(\hat{n}_{i\downarrow} - \frac{1}{2} \right) = U \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \frac{U}{2} \hat{n}_i + \frac{U}{4}. \quad (3)$$

Summing over sites,

$$U \sum_i \left(\hat{n}_{i\uparrow} - \frac{1}{2} \right) \left(\hat{n}_{i\downarrow} - \frac{1}{2} \right) = U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \frac{U}{2} \sum_i \hat{n}_i + \frac{U}{4} N_s, \quad (4)$$

where N_s is the number of lattice sites. Therefore, compared with the more common form $U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \mu \sum_i \hat{n}_i$, the shifted form is exactly equivalent to the replacement

$$\mu \longrightarrow \mu + \frac{U}{2}, \quad (5)$$

up to an additive constant $UN_s/4$ which does not affect dynamics or thermodynamics.

Why it is useful. This form makes the particle–hole symmetry around half filling ($\mu = 0$ in this convention) manifest, and simplifies the particle–hole mapping discussed in Chapter 2.

1.2 Canonical ensemble description: conserved charges and constraints

In the canonical ensemble we fix particle numbers instead of introducing μ and h . Dropping the μ and h terms, the Hamiltonian is

$$\hat{H}_{\text{FH}} = -J \sum_{\langle ij \rangle, \sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{h.c.}) + U \sum_i \left(\hat{n}_{i\uparrow} - \frac{1}{2} \right) \left(\hat{n}_{i\downarrow} - \frac{1}{2} \right). \quad (6)$$

The conserved particle numbers are

$$N_\sigma \equiv \sum_i \langle \hat{n}_{i\sigma} \rangle, \quad N \equiv N_\uparrow + N_\downarrow. \quad (7)$$

It is common to package them into

$$\delta \equiv N - N_s, \quad m \equiv N_\uparrow - N_\downarrow, \quad (8)$$

Here δ measures deviation from half filling, and is referred to as *doping*. m measures spin polarization, and is referred to as *spin imbalance*.

Because $0 \leq N \leq 2N_s$, one has $-N_s \leq \delta \leq N_s$; similarly $-N_s \leq m \leq N_s$.

Grand-canonical vs canonical: what does “impose constraints” mean?

Two equivalent viewpoints.

We recommend the readers to Appendix A for a more detailed discussion on ensembles.

- In the grand-canonical ensemble, one minimizes the thermodynamic potential with Lagrange multipliers:

$$\hat{H}_{\text{GC}} = \hat{H}_{\text{FH}} - \mu \hat{N} - 2h \hat{S}^z, \quad \hat{N} \equiv \sum_i \hat{n}_i, \quad \hat{S}^z \equiv \sum_i \hat{S}_{zi}. \quad (9)$$

Here μ and h fix $\langle \hat{N} \rangle$ and $\langle \hat{S}^z \rangle$ on average, allowing fluctuations.

- In the canonical ensemble, one restricts the Hilbert space to the sector with fixed $(N_\uparrow, N_\downarrow)$, equivalently fixed (δ, m) . This is what “impose constraints” means: δ and m are *sharp* quantum numbers and do not fluctuate.

Why use canonical language here. In many cold-atom realizations, N_\uparrow and N_\downarrow are (to good approximation) fixed by preparation, so δ and m are control parameters rather than fluctuating thermodynamic variables. The grand-canonical description is still useful (and becomes equivalent in the thermodynamic limit), but the particle-hole mapping in Chapter 2 acts very transparently on (δ, m) .

1.3 Spin rotational symmetry

In this section, we will repeatedly use the completeness (Fierz) identity:

$$\sum_{a=1}^3 (\sigma^a)_{\alpha\beta} (\sigma^a)_{\gamma\delta} = 2\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\beta}\delta_{\gamma\delta}, \quad (10)$$

and the canonical fermion anticommutation relation (CAR):

$$\{\hat{c}_{i\sigma}, \hat{c}_{j\sigma'}^\dagger\} = \delta_{ij} \delta_{\sigma\sigma'}, \quad \{\hat{c}_{i\sigma}, \hat{c}_{j\sigma'}\} = \{\hat{c}_{i\sigma}^\dagger, \hat{c}_{j\sigma'}^\dagger\} = 0. \quad (11)$$

The spin operator. Define the on-site spin operator by the standard spinor bilinear

$$\hat{S}_i \equiv \frac{1}{2} \hat{c}_{ia}^\dagger \sigma_{\alpha\beta} \hat{c}_{i\beta}, \quad (12)$$

where $\sigma = (\sigma^x, \sigma^y, \sigma^z)$ are Pauli matrices and repeated spin indices $\alpha, \beta \in \{\uparrow, \downarrow\}$ are summed.

Derivation of $\frac{1}{2}\hat{n}_i^2 = \hat{n}_i - \frac{2}{3}\hat{S}_i^2$

Step 1: compute \hat{S}_i^2 using completeness.

Starting from (12),

$$\hat{S}_i^2 = \sum_{a=1}^3 \hat{S}_i^a \hat{S}_i^a = \frac{1}{4} \sum_a (\hat{c}_{i\alpha}^\dagger (\sigma^a)_{\alpha\beta} \hat{c}_{i\beta}) (\hat{c}_{i\gamma}^\dagger (\sigma^a)_{\gamma\delta} \hat{c}_{i\delta}). \quad (13)$$

Insert (10):

$$\hat{S}_i^2 = \frac{1}{4} [2 \hat{c}_{i\alpha}^\dagger \hat{c}_{i\beta} \hat{c}_{i\beta}^\dagger \hat{c}_{i\alpha} - \hat{c}_{i\alpha}^\dagger \hat{c}_{i\alpha} \hat{c}_{i\gamma}^\dagger \hat{c}_{i\gamma}]. \quad (14)$$

Use $\hat{c}_{i\beta} \hat{c}_{i\beta}^\dagger = 1 - \hat{n}_{i\beta}$ and fermionic anticommutation to simplify. (The detailed derivation is left in the end of this box.) One finds the standard result

$$\hat{S}_i^2 = \frac{3}{4} (\hat{n}_i - 2\hat{D}_i), \quad \hat{D}_i \equiv \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}. \quad (15)$$

Step 2: relate \hat{n}_i^2 to \hat{D}_i . Since $\hat{n}_{i\sigma}^2 = \hat{n}_{i\sigma}$ for fermions,

$$\hat{n}_i^2 = (\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow})^2 = \hat{n}_i + 2\hat{D}_i. \quad (16)$$

Step 3: eliminate \hat{D}_i . From (??), $\hat{D}_i = \frac{1}{2}\hat{n}_i - \frac{2}{3}\hat{S}_i^2$. Insert into (16):

$$\hat{n}_i^2 = \hat{n}_i + 2\left(\frac{1}{2}\hat{n}_i - \frac{2}{3}\hat{S}_i^2\right) = 2\hat{n}_i - \frac{4}{3}\hat{S}_i^2. \quad (17)$$

Therefore

$$\boxed{\frac{1}{2}\hat{n}_i^2 = \hat{n}_i - \frac{2}{3}\hat{S}_i^2.} \quad (18)$$

■ **Derivation:** Eq. (14) \Rightarrow Eq. (15).

Start from Eq. (14):

$$\hat{S}_i^2 = \frac{1}{4} [2 \hat{c}_{i\alpha}^\dagger \hat{c}_{i\beta} \hat{c}_{i\beta}^\dagger \hat{c}_{i\alpha} - \hat{c}_{i\alpha}^\dagger \hat{c}_{i\alpha} \hat{c}_{i\gamma}^\dagger \hat{c}_{i\gamma}].$$

We simplify the two brackets separately.

