Charge and Spin transport in Hubbard lattice

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Abstract: In this note, I summarize our discussion on the charge and spin transport in Hubbard lattice.

1 Overview

In recent experiments, people do transport measurements in repulsive Hubbard interacting systems. Some transport constants, such as the spin diffusion and charge diffusion, are extracted from the measurements. (spin diffusion: arXiv:1802.10018. charge diffusion: arXiv:1802.09456.)

Although appearing quite differently at first sight, the two transport process, the charge transport and the spin transport, are actually deeply related to each other in such a system. Revealed by several symmetries of the system, the dynamical evolution of one quantity reflects that of the other, as its counterpart, under certain conditions. In this work, we give a thorough study to this discovery.

1.1 Bipartite Hubbard Lattice

Bipartite lattice is one that could be divided into A/B sublattices such that there is no intra-sublattice hopping but only inter-sublattice hopping. For example, a two-dimensional (2D) square lattice with nearest neighboring tunneling is a bipartite lattice. The sites of a bipartite lattice can be numbered such that the number of sites in A are odd integers and that of B sites are even integers. That is, $\forall i \in A, i \equiv 1 \mod 2$, and $\forall i \in B, i \equiv 0 \mod 2$.

Hubbard interaction can be included in the model, with such onsite interacting term as $U\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$ added into the model Hamiltonian. Hence, the Hamiltonian of a tight-binding model with Hubbard interaction on a bipartite lattice can be written as

$$\hat{H} = \sum_{\langle i,j\rangle,\sigma} -t\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + \sum_i U\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \tag{1}$$

where $\langle i, j\rangle$ denotes the nearest neighboring sites, with $i \in A$ and $j \in B$.

1.2 Many-body systems

If we consider many-particle systems, where the chemical potential can be tuned either locally or globally, such term as $\mu_i\hat{n}_i$ can be added in (1). The Hamiltonian is therefore written as

$$\hat{H} = \sum_{\langle i,j\rangle,\sigma} -t\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + \sum_i U\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - \sum_i \mu_i\hat{n}_i \tag{2}$$

for local chemical potentials μ_i, or

$$\hat{H} = \sum_{\langle i,j\rangle,\sigma} -t\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + \sum_i U\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - \mu\hat{N} \tag{3}$$

for a total chemical potential μ.

If the particle number is fixed, for example when considering the dynamics of a product Fock state, then there is no need of writing down the $\mu\hat{N}$ term.

For a half-filled system, $\mu = U/2$, another way to write the Hamiltonian is

$$\hat{H} = \sum_{\langle i,j\rangle,\sigma} -t\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + \sum_i U(\hat{n}_{i\uparrow} - 1/2)(\hat{n}_{i\downarrow} - 1/2) \tag{4}$$

2 Symmetry

2.1 Particle-hole symmetry at half filling

The model Hamiltonian has a particle-hole symmetry at half filling.

Definition 1: Define particle-hole transformation $\mathcal{P}$ as

$$\begin{aligned} \mathcal{P}: \ \hat{c}_{i\uparrow} &\to (-1)^i\hat{c}^\dagger_{i\uparrow}, \\ \hat{c}_{i\downarrow} &\to \hat{c}_{i\downarrow}. \end{aligned} \tag{5}$$

In a more specific way, the particle-hole transformation executes the following operator equations,

$$\mathcal{P}\hat{c}_{i\uparrow}\mathcal{P}^{-1} = (-1)^i\hat{c}^\dagger_{i\uparrow}, \quad \mathcal{P}\hat{c}_{i\downarrow}\mathcal{P}^{-1} = \hat{c}_{i\downarrow}, \tag{6}$$

and the state equations,[1]

$$\mathcal{P}|n_{i\uparrow}=0\rangle=|n_{i\uparrow}=1\rangle,\quad \mathcal{P}|n_{i\uparrow}=1\rangle=|n_{i\uparrow}=0\rangle. \tag{7}$$

Theorem 1: For the half-filled Fermi-Hubbard Hamiltonian (4), $\mathcal{P}$ maps the repulsive one ($U>0$) and the attractive one ($U<0$) of the same interaction strength $|U|$ into each other.

Theorem 1 states, in another word, $\mathcal{P}\hat{H}(+U)\mathcal{P}^{-1}=\hat{H}(-U)$. The proof is straightforward.

Definition 2: Local charge density is defined as the particle density $\hat{n}_i$, where $\hat{n}_i=\hat{n}_{i\uparrow}+\hat{n}_{i\downarrow}$. Local spin density is defined as $\hat{S}_i=\hat{n}_{i\uparrow}-\hat{n}_{i\downarrow}$.