(I) The first bracket. Using the CAR $\{\hat{c}_{i\beta}, \hat{c}_{i\beta}^\dagger\} = 1$, we have

$$\hat{c}_{i\beta} \hat{c}_{i\beta}^\dagger = 1 - \hat{n}_{i\beta}. \quad (19)$$

Hence

$$\begin{aligned} \hat{c}_{i\alpha}^\dagger \hat{c}_{i\beta} \hat{c}_{i\beta}^\dagger \hat{c}_{i\alpha} &= \hat{c}_{i\alpha}^\dagger (1 - \hat{n}_{i\beta}) \hat{c}_{i\alpha} \\ &= \hat{c}_{i\alpha}^\dagger \hat{c}_{i\alpha} - \hat{c}_{i\alpha}^\dagger \hat{n}_{i\beta} \hat{c}_{i\alpha}. \end{aligned} \quad (20)$$

Now note that $\hat{n}_{i\beta}$ is an even (bilinear) operator, so it commutes with $\hat{c}_{i\alpha}$ and $\hat{c}_{i\alpha}^\dagger$ (for any spin indices):

$$[\hat{n}_{i\beta}, \hat{c}_{i\alpha}] = 0, \quad [\hat{n}_{i\beta}, \hat{c}_{i\alpha}^\dagger] = 0. \quad (21)$$

Therefore

$$\hat{c}_{i\alpha}^\dagger \hat{n}_{i\beta} \hat{c}_{i\alpha} = \hat{n}_{i\beta} \hat{c}_{i\alpha}^\dagger \hat{c}_{i\alpha} = \hat{n}_{i\beta} \hat{n}_{i\alpha}. \quad (22)$$

Summing over $\alpha, \beta \in \{\uparrow, \downarrow\}$,

$$\begin{aligned} \sum_{\alpha, \beta} \hat{c}_{i\alpha}^\dagger \hat{c}_{i\beta} \hat{c}_{i\beta}^\dagger \hat{c}_{i\alpha} &= \sum_{\alpha, \beta} (\hat{n}_{i\alpha} - \hat{n}_{i\beta} \hat{n}_{i\alpha}) \\ &= \sum_{\alpha} (2\hat{n}_{i\alpha} - \hat{n}_i \hat{n}_{i\alpha}) \\ &= 2\hat{n}_i - \hat{n}_i^2. \end{aligned} \quad (23)$$

(II) The second bracket. The second term is simply

$$\sum_{\alpha, \gamma} \hat{c}_{i\alpha}^\dagger \hat{c}_{i\alpha} \hat{c}_{i\gamma}^\dagger \hat{c}_{i\gamma} = \left(\sum_{\alpha} \hat{n}_{i\alpha} \right) \left(\sum_{\gamma} \hat{n}_{i\gamma} \right) = \hat{n}_i^2. \quad (24)$$

(III) Combine. Plugging (23) and (24) into \hat{S}_i^2 ,

$$\hat{S}_i^2 = \frac{1}{4} [2(2\hat{n}_i - \hat{n}_i^2) - \hat{n}_i^2] = \hat{n}_i - \frac{3}{4} \hat{n}_i^2. \quad (25)$$

Finally, use $\hat{n}_{i\sigma}^2 = \hat{n}_{i\sigma}$ for fermions, so

$$\begin{aligned} \hat{n}_i^2 &= (\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow})^2 \\ &= \hat{n}_{i\uparrow}^2 + \hat{n}_{i\downarrow}^2 + 2\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \\ &= \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} + 2\hat{D}_i = \hat{n}_i + 2\hat{D}_i, \end{aligned} \quad (26)$$

where $\hat{D}_i \equiv \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$. Therefore

$$\hat{S}_i^2 = \hat{n}_i - \frac{3}{4}(\hat{n}_i + 2\hat{D}_i) = \frac{3}{4}(\hat{n}_i - 2\hat{D}_i). \quad (27)$$

This proves (15).

Rewriting the Hamiltonian and reading off symmetries. Using (15) and (3), one can rewrite the on-site interaction as

$$U\left(\hat{n}_{i\uparrow} - \frac{1}{2}\right)\left(\hat{n}_{i\downarrow} - \frac{1}{2}\right) = -\frac{2U}{3}\hat{S}_i^2 + \frac{U}{4}. \quad (28)$$

Thus (2) becomes

$$\hat{H}_{\text{FH}} = -J \sum_{\langle ij \rangle, \sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{h.c.}) - \frac{2U}{3} \sum_i \hat{S}_i^2 - \mu \sum_i \hat{n}_i - 2h \sum_i \hat{S}_{zi} + \frac{U}{4} N_s. \quad (29)$$

Dropping the constant $UN_s/4$ yields the commonly quoted form

$$\hat{H}_{\text{FH}} = -J \sum_{\langle ij \rangle, \sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{h.c.}) - \frac{2U}{3} \sum_i \hat{S}_i^2 - \mu \sum_i \hat{n}_i - 2h \sum_i \hat{S}_{zi}. \quad (30)$$

Spin symmetry at a glance.

- The on-site terms $\sum_i \hat{S}_i^2$ and $\sum_i \hat{n}_i$ are invariant under *independent* $SU(2)$ rotations on each site (local rotations), because they are built from on-site scalar bilinears.

- The hopping term couples different sites and is only invariant under a *global* $SU(2)$ rotation generated by total spin $\hat{S} \equiv \sum_i \hat{S}_i$. The generators are listed at the end of this box.
- If $h = 0$, the Hamiltonian has global $SU(2)$ spin rotational symmetry. If $h \neq 0$, the Zeeman term picks \hat{z} and reduces symmetry to $U(1)$ rotations about \hat{z} .

The generators of the global rotation symmetry are:

$$\hat{S}^x = \frac{1}{2} \sum_i (\hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow} + \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\uparrow}), \quad (31)$$

$$\hat{S}^y = \frac{i}{2} \sum_i (\hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow} - \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\uparrow}), \quad (32)$$

$$\hat{S}^z = \frac{1}{2} \sum_i (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}). \quad (33)$$

2 Particle–Hole Transformation

2.1 Why introduce a particle–hole transformation?

Relating different Hamiltonians by a unitary map.

If two Hamiltonians satisfy $\hat{H}' = \hat{U}^\dagger \hat{H} \hat{U}$, then their spectra are identical and their eigenstates are mapped by \hat{U}^\dagger . This allows us to deduce properties of one regime from another.

In FHM: repulsive \leftrightarrow attractive and $\mu \leftrightarrow h$.

A particularly useful symmetry in the FHM is a particle–hole (PH) transformation applied to one spin component. On bipartite lattices, it maps $U \rightarrow -U$ while exchanging the roles of μ and h , and it swaps the canonical labels (δ, m).

2.2 Naive PH transformation on one spin component

Definition (naive version).

Keep spin-up operators unchanged, and transform only spin-down:

$$\hat{c}_{i\uparrow} \rightarrow \hat{c}_{i\uparrow} ; \quad \hat{c}_{i\downarrow} \rightarrow \hat{c}_{i\downarrow}^\dagger , \quad \hat{c}_{i\downarrow}^\dagger \rightarrow \hat{c}_{i\downarrow}. \quad (34)$$

In the following we list the operator identities under (34).

◦ **Number operator.** Using $\hat{n}_{i\downarrow} = \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow}$ and the canonical anticommutation,

$$\hat{n}_{i\downarrow} \longrightarrow \hat{c}_{i\downarrow} \hat{c}_{i\downarrow}^\dagger = 1 - \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow} = 1 - \hat{n}_{i\downarrow}. \quad (35)$$

◦ **Shifted interaction flips sign.** Since $\hat{n}_{i\downarrow} - \frac{1}{2} \rightarrow -(\hat{n}_{i\downarrow} - \frac{1}{2})$, we have

$$U\left(\hat{n}_{i\uparrow} - \frac{1}{2}\right)\left(\hat{n}_{i\downarrow} - \frac{1}{2}\right) \longrightarrow -U\left(\hat{n}_{i\uparrow} - \frac{1}{2}\right)\left(\hat{n}_{i\downarrow} - \frac{1}{2}\right). \quad (36)$$

◦ **Chemical potential and Zeeman terms exchange.**

Under $\hat{n}_{i\downarrow} \rightarrow 1 - \hat{n}_{i\downarrow}$,

$$\hat{n}_i = \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} \longrightarrow \hat{n}_{i\uparrow} + 1 - \hat{n}_{i\downarrow} = (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}) + 1, \quad (37)$$

$$(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}) \longrightarrow \hat{n}_{i\uparrow} - (1 - \hat{n}_{i\downarrow}) = (\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}) - 1. \quad (38)$$

Therefore

$$-\mu \sum_i \hat{n}_i \longrightarrow -\mu \sum_i (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}) - \mu N_s, \quad (39)$$

$$-2h \sum_i \hat{S}_{zi} = -h \sum_i (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}) \longrightarrow -h \sum_i (\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}) + hN_s. \quad (40)$$

Thus μ and h exchange roles, modulo additive constants.