Theorem 2: Local charge density and local spin density are mapped to each other under $\mathcal{P}$, up to a constant. $\mathcal{P}\hat{S}_i\mathcal{P}^{-1}=1-\hat{n}_i$.

The proof is straightforward.

Now consider two classes of states, both are product Fock state at half filling, one with inhomogeneous local charge density and homogeneous local spin density, the other, on the contrary, with homogeneous local charge density and inhomogeneous local spin density. For example, $|\psi_1\rangle$ and $|\psi_2\rangle$ introduced here in a one-dimensional (1D) lattice,

$$|\psi_1\rangle=\prod_{i\leq\frac{N}{2}}\hat{c}^\dagger_{i\uparrow}\hat{c}^\dagger_{i\downarrow}|0\rangle,\quad |\psi_2\rangle=\prod_{i\leq\frac{N}{2}}\prod_{j\geq\frac{N}{2}}\hat{c}^\dagger_{i\downarrow}\hat{c}^\dagger_{j\uparrow}|0\rangle, \tag{8}$$

are two typical states of the two classes, respectively. Rigorously, the two classes of states can be defined as follows.

Definition 3: half-filled product Fock state is defined as $|\psi\rangle=\prod_{i\sigma}\hat{c}^\dagger_{i\sigma}|0\rangle$ and $|\psi\rangle$ satisfies $\langle\psi|\hat{N}|\psi\rangle=N$, where $\hat{N}=\sum_i\hat{n}_i$ and N is the total number of lattice sites. Class 1: the set of $|\psi\rangle$ where $|\psi\rangle$ is a half-filled product Fock state and satisfying i) $\forall i,\langle\psi|\hat{S}_i|\psi\rangle=0$, ii) $\exists i,\langle\psi|\hat{n}_i|\psi\rangle\neq 1$. Class 2: the set of $|\psi\rangle$ where $|\psi\rangle$ is a half-filled product Fock state and satisfying i) $\forall i,\langle\psi|\hat{n}_i|\psi\rangle=1$, ii) $\exists i,\langle\psi|\hat{S}_i|\psi\rangle\neq 0$.

Then there comes a theorem for states also, regarding these two classes just introduced above.

Theorem 3: Regarding the two classes defined in Definition 3, Class 1 and Class 2. The particle-hole transformation $\mathcal{P}$ maps the two classes into each other. Or in other words, $\forall|\psi_1\rangle\in$ Class 1, $\exists|\psi_2\rangle\in$ Class 2, s.t. $\mathcal{P}|\psi_1\rangle=|\psi_2\rangle$; and $\forall|\psi_2\rangle\in$ Class 2, $\exists|\psi_1\rangle\in$ Class 1, s.t. $\mathcal{P}|\psi_2\rangle=|\psi_1\rangle$. That is to say, for any state in Class 1, there is a counterpart in Class 2 (and vice versa), who are related through $\mathcal{P}$.

The proof is straightforward. For example, for the two states in Eq.(8), easy to verify $\mathcal{P}|\psi_1\rangle=|\psi_2\rangle$.

Combining these three theorems, we conclude that, the dynamics of a state, starting from one in Class 1 and governed by the repulsive interacting Hamiltonian, is equivalent to the dynamics of the state starting from the counterpart one in Class 2 and governed by the counterpart attractive interacting Hamiltonian. And measured in these two states respectively, the evolution of local charge density in a repulsive system is equivalent to the evolution of local spin density in an attractive system.

Formally,

$$\mathcal{P}e^{-iH(+U)t}|\psi_1\rangle=e^{-iH(-U)t}|\psi_2\rangle \tag{9}$$

$$\mathcal{P}\hat{n}_i\mathcal{P}^{-1}=1-\hat{S}_i \tag{10}$$

[1] $\mathcal{P}$ does not change $|n_{i\downarrow}\rangle$ state.

2.2 Symmetry protected dynamical symmetry

In our previous work [Physical Review Letter **119** 225302 (2017)], we proposed a theorem called *Symmetry protected dynamical symmetry* in generalized Hubbard models. We presented there three examples, the first of which is the bipartite Fermi-Hubbard model. By finding such a unitary transformation $W\hat{c}_{i\sigma}W^{-1} = (-1)^i\hat{c}_{i\sigma}$, combined with the antiunitary transformation $TiT^{-1} = -i$, to get an antiunitary transformation $R = TW$, such that $\{R, \hat{H}_0\} = 0$, $[R, \hat{V}] = 0$, where $\hat{H}_0$ is the single-particle part of the Hamiltonian, and $\hat{V}$ is the Hubbard interaction, the dynamics governed by the attractive interacting Hamiltonian is related to the dynamics governed by the repulsive interacting Hamiltonian for certain states and certain observables.