◦ **Kinetic term changes sign for \downarrow .**

For $i \neq j$, $\hat{c}_{i\downarrow}^\dagger \hat{c}_{j\downarrow} \rightarrow \hat{c}_{i\downarrow} \hat{c}_{j\downarrow}^\dagger = -\hat{c}_{j\downarrow}^\dagger \hat{c}_{i\downarrow}$. This flips the sign of the \downarrow -hopping term (after relabeling bonds).

Thus, this naive particle-hole transformation does not preserve the kinetic term, motivating an improved version.

2.3 Bipartite lattices and the momentum-space form

The naive PH map flips the sign of the \downarrow kinetic energy. On a bipartite lattice one can restore invariance by attaching a sublattice-dependent sign.

■ **Definition of Bipartite lattice.**

A lattice is bipartite if sites can be split into A and B sublattices such that hopping occurs only between A and B , never within A or within B . Nearest-neighbor square, honeycomb, and cubic lattices are bipartite; the triangular lattice is not. Including next-nearest-neighbor hopping typically breaks bipartiteness.

Modified PH transformation. Choose $\eta_i = \pm 1$ with $\eta_i \eta_j = -1$ for any nearest-neighbor bond $\langle ij \rangle$. For the square lattice with $R_i = (i_x, i_y)$, a standard choice is

$$\eta_i = (-1)^{i_x + i_y} = e^{iQ \cdot R_i}, \quad Q = (\pi, \pi). \quad (41)$$

Define the bipartite PH map by

$$\hat{c}_{i\uparrow} \rightarrow \hat{c}_{i\uparrow}, \quad \hat{c}_{i\downarrow} \rightarrow \eta_i \hat{c}_{i\downarrow}^\dagger, \quad \hat{c}_{i\downarrow}^\dagger \rightarrow \eta_i \hat{c}_{i\downarrow}. \quad (42)$$

Why (42) keeps the kinetic term invariant

Bond-by-bond cancellation of the sign flip. Consider a single bond $\langle ij \rangle$ and the hopping term $-J(\hat{c}_{i\downarrow}^\dagger \hat{c}_{j\downarrow} + \text{h.c.})$. Under (42),

$$\hat{c}_{i\downarrow}^\dagger \hat{c}_{j\downarrow} \longrightarrow (\eta_i \hat{c}_{i\downarrow})(\eta_j \hat{c}_{j\downarrow}^\dagger) = \eta_i \eta_j \hat{c}_{i\downarrow} \hat{c}_{j\downarrow}^\dagger = -\eta_i \eta_j \hat{c}_{j\downarrow}^\dagger \hat{c}_{i\downarrow}. \quad (43)$$

On a bipartite nearest-neighbor bond, $\eta_i \eta_j = -1$, so the extra minus sign cancels:

$$-\eta_i \eta_j = 1, \quad \Rightarrow \quad \hat{c}_{i\downarrow}^\dagger \hat{c}_{j\downarrow} \rightarrow \hat{c}_{j\downarrow}^\dagger \hat{c}_{i\downarrow}. \quad (44)$$

After adding the Hermitian conjugate and summing over undirected bonds $\langle ij \rangle$, the kinetic term is unchanged.

Momentum-space form and dispersion condition.

We fix the Fourier transform convention as

$$\hat{c}_{i\sigma} = \frac{1}{\sqrt{N}} \sum_k e^{ik \cdot R_i} \hat{c}_{k\sigma}, \quad \hat{c}_{k\sigma} = \frac{1}{\sqrt{N}} \sum_i e^{-ik \cdot R_i} \hat{c}_{i\sigma}, \quad (45)$$

where the sum over k runs over the first Brillouin zone.

Under the particle-hole transformation on the down-spin sector,

$$\hat{c}_{i\downarrow} \longrightarrow \eta_i \hat{c}_{i\downarrow}^\dagger, \quad \eta_i = e^{i\mathbf{Q}\cdot\mathbf{R}_i}, \quad (46)$$

the momentum-space operator transforms as

$$\begin{aligned} \hat{c}_{k\downarrow} &\longrightarrow \frac{1}{\sqrt{N}} \sum_i e^{-ik\cdot R_i} \eta_i \hat{c}_{i\downarrow}^\dagger = \frac{1}{\sqrt{N}} \sum_i e^{-i(k-Q)\cdot R_i} \hat{c}_{i\downarrow}^\dagger \\ &= \hat{c}_{Q-k,\downarrow}^\dagger. \end{aligned} \quad (47)$$

For nearest-neighbor hopping on the square lattice, the single-particle dispersion is

$$\epsilon(k) = -2J(\cos k_x + \cos k_y). \quad (48)$$

Choosing the antiferromagnetic wavevector $\mathbf{Q} = (\pi, \pi)$, one finds

$$\epsilon(Q - k) = -\epsilon(k). \quad (49)$$

Under the transformation (47), the kinetic term becomes

$$\begin{aligned} \sum_k \epsilon(k) \hat{c}_{k\downarrow}^\dagger \hat{c}_{k\downarrow} &\longrightarrow \sum_k \epsilon(k) \hat{c}_{Q-k,\downarrow}^\dagger \hat{c}_{Q-k,\downarrow} \\ &= \sum_k \epsilon(k) (1 - \hat{c}_{Q-k,\downarrow}^\dagger \hat{c}_{Q-k,\downarrow}) \\ &= \sum_k \epsilon(k) - \sum_k \epsilon(k) \hat{c}_{Q-k,\downarrow}^\dagger \hat{c}_{Q-k,\downarrow}. \end{aligned} \quad (50)$$

Relabeling the momentum $k \rightarrow Q - k$ in the second term and using $\epsilon(Q - k) = -\epsilon(k)$, we obtain

$$\sum_k \epsilon(k) \hat{c}_{k\downarrow}^\dagger \hat{c}_{k\downarrow} \longrightarrow \sum_k \epsilon(k) \hat{c}_{k\downarrow}^\dagger \hat{c}_{k\downarrow} + \sum_k \epsilon(k). \quad (51)$$

The last term is a c -number constant and therefore does not affect the dynamics, establishing the invariance of the kinetic energy up to an additive constant.

2.4 Parameter mapping between repulsive and attractive models

Grand-canonical parameter map.

On a bipartite lattice, the PH map (42) yields

$$(U, \mu, h) \longrightarrow (-U, h, \mu), \quad (52)$$

up to additive constants in the Hamiltonian.

Canonical map: (δ, m) exchange.

In the Canonical ensemble case, the interaction similarly changes sign $U \rightarrow -U$. The notion of (μ, h) becomes (δ, m) .

Using $\hat{n}_{i\downarrow} \rightarrow 1 - \hat{n}_{i\downarrow}$, the total numbers transform as

$$N_\downarrow \rightarrow N_s - N_\downarrow, \quad N_\uparrow \rightarrow N_\uparrow. \quad (53)$$

Therefore

$$\delta = N - N_s \longrightarrow (N_\uparrow - N_\downarrow) = m, \quad m = N_\uparrow - N_\downarrow \longrightarrow (N - N_s) = \delta. \quad (54)$$

A compact summary of the PH correspondence.

- Repulsive ($U > 0$) \leftrightarrow attractive ($U < 0$).
- Chemical potential $\mu \leftrightarrow$ Zeeman field h .
- Doping $\delta \leftrightarrow$ spin imbalance m .
- On bipartite lattices with appropriate η_i , the kinetic term is invariant.

3 Pairing and Antiferromagnetism: an exact correspondence

3.1 Attractive FHM with balanced spins: pairing order and competing CDW

Cooper instability and pairing order.

Consider attractive interaction ($U = -U_0 < 0$) with equal spin populations $N_\uparrow = N_\downarrow$ (i.e. $m = 0$). The attractive interaction produces a Cooper instability: arbitrarily weak attraction destabilizes the Fermi surface toward pairing. A standard pairing order parameter is

$$\Delta \equiv \sum_k \langle \hat{c}_{-k\downarrow} \hat{c}_{k\uparrow} \rangle \neq 0, \quad \Delta^* \equiv \sum_k \langle \hat{c}_{k\uparrow}^\dagger \hat{c}_{-k\downarrow}^\dagger \rangle \neq 0. \quad (55)$$

In three dimensions, this supports a finite-temperature transition into a phase with long-range pairing order.