Here, the observables we consider are local charge density $\hat{n}_i$ and local spin density $\hat{S}_i$. Easy to verify $[R, \hat{n}_i] = 0$, $[R, \hat{S}_i] = 0$. And the states we consider here are $|\psi_1\rangle$ in Class 1 and $|\psi_2\rangle$ in Class 2. Easy to verify $R|\psi_1\rangle = |\psi_1\rangle$, $R|\psi_2\rangle = |\psi_2\rangle$.

By (9) and (10),

$$\begin{aligned}
\langle\hat{n}_i(t)\rangle_{\psi_1,+U} &= \langle\psi_1|e^{iH(+U)t}\hat{n}_i e^{-iH(+U)t}|\psi_1\rangle \\
&= \langle\psi_1|e^{iH(+U)t}\mathcal{P}^{-1}\mathcal{P}\hat{n}_i\mathcal{P}^{-1}\mathcal{P}e^{-iH(+U)t}|\psi_1\rangle \\
&= \langle\psi_2|e^{iH(-U)t}(1-\hat{S}_i)e^{-iH(-U)t}|\psi_2\rangle \\
&= 1 - \langle\psi_2|e^{iH(-U)t}\hat{S}_i e^{-iH(-U)t}|\psi_2\rangle \\
&= 1 - \langle\hat{S}_i(t)\rangle_{\psi_2,-U},
\end{aligned} \tag{11}$$

and by the *Symmetry protected dynamical symmetry*

$$\langle\hat{S}_i(t)\rangle_{\psi_2,-U} = \langle\hat{S}_i(t)\rangle_{\psi_2,+U}, \tag{12}$$

thus

$$\langle\hat{n}_i(t)\rangle_{\psi_1,+U} = 1 - \langle\hat{S}_i(t)\rangle_{\psi_2,+U}. \tag{13}$$

2.3 Away from half filling

Consider the case away from half filling. When the total particle number is given, there is no need of the $\mu\hat{N}$ term and the total particle number is conserved. If the initial states we consider are also product Fock state, the conclusion is unchanged.

3 Transport

diffusive process is characterized by the evolution of the local density n and local current $\vec{j}$ who satisfy

$$\partial_t n + \nabla\cdot\vec{j} = 0, \tag{14}$$

$$\vec{j} = -D_c\nabla n. \tag{15}$$

It results in the diffusion equation

$$\partial_t n - D_c\nabla^2 n = 0 \tag{16}$$

where D_c is known as the diffusion constant.

Regarding the charge diffusion and spin diffusive process as discussed above, the local density n should be substituted with the measurement of local charge density, $\langle\hat{n}_i\rangle$, and local spin density, $\langle\hat{S}_i\rangle$, respectively.

By Eq.(13),

$$\partial_t \langle \hat{n}_i(t) \rangle_{\psi_1,+U} = -\partial_t \langle \hat{S}_i(t) \rangle_{\psi_2,+U} \tag{17}$$

$$\nabla^2 \langle \hat{n}_i(t) \rangle_{\psi_1,+U} = -\nabla^2 \langle \hat{S}_i(t) \rangle_{\psi_2,+U} \tag{18}$$

Therefore, starting from the certain initial states as considered, the diffusion constant D_c for the charge diffusive process and the spin diffusive process are the same, for the same repulsive Hamiltonian.

3.1 Temperature effect

If the temperature effect is taken into account, then it is not merely a certain state, but the density matrix $\rho = e^{-\beta H}$ that we should consider. The observable becomes $n = tr(\rho \hat{n})$. If we want to show the diffusion constants are the same, then we ought to prove that the ensemble averaged expectation value of charge density and spin density have some relations, which is not that straightforward. But there is a special case.

A special case is the infinite temperature. $\mathcal{P} e^{-\beta H(+U)} \mathcal{P}^{-1} = e^{-\beta H(-U)}$, $R e^{-\beta H(-U)} R^{-1} = e^{\beta H(+U)}$. Hence, when temperature is infinite, $\beta = 0$, the combination transformation $\mathcal{P}R$ maps the density matrix into itself. By the logic of Sec. 2, the diffusive process for charge and spin are equivalent, as well as the diffusion constants D_c in each process.

4 Numerical Demonstration

To be continued..

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