Pairing vs. CDW in real space, and why they can be degenerate at half filling

The s-wave pairing order parameter $\Delta \equiv \sum_k \langle \hat{c}_{-k\downarrow} \hat{c}_{k\uparrow} \rangle$ signals a condensate of zero center-of-mass Cooper pairs. Indeed, using the Fourier transform $\hat{c}_{k\sigma} = \frac{1}{\sqrt{N}} \sum_j e^{-ik \cdot R_j} \hat{c}_{j\sigma}$, we find

$$\sum_k \hat{c}_{-k\downarrow} \hat{c}_{k\uparrow} = \frac{1}{N} \sum_k \sum_{ij} e^{ik(R_i - R_j)} \hat{c}_{i\downarrow} \hat{c}_{j\uparrow} = \sum_i \hat{c}_{i\downarrow} \hat{c}_{i\uparrow}, \quad (56)$$

so $\Delta \neq 0$ is equivalent to a *uniform on-site pair amplitude* $\langle \hat{c}_{i\downarrow} \hat{c}_{i\uparrow} \rangle \neq 0$, i.e. broken global $U(1)$ charge symmetry. By contrast, a commensurate CDW order at wavevector \mathbf{Q} is $\Phi_{\text{CDW}} \equiv \sum_{k,\sigma} \langle \hat{c}_{k\sigma}^\dagger \hat{c}_{k+\mathbf{Q},\sigma} \rangle$. Fourier transforming gives

$$\sum_{k,\sigma} \hat{c}_{k\sigma}^\dagger \hat{c}_{k+\mathbf{Q},\sigma} = \frac{1}{N} \sum_{k,\sigma} \sum_{ij} e^{-ikR_i} e^{i(k+\mathbf{Q})R_j} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} = \sum_j e^{i\mathbf{Q} \cdot \mathbf{R}_j} \hat{n}_j, \quad (57)$$

hence $\Phi_{\text{CDW}} \neq 0$ implies a *density modulation* $\langle \hat{n}_j \rangle = n_0 + A \cos(\mathbf{Q} \cdot \mathbf{R}_j + \varphi)$, i.e. broken translation symmetry. On a bipartite lattice at half filling, these seemingly different orders become degenerate due to an exact mapping: perform a particle-hole transformation on the \downarrow fermions, $\hat{c}_{j\downarrow} \mapsto (-1)^j \hat{c}_{j\downarrow}^\dagger$ with $(-1)^j = e^{i\mathbf{Q} \cdot \mathbf{R}_j}$. Under this mapping, the CDW operator turns into the staggered spin density,

$$\sum_j (-1)^j (\hat{n}_{j\uparrow} + \hat{n}_{j\downarrow} - 1) \mapsto \sum_j (-1)^j (\hat{n}_{j\uparrow} - \hat{n}_{j\downarrow}), \quad (58)$$

while the pairing operator turns into the transverse staggered spin component,

$$\sum_j \hat{c}_{j\downarrow} \hat{c}_{j\uparrow} \mapsto \sum_j (-1)^j \hat{c}_{j\downarrow}^\dagger \hat{c}_{j\uparrow} = \sum_j (-1)^j \hat{S}_j^+. \quad (59)$$

Therefore, at half filling the attractive Hubbard model is mapped to the repulsive Hubbard model, where the three components of the Néel order parameter are related by spin $SU(2)$; mapping back implies an $SU(2)$ *pseudospin* symmetry that rotates CDW (η^z) into pairing ($\eta^{x,y}$), explaining why CDW and s-wave pairing can be exactly degenerate in this special case.

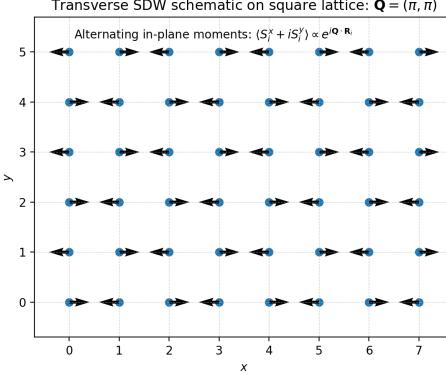


Figure 1: Schematic illustration of Spin-Density Wave Order. Note we take θ in Eq. (65) to be 0.

3.2 Mapping to repulsive half-filled FHM: SDW/AFM order parameter

Parameter mapping in the canonical language. The attractive model with ($U = -U_0, \mu = x, h = 0$) maps to a repulsive model at half filling ($U = +U_0, \mu = 0, h = x$), or in canonical variables ($U = -U_0, \delta = x, m = 0 \mapsto (U = +U_0, \delta = 0, m = x)$).

Order-parameter mapping: pairing \leftrightarrow in-plane spin density wave.

Under the bipartite PH map, one finds (up to a relabeling of k)

$$\hat{c}_{-k\downarrow} \longrightarrow \hat{c}_{k+Q,\downarrow}^\dagger. \quad (60)$$

Therefore the pairing order Δ in (55) transforms to

$$\Delta \longrightarrow \sum_k \langle \hat{c}_{k+Q,\downarrow}^\dagger \hat{c}_{k\uparrow} \rangle \equiv \langle \hat{S}_Q^- \rangle, \quad (61)$$

and similarly

$$\Delta^* \longrightarrow \sum_k \langle \hat{c}_{k\uparrow}^\dagger \hat{c}_{k+Q,\downarrow} \rangle \equiv \langle \hat{S}_Q^+ \rangle. \quad (62)$$

These are transverse¹ spin-density-wave (SDW) order parameters at momentum Q . A spin-density-wave (SDW) order implies that the spin expectation values develop a well-defined periodic pattern in space. In the present case, the ordering wavevector $Q = (\pi, \pi)$ leads to a checkerboard-like staggered arrangement of the in-plane spin moments, as illustrated in Fig. 1. It's also referred to as the *antiferromagnetic order* (AFM).

Concrete derivation of the SDW physical picture

We focus on the transverse SDW order parameter $S_Q^- \equiv \sum_k \hat{c}_{k+Q,\downarrow}^\dagger \hat{c}_{k\uparrow}$. In momentum space, S_Q^- acts as

- Annihilating an electron in the (k, \uparrow) state,
- Creating an electron in the $(k + Q, \downarrow)$ state.

Equivalently,

The system supports a macroscopic coherent process that converts a spin-up fermion into a spin-down fermion with a fixed momentum transfer Q .

¹Transverse means “in-plane”, i.e. spins rest in the plane and $\langle S_z \rangle = 0$.

To reveal the real-space pattern, transform back using $\hat{c}_{k\sigma} = \frac{1}{\sqrt{N}} \sum_i e^{-ik \cdot R_i} \hat{c}_{i\sigma}$. One finds

$$\begin{aligned} S_Q^- &= \sum_k \hat{c}_{k+Q,\downarrow}^\dagger \hat{c}_{k\uparrow} = \sum_i e^{-iQ \cdot R_i} \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\uparrow} \\ &= \sum_i e^{-iQ \cdot R_i} (S_i^x - iS_i^y), \end{aligned} \quad (63)$$

where $S_i^\alpha \equiv \frac{1}{2} \sum_{\sigma\sigma'} \hat{c}_{i\sigma}^\dagger (\sigma^\alpha)_{\sigma\sigma'} \hat{c}_{i\sigma'}$, as defined in Eq. (31),(32),(33). Hence a nonzero expectation value $\langle S_Q^- \rangle \neq 0$ implies an in-plane spin texture. It is convenient to parametrize the transverse local moment as

$$\langle S_i^x + iS_i^y \rangle = \Phi e^{iQ \cdot R_i} \quad (Q = (\pi, \pi)), \quad (64)$$

where $\Phi \equiv |\Phi|e^{i\theta}$ is the complex SDW amplitude: $|\Phi|$ measures the magnitude of the in-plane ordered moment, while its phase θ fixes the common spin direction within the $x-y$ plane.

Splitting into components,

$$\langle S_i^x \rangle = |\Phi| \cos(Q \cdot R_i + \theta), \quad \langle S_i^y \rangle = |\Phi| \sin(Q \cdot R_i + \theta), \quad (65)$$

we see that each lattice site carries a transverse (in-plane) spin expectation value, and this transverse moment alternates in space with wavevector Q . In particular, for $Q = (\pi, \pi)$ on the square lattice, $Q \cdot R_i = \pi(x_i + y_i)$, so

$$\langle S_i^x \rangle = |\Phi|(-1)^{x_i+y_i} \cos \theta, \quad \langle S_i^y \rangle = |\Phi|(-1)^{x_i+y_i} \sin \theta, \quad (66)$$

i.e. neighboring sites (opposite sublattices) carry opposite in-plane moments: a checkerboard-like staggered pattern.

S_Q^+ is not an independent order parameter. Since $S_Q^+ = (S_Q^-)^\dagger$, their expectation values satisfy $\langle S_Q^+ \rangle = \langle S_Q^- \rangle^*$. Thus S_Q^\pm are simply the complex representations of the same transverse (in-plane) SDW order, encoding the two real components $\langle S^x \rangle$ and $\langle S^y \rangle$.

Transverse vs. longitudinal SDW.. The present order is *transverse* because it involves $\langle S_i^{x,y} \rangle \neq 0$ (equivalently $\langle S_Q^\pm \rangle \neq 0$). By contrast, a *longitudinal* SDW is characterized by a staggered $\langle S_i^z \rangle \neq 0$ (equivalently $\langle S_Q^z \rangle \neq 0$), describing an Ising-like modulation of the spin polarization along the quantization axis.

3.3 $U(1)$ degeneracy: pairing phase vs spin azimuth

Pairing phase degeneracy. In the attractive pairing state, $\Delta = |\Delta|e^{i\theta}$ has an arbitrary global phase θ due to $U(1)$ symmetry, leading to a continuous degeneracy of mean-field ground states.

Mapped to azimuthal angle of transverse AFM order. Under the PH map, $\Delta \leftrightarrow \langle \hat{S}_Q^- \rangle$. The phase θ becomes the azimuthal angle of the staggered spin in the xy plane. If $h \neq 0$, the spin symmetry is reduced to rotations about \hat{z} , i.e. a $U(1)$ symmetry, matching the $U(1)$ phase degeneracy.

3.4 Why infinitesimal interaction can order in weak coupling

Attractive side: Cooper instability. In BCS theory, the pairing susceptibility diverges logarithmically at the Fermi surface, so any $U < 0$ triggers pairing. Quantitatively, a weak-coupling

estimate has the form

$$T_c \sim E_F \exp\left(-\frac{1}{|U|D(E_F)}\right), \quad (67)$$

where $D(E_F)$ is the density of states at the Fermi energy.

Repulsive half-filled side: nesting and SDW instability. At half filling on a bipartite lattice with $\epsilon(k) = -\epsilon(k + Q)$, the Fermi surface is nested by Q . The particle–hole susceptibility at Q is strongly enhanced, favoring SDW/AFM order for arbitrarily small $U > 0$ (with an exponentially small ordering scale in weak coupling).

4 Transition-temperature scales and strong-coupling effective models

4.1 Weak-coupling estimates

In the Weak-coupling regime $U \ll J$, the estimation is:

$$T_c \sim E_F \exp\left(-\frac{1}{|U|D(E_F)}\right), \quad (68)$$

which indicates that transition temperature increases as U increases.

4.2 Strong coupling on the repulsive side: superexchange and Heisenberg limit

Set-up: strong coupling at half filling and the low-energy (Mott) subspace. We start from the canonical-ensemble Fermi–Hubbard Hamiltonian in Eq. (6) and rewrite it as

$$\hat{H} = \hat{H}_0 + \hat{T}, \quad \text{where: } \hat{H}_0 = U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}, \quad \hat{T} = -J \sum_{\langle ij \rangle, \sigma} (\hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + \text{h.c.}), \quad (69)$$

with $U > 0$. We focus on the *half-filled*² and *strong-coupling* regime $U \gg J$, where charge fluctuations are suppressed and the low-energy physics lives in the “Mott” subspace with $\hat{n}_i \simeq 1$ (one fermion per site and essentially no doublons/holons³).

Unperturbed spectrum: 2^N degenerate ground manifold and charge excitations at scale U .

In the unperturbed limit $J = 0$, \hat{H}_0 assigns zero energy to any configuration with no double occupancy. At half filling this “no-doublon” manifold contains precisely one fermion per site, with an independent spin- $\frac{1}{2}$ degree of freedom on each site. Hence the unperturbed ground space is 2^N -fold degenerate (for N lattice sites). The lowest charge excitations are doublon–holon configurations created by moving one fermion onto an occupied site, producing one doubly-occupied site and one empty site; such intermediate states cost an energy of order U under \hat{H}_0 .

First-order degenerate perturbation: vanishes at strict half filling.

Within the degenerate ground manifold, the first-order effective Hamiltonian is given by the standard (degenerate) perturbation-theory matrix element

$$\left(H_{\text{eff}}^{(1)}\right)_{\alpha\beta} = \langle \alpha | \hat{T} | \beta \rangle, \quad |\alpha\rangle, |\beta\rangle \in \mathcal{H}_{\text{GS}}(H_0). \quad (70)$$

At strict half filling with no holes, any single hop necessarily creates a doublon–holon pair and therefore takes the state *out* of the no-doublon ground manifold. Consequently $\langle \alpha | \hat{T} | \beta \rangle = 0$ for all ground-manifold states, i.e.

$$\hat{H}_{\text{eff}}^{(1)} = 0. \quad (71)$$

²“Half-filled” means $N_\uparrow + N_\downarrow = N_s$.

³Doublon means there are two fermions on the site, while holon means there is no fermion on the site.

Second-order degenerate perturbation: virtual doublon–holon processes on each bond.

The leading nontrivial contribution arises at second order. The standard undergraduate formula for the effective matrix element within the ground manifold reads

$$(H_{\text{eff}}^{(2)})_{\alpha\beta} = \sum_{m \notin \mathcal{H}_{\text{GS}}(H_0)} \frac{\langle \alpha | \hat{T} | m \rangle \langle m | \hat{T} | \beta \rangle}{E_0 - E_m}, \quad (72)$$

where E_0 is the unperturbed ground energy ($E_0 = 0$ here) and $|m\rangle$ runs over excited eigenstates of \hat{H}_0 . In the present problem, \hat{T} connects the ground manifold to intermediate states with exactly one doublon–holon pair on a nearest-neighbor bond, whose energy is $E_m = U$. Therefore the energy denominator in (72) is $-U$, and the scale of the induced interaction is J^2/U .

Bond-by-bond reduction and the two-site effective Hamiltonian.

Because $\hat{T} = \sum_{\langle ij \rangle} \hat{T}_{ij}$ is a sum of nearest-neighbor hoppings, the second-order processes in (72) are local: starting from the half-filled no-doublon manifold, one hop \hat{T}_{ij} can only create a single doublon–holon pair on the *same* bond $\langle ij \rangle$, costing energy U . In order to return to the low-energy manifold after the second hop, the second hopping must remove that doublon–holon pair, which again can be done only by acting on the same bond. Thus the second-order effective Hamiltonian decomposes into a sum of independent bond terms,

$$\hat{H}_{\text{eff}}^{(2)} = \sum_{\langle ij \rangle} \hat{H}_{ij}^{(2)}, \quad \hat{H}_{ij}^{(2)} \sim -\frac{1}{U} \hat{T}_{ij} \hat{T}_{ij} \quad (\text{within the no-doublon subspace}). \quad (73)$$

Therefore it suffices to solve a *two-site problem* on a single bond and then sum the resulting bond Hamiltonian over the lattice.

Fix a bond $\langle ij \rangle$ at half filling. The low-energy subspace has four spin states $|\uparrow, \uparrow\rangle, |\downarrow, \downarrow\rangle, |\uparrow, \downarrow\rangle, |\downarrow, \uparrow\rangle$. A single hop is Pauli-blocked for the polarized states $|\uparrow, \uparrow\rangle$ and $|\downarrow, \downarrow\rangle$, hence they receive no second-order shift:

$$E_{\uparrow\uparrow}^{(2)} = E_{\downarrow\downarrow}^{(2)} = 0. \quad (74)$$

Nontrivial virtual processes exist only in the subspace spanned by $\{|\uparrow, \downarrow\rangle, |\downarrow, \uparrow\rangle\}$. Using the standard second-order formula (72), there are two intermediate doublon–holon states, $|\uparrow\downarrow, 0\rangle$ and $|0, \uparrow\downarrow\rangle$, both at energy U . Evaluating the second-order matrix elements gives (within this two-dimensional subspace)

$$\hat{H}_{ij}^{(2)} = -\frac{2J^2}{U} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}_{\{|\uparrow, \downarrow\rangle, |\downarrow, \uparrow\rangle\}}.$$

(75)

Diagonalizing (75) yields eigenstates and eigenvalues

$$|T_0\rangle = \frac{|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle}{\sqrt{2}}, \quad E_{T_0}^{(2)} = 0, \quad (76)$$

$$|S\rangle = \frac{|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle}{\sqrt{2}}, \quad E_S^{(2)} = -\frac{4J^2}{U}. \quad (77)$$

Together with $E_{\uparrow\uparrow}^{(2)} = E_{\downarrow\downarrow}^{(2)} = 0$, this shows that the singlet is lowered relative to the triplet manifold, i.e. the induced interaction is antiferromagnetic.

To identify the operator form, recall that for two spin- $\frac{1}{2}$ degrees of freedom,

$$\hat{S}_i \cdot \hat{S}_j = \begin{cases} +\frac{1}{4}, & \text{triplet,} \\ -\frac{3}{4}, & \text{singlet.} \end{cases} \quad (78)$$

Hence the unique (up to an additive constant) rotationally invariant operator that yields $E_T = 0$ and $E_S = -4J^2/U$ is

$$\hat{H}_{ij}^{(2)} = J_{\text{ex}} \left(\hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j - \frac{1}{4} \right), \quad J_{\text{ex}} = \frac{4J^2}{U}. \quad (79)$$

Summing (79) over all nearest-neighbor bonds gives the many-body Heisenberg limit (up to a constant shift),

$$\hat{H}_{\text{eff}} = J_{\text{ex}} \sum_{\langle ij \rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j + \text{const.}, \quad J_{\text{ex}} = \frac{4J^2}{U}. \quad (80)$$

Formal projector derivation (Schrieffer–Wolff / degenerate PT viewpoint)

The physical picture above can be packaged into a compact formalism using projectors onto the low-energy Mott subspace. Let \mathcal{P} project onto the no-doublon subspace (at half filling, $\hat{n}_i \simeq 1$), and $Q = 1 - \mathcal{P}$. To second order in \hat{T} , the effective Hamiltonian acting within \mathcal{P} is

$$\hat{H}_{\text{eff}} = \mathcal{P} \hat{H} \mathcal{P} - \mathcal{P} \hat{T} Q \frac{1}{\hat{H}_0} Q \hat{T} \mathcal{P} + O\left(\frac{J^3}{U^2}\right). \quad (81)$$

At strict half filling, $\mathcal{P} \hat{H} \mathcal{P} = \mathcal{P} \hat{T} \mathcal{P} = 0$, and the intermediate states reached by a single hop have one doublon costing energy U , so $1/\hat{H}_0 \rightarrow 1/U$ in this order. Evaluating the two-step process on each bond leads to the standard fermionic exchange form

$$\hat{H}_{\text{eff}} = -\frac{J^2}{U} \sum_{\langle ij \rangle} \sum_{ss'} (\hat{c}_{is}^\dagger \hat{c}_{js} \hat{c}_{js'}^\dagger \hat{c}_{is'} + \text{h.c.}), \quad (82)$$

which, upon rewriting in terms of spin operators and using $\hat{n}_i \simeq 1$, reduces to the antiferromagnetic Heisenberg model in Eq. (??).

Temperature scales for $U \gg J$ (repulsive, half filling).

- Charge (Mott) scale: $T \sim U$ controls suppression of double occupancy and onset of insulating behavior.
- Spin (AFM) scale: $T \sim J_{\text{ex}} = 4J^2/U \ll U$ controls antiferromagnetic ordering/correlations.
- Therefore there is a broad intermediate regime $J_{\text{ex}} \ll T \ll U$ where the system is insulating but not spin ordered.

4.3 Strong coupling on the attractive side: pair formation vs pair condensation

Local pairs and two distinct scales. For $U = -|U|$ with $|U| \gg J$, the low-energy on-site configurations are empty $|0\rangle$ and doubly occupied $|\uparrow\downarrow\rangle$; singly occupied states are gapped by $\sim |U|$. Thus pair *formation* occurs at $T \sim |U|$, while pair *motion/condensation* is controlled by a much smaller scale $\sim J^2/|U|$.

Pair hopping amplitude is $O(J^2/|U|)$ (prefactor depends on convention)

A doublon $|\uparrow\downarrow\rangle$ hopping from site i to an empty neighbor j requires two single-particle hops. Each hop contributes a factor J , and the intermediate singly-occupied configuration costs energy $|U|$. Therefore the effective pair-hopping amplitude scales as

$$t_{\text{pair}} \sim \frac{J^2}{|U|}. \quad (83)$$

Depending on operator conventions and how “paths” are counted, one commonly finds $t_{\text{pair}} = 2J^2/|U|$, while some presentations quote $4J^2/|U|$; the robust point is the parametric scale $J^2/|U|$.

Temperature scales for $|U| \gg J$ (attractive).

- Pair formation (binding) scale: $T \sim |U|$.
- Pair condensation/superfluid coherence scale: $T \sim t_{\text{pair}} \sim J^2/|U| \ll |U|$.
- Hence an intermediate “preformed-pair” (pseudo-gap) regime can exist: pairs form without long-range phase coherence.

5 $SO(4)$ Symmetry at $\mu = h = 0$ and its consequences

5.1 Two commuting $SU(2)$'s and the $SU(2) \times SU(2)/\mathbb{Z}_2$ structure

Spin $SU(2)$ at $h = 0$. When $h = 0$, the model has a global spin $SU(2)$ generated by total spin operators $\hat{S}^a = \sum_i \hat{S}_i^a$.

Pseudospin $SU(2)$ (“ η -pairing”) at $\mu = 0$. When $\mu = 0$, the Hamiltonian is mapped by PH to a model at $h = 0$, implying another $SU(2)$. The corresponding generators are

$$\hat{L}^x \equiv \frac{1}{2} \sum_i \eta_i (\hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger + \hat{c}_{i\downarrow} \hat{c}_{i\uparrow}), \quad (84)$$

$$\hat{L}^y \equiv \frac{i}{2} \sum_i \eta_i (\hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow}^\dagger - \hat{c}_{i\downarrow} \hat{c}_{i\uparrow}), \quad (85)$$

$$\hat{L}^z \equiv \frac{1}{2} \left(\sum_i \hat{n}_i - N_s \right) = \frac{1}{2} \hat{\delta}, \quad (86)$$

where $\eta_i = (-1)^{i_x+i_y}$ on the square lattice and $\hat{\delta} \equiv \hat{N} - N_s$.

Enlarged symmetry at $\mu = h = 0$. At $\mu = h = 0$, both $SU(2)$ symmetries coexist, giving $SU(2) \times SU(2)$. However, not all representations occur because $(-1, -1)$ acts trivially on physical states: for fixed N_s , $\hat{S}^z + \hat{L}^z = N_\uparrow - N_s/2$ is always an integer or half-integer, restricting allowed multiplets. Thus the actual symmetry group is

$$SU(2) \times SU(2)/\mathbb{Z}_2 \simeq SO(4). \quad (87)$$

5.2 Two-dimensional consequence: order-parameter manifold and KT transition

Repulsive side in 2D: $U(1) \rightarrow S^2$ and KT suppression. For repulsive FHM in 2D, away from $h = 0$ the transverse AFM order has a $U(1)$ degeneracy (azimuthal angle), supporting a Kosterlitz–Thouless (KT) transition driven by vortex proliferation.

When $h = 0$, full spin $SU(2)$ is restored, and the AFM order parameter can point along any direction, so the degeneracy manifold is S^2 instead of $U(1)$. Because S^2 does not support vortex defects in 2D, the finite-temperature KT transition is suppressed: the KT transition temperature vanishes at $h = 0$ (or $N_\uparrow = N_\downarrow$).

Fixing a common notational slip about AFM order parameters

Longitudinal (staggered z -spin) AFM order is

$$M_Q^z \equiv \sum_k \langle \hat{c}_{k\uparrow}^\dagger \hat{c}_{k+Q,\uparrow} - \hat{c}_{k\downarrow}^\dagger \hat{c}_{k+Q,\downarrow} \rangle \neq 0. \quad (88)$$

Transverse (in-plane) AFM order is captured by

$$M_Q^- \equiv \sum_k \langle \hat{c}_{k+Q,\downarrow}^\dagger \hat{c}_{k\uparrow} \rangle \neq 0, \quad M_Q^+ = (M_Q^-)^*. \quad (89)$$

If a text accidentally repeats the same expression for both cases, it is a typographical duplication.

Attractive side in 2D: pairing vs CDW and KT suppression at $\mu = 0$. By PH mapping, at $\mu = h = 0$ the attractive FHM is mapped to the repulsive FHM with the same $|U|$, so the degeneracy between AFM orientations maps to a degeneracy between pairing and CDW: in-plane AFM \leftrightarrow zero-momentum pairing, while longitudinal AFM \leftrightarrow CDW at Q . Hence at half filling and spin balance, the attractive model has an S^2 order-parameter manifold, and the KT transition temperature is suppressed to zero at $\mu = 0$.

5.3 Experimental signatures under the mapping

Correlators related by PH transformation. Short-range spin correlations in the repulsive half-filled model are related to short-range density correlations and pairing correlations in the attractive model. Qualitatively, the mapping predicts that:

- at zero spin polarization, longitudinal and transverse spin correlations nearly coincide;
 - at half filling, density correlations nearly coincide with pairing correlations;
- Away from these special points, the “non-degenerate” channel is weaker.

6 Open problems and physical pictures

6.1 Near half-filling in 2D: d -wave superconductivity?

Motivation from cuprates and the limitation of FHM. Cuprate materials have complicated microscopic structure, so it is nontrivial whether a single-band FHM fully captures them. Nevertheless, their parent compounds are antiferromagnetic Mott insulators at (approximately) half filling, echoing the repulsive FHM at $\delta = 0$.

Central unsolved question. When slightly doped away from half filling ($n \sim 1$ in 2D), can a repulsive FHM develop d -wave pairing? There is no theoretical consensus across the full parameter regime.

d -wave order parameter and its PH image. A standard d -wave pairing order parameter is

$$\Delta_d^* \equiv \sum_k f_d(k) \langle \hat{c}_{k\uparrow}^\dagger \hat{c}_{-k\downarrow}^\dagger \rangle, \quad f_d(k) \propto k_x^2 - k_y^2. \quad (90)$$

Under PH mapping, it corresponds to a d -wave SDW/AFM-like order:

$$\sum_k f_d(k) \langle \hat{c}_{k\uparrow}^\dagger \hat{c}_{k+Q,\downarrow} \rangle, \quad (91)$$

i.e. a form-factor-modulated staggered spin order.

Cold-atom quantum simulation: the main bottleneck is temperature. Even if such a phase exists, current ultracold lattice systems typically cannot reach the (dimensionless) transition temperature, because the relevant scale is small in units of E_F , and translating to atomic-gas energy scales makes it experimentally challenging.

6.2 Low density: itinerant ferromagnetism vs strong-correlation alternatives

Stoner picture at $n \ll 1$. In the low-density regime one may approximate the dispersion by $\epsilon_k = k^2/(2m^*)$. A uniform Hartree estimate gives

$$E_{\text{int}} = Un_{\uparrow}n_{\downarrow} = U\left(\frac{n^2}{4} - S_z^2\right), \quad S_z = \frac{n_{\uparrow} - n_{\downarrow}}{2}, \quad (92)$$

which favors maximizing $|S_z|$ (ferromagnetism), while the kinetic energy cost favors $S_z = 0$. This competition yields the Stoner scenario with a critical U_c , and full polarization at very large U .

Why the issue is nontrivial. A nonmagnetic but strongly correlated state can also suppress double occupancy without polarizing. A classic variational example is the Gutzwiller wave function

$$|\Psi\rangle = \prod_i (1 - \alpha \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}) |FS\rangle, \quad (93)$$

where $|FS\rangle$ is a spin-balanced Fermi sea. Here $\alpha = 0$ gives the free Fermi gas, while $\alpha = 1$ projects out all doubly occupied sites (typo-corrected), driving the interaction energy toward zero at the cost of increased kinetic energy. Determining the true ground state requires an energy comparison among increasingly optimized correlated states, so the ferromagnetism question remains open in generic non-flat bands.

PH reinterpretation. Under the PH map, ferromagnetism on the repulsive side corresponds to density inhomogeneity tendencies on the attractive side, so the question is equivalent to whether an attractive FHM develops density inhomogeneity when a nearly fully polarized configuration is realized.

A Ensemble theory primer: microcanonical, canonical, and grand-canonical

A.1 Why ensembles at all?

Macroscopic constraints vs microscopic description.

In lattice many-body problems (such as the Fermi–Hubbard model), one typically has several *conserved* quantities, most importantly the total particle number \hat{N} and (when spin-flip terms are absent) the total spin polarization \hat{S}^z . An “ensemble” is simply a systematic way to incorporate which quantities are held fixed and which are allowed to fluctuate, and to organize the corresponding thermodynamics in terms of appropriate potentials.

Core message. Different ensembles correspond to different choices of *control variables* (e.g. (E, N, S^z) vs (T, N, S^z) vs (T, μ, h)). They are related by Laplace transforms and Legendre transforms. In the thermodynamic limit and under standard convexity conditions, they give the same local physics once the mean values match.

A.2 Microcanonical ensemble: fixed (E, N, S^z)

Definition (hard constraints on energy and charges). The microcanonical ensemble fixes the energy and conserved charges sharply. For a quantum system, define the density of states in an energy window $[E, E + \Delta E]$ by

$$\Omega(E, N, S^z; \Delta E) \equiv \text{Tr} \left[1_{[E, E + \Delta E]}(\hat{H}) \delta_{\hat{N}, N} \delta_{\hat{S}^z, S^z} \right], \quad (94)$$

where $1_{[E, E + \Delta E]}(\hat{H})$ projects onto eigenstates with energies in the given window, and $\delta_{\hat{N}, N}$, $\delta_{\hat{S}^z, S^z}$ project onto the (N, S^z) sector. The microcanonical entropy is

$$S(E, N, S^z) \equiv \ln \Omega(E, N, S^z; \Delta E), \quad (95)$$

where we set $k_B = 1$. Thermodynamic conjugates are defined by derivatives of S :

$$\frac{1}{T} = \frac{\partial S}{\partial E} \Big|_{N, S^z}, \quad \frac{\mu}{T} = -\frac{\partial S}{\partial N} \Big|_{E, S^z}, \quad \frac{2h}{T} = -\frac{\partial S}{\partial S^z} \Big|_{E, N}. \quad (96)$$

Remark: why an energy window ΔE ?

Remark: In finite quantum systems the spectrum is discrete, so one typically counts states in an energy shell. Thermodynamics becomes insensitive to the precise choice of ΔE in the thermodynamic limit as long as ΔE is large compared to the many-body level spacing but small on macroscopic scales.

A.3 Canonical ensemble: fixed (N, S^z) , fluctuating E

Restricted trace and Helmholtz free energy. In the canonical ensemble one fixes (N, S^z) but allows energy fluctuations at temperature T . The canonical partition function is

$$Z_C(N, S^z, T) = \text{Tr}_{N, S^z} e^{-\beta \hat{H}}, \quad \beta \equiv \frac{1}{T}, \quad (97)$$

where Tr_{N, S^z} denotes the trace restricted to the (N, S^z) sector. The corresponding Helmholtz free energy is

$$F(N, S^z, T) \equiv -T \ln Z_C(N, S^z, T). \quad (98)$$

Standard identities include

$$\langle \hat{H} \rangle_{N, S^z} = -\frac{\partial}{\partial \beta} \ln Z_C, \quad S(N, S^z, T) = -\frac{\partial F}{\partial T} \Big|_{N, S^z}, \quad (99)$$

and the energy fluctuation is controlled by the heat capacity:

$$(\Delta E)^2 \equiv \langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2 = T^2 C_{N, S^z}, \quad C_{N, S^z} \equiv \frac{\partial \langle \hat{H} \rangle}{\partial T} \Big|_{N, S^z}. \quad (100)$$

Recap: canonical as a Laplace transform of microcanonical data

Recap: Formally, the canonical partition function can be written as a Laplace transform of the microcanonical density of states:

$$Z_C(N, S^z, T) = \int dE \Omega(E, N, S^z; \Delta E) e^{-\beta E}. \quad (101)$$

In the thermodynamic limit, this integral is dominated by a saddle point E_* satisfying $\beta = \partial S / \partial E|_{E_*}$, i.e. $T^{-1} = \partial S / \partial E$, which realizes the equivalence between microcanonical and canonical ensembles for typical phases.

A.4 Grand-canonical ensemble: fixed (T, μ, h) , fluctuating (E, N, S^z)

Lagrange multipliers and grand potential. In the grand-canonical ensemble one introduces chemical potential μ and Zeeman field h as Lagrange multipliers that control N and S^z on average:

$$\hat{H}_{\text{GC}} = \hat{H} - \mu \hat{N} - 2h \hat{S}^z, \quad \hat{N} \equiv \sum_i \hat{n}_i, \quad \hat{S}^z \equiv \sum_i \hat{S}_{zi}. \quad (102)$$

The grand partition function and grand potential are

$$Z_{\text{GC}}(\mu, h, T) = \text{Tr } e^{-\beta(\hat{H} - \mu \hat{N} - 2h \hat{S}^z)}, \quad \Omega(\mu, h, T) \equiv -T \ln Z_{\text{GC}}. \quad (103)$$

Thermodynamic averages follow from derivatives of Ω :

$$\langle \hat{N} \rangle_{\mu, h} = -\frac{\partial \Omega}{\partial \mu}, \quad \langle \hat{S}^z \rangle_{\mu, h} = -\frac{1}{2} \frac{\partial \Omega}{\partial h}. \quad (104)$$

Because the trace in Z_{GC} runs over all charge sectors, \hat{N} and \hat{S}^z fluctuate:

$$(\Delta N)^2 = \langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2 = T \frac{\partial \langle \hat{N} \rangle}{\partial \mu}, \quad (\Delta S^z)^2 = \langle \langle \hat{S}^z \rangle^2 \rangle - \langle \hat{S}^z \rangle^2 = \frac{T}{4} \frac{\partial \langle \hat{S}^z \rangle}{\partial h}. \quad (105)$$

A.5 Legendre transforms: switching the control variables

Differentials and conjugate pairs. The cleanest way to remember the Legendre structure is via differentials. For a system with conserved (N, S^z) , the internal energy E (as a function of entropy S and charges) satisfies

$$dE = T dS + \mu dN + 2h dS^z. \quad (106)$$

One may then define thermodynamic potentials by subtracting the “work terms” corresponding to variables one wishes to control:

■ **From microcanonical to canonical (fix T instead of S).** Define the Helmholtz free energy

$$F(T, N, S^z) \equiv E - TS, \quad (107)$$

so that

$$dF = -S dT + \mu dN + 2h dS^z. \quad (108)$$

■ **From canonical to grand-canonical (fix μ, h instead of N, S^z).** Define the grand potential

$$\Omega(T, \mu, h) \equiv F - \mu N - 2h S^z, \quad (109)$$

so that

$$d\Omega = -S dT - N d\mu - 2S^z dh. \quad (110)$$

Remark: Legendre transform as an optimization principle

Remark: At fixed (T, μ, h) , the equilibrium state minimizes Ω . At fixed (T, N, S^z) , it minimizes F . This is the variational meaning behind “introducing Lagrange multipliers”: the multipliers μ, h are chosen so that the minimizer has the desired average charges. In the thermodynamic limit, these minimizations are equivalent to the Legendre transform relations among potentials.

A.6 Hard constraint vs Lagrange multiplier (and why canonical is often natural for cold atoms)

Two operational viewpoints.

Two equivalent viewpoints (hard constraint vs Lagrange multiplier)

■ **Hard constraint (canonical/microcanonical).** One restricts the Hilbert space to a fixed sector, e.g.

$$\mathcal{H}_{N,S^z} = \left\{ |\Psi\rangle : \hat{N}|\Psi\rangle = N|\Psi\rangle, \hat{S}^z|\Psi\rangle = S^z|\Psi\rangle \right\}, \quad (111)$$

and computes $Z_C = \text{Tr}_{\mathcal{H}_{N,S^z}} e^{-\beta \hat{H}}$. Then $\Delta N = \Delta S^z = 0$ by construction.

■ **Lagrange multipliers (grand-canonical).** One keeps the full Hilbert space but weights each sector by $e^{\beta \mu \hat{N} + \beta 2h \hat{S}^z}$, equivalently replacing \hat{H} by $\hat{H} - \mu \hat{N} - 2h \hat{S}^z$. Then N, S^z fluctuate, but their mean values are controlled by μ, h via (104).

FHM-specific bookkeeping: density, doping, and spin imbalance. For the Fermi–Hubbard model on N_s lattice sites, it is often useful to define

$$n \equiv \frac{N_\uparrow + N_\downarrow}{N_s} = \frac{N}{N_s}, \quad \delta \equiv N - N_s, \quad m \equiv N_\uparrow - N_\downarrow = 2S^z. \quad (112)$$

In many ultracold-atom experiments, N_\uparrow and N_\downarrow are prepared and (approximately) conserved on experimental time scales, so (δ, m) are naturally treated as fixed quantum numbers (canonical viewpoint). In contrast, in electronic settings one often effectively controls μ (and sometimes h) via reservoirs/fields (grand-canonical viewpoint).

A.7 When can ensembles differ? (phase separation and convexity)

Equivalence and its caveats. Although ensembles are usually equivalent in the thermodynamic limit for short-range interacting systems, care is needed near first-order transitions and phase separation. A standard diagnostic is the convexity of the free energy (or, equivalently, positivity of compressibility/susceptibility).

Remark: convexity, Maxwell construction, and “negative compressibility”

Remark: In the grand-canonical ensemble one may encounter regimes where $\partial \langle N \rangle / \partial \mu < 0$ (formally “negative compressibility”), signaling that the homogeneous state is unstable and the true equilibrium involves coexistence of phases. In the canonical ensemble, this manifests as phase separation at fixed N . The consistent thermodynamics corresponds to the convex envelope of the free energy (Maxwell construction), which restores stability and ensemble equivalence at the level of equilibrium states.

B Pauli matrices, spinor bilinears, and $SU(2)$ generators

B.1 Pauli algebra and completeness (Fierz) identity

Basic algebra. Pauli matrices satisfy

$$\sigma^a \sigma^b = \delta^{ab} \mathbb{I} + i\epsilon^{abc} \sigma^c, \quad \text{tr}(\sigma^a) = 0, \quad \text{tr}(\sigma^a \sigma^b) = 2\delta^{ab}. \quad (113)$$

The completeness identity (10) is a Fierz rearrangement and is the key tool for reducing products of spinor bilinears.

B.2 The generator S

Spinor language. On each site define the spinor $\hat{\psi}_i \equiv (\hat{c}_{i\uparrow}, \hat{c}_{i\downarrow})^\top$. A global spin rotation acts as

$$\hat{\psi}_i \rightarrow U \hat{\psi}_i, \quad U = \exp(-i\theta \cdot \sigma/2) \in SU(2). \quad (114)$$

“The unique natural $SU(2)$ generator inside $\hat{\psi}^\dagger(\cdot)\hat{\psi}$ ”. Any on-site quadratic operator has the form $\hat{\psi}_i^\dagger M \hat{\psi}_i$ with a 2×2 matrix M . Under $SU(2)$ rotations, it transforms by conjugation $M \rightarrow U^\dagger M U$. The Lie algebra generators are therefore precisely the traceless Hermitian matrices, i.e. linear combinations of σ^a . Thus the only nontrivial on-site bilinear that generates spin rotations is

$$\hat{S}_i^a = \frac{1}{2} \hat{\psi}_i^\dagger \sigma^a \hat{\psi}_i, \quad (115)$$

with the factor $1/2$ ensuring $[\hat{S}^a, \hat{S}^b] = i\epsilon^{abc} \hat{S}^c$. This is the precise mathematical meaning of “the unique natural $SU(2)$ generator structure” inside $\hat{\psi}^\dagger(\cdot)\hat{\psi}$.

B.3 Useful operator identities on a single site

Double occupancy and spin-length identity. Define $\hat{D}_i \equiv \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$. Then the following identities hold:

$$\hat{n}_i^2 = \hat{n}_i + 2\hat{D}_i, \quad \hat{S}_i^2 = \frac{3}{4}(\hat{n}_i - 2\hat{D}_i), \quad \frac{1}{2}\hat{n}_i^2 = \hat{n}_i - \frac{2}{3}\hat{S}_i^2. \quad (116)$$

They are particularly useful for rewriting interaction terms and for making symmetries manifest.