

Unitary Renormalization Group Approach to Single-Impurity Anderson Model

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Sensing Fermi volume from entanglement entropy of non-interacting ground state

0.1 Description of the ground state wavefunction

For an (effectively) *non-interacting system of N spin-less Fermions*, the momenta are good quantum numbers, and the ground state wavefunction can be labeled as

$$|k_1, k_2, \dots, k_N\rangle \quad (0.1)$$

The set k_1 through k_N is the set of momenta values that are occupied. It is understood that all other momenta are unoccupied. For a metallic ground state, k_N would be the Fermi momentum. The ground state, when written in terms of single-particle states, would have to be antisymmetrised. Let $|k_a\rangle_1 |k_b\rangle_2 \dots |k_q\rangle_N$ represent the state in which the first electron has momentum k_a , the second one has momentum k_b , and so on and the last one has momentum k_q . The antisymmetrised form is

$$|\Psi^N\rangle = |k_1, k_2, \dots, k_N\rangle = \frac{1}{\sqrt{N!}} \sum_{p \in S_N} (-1)^p \prod_{i=1}^N |k_{p_i}\rangle_i \quad (0.2)$$

S_N is the set of all permutations of the set $\{1, 2, \dots, N\}$. p is a string of numbers $p_1 p_2 \dots p_N$, and runs through all such permutations. $p(i)$ then refers to the i^{th} element of such a permutation. One permutation can thus be represented as

$$\begin{pmatrix} 1 & 2 & 3 & \dots & N \\ p_1 & p_2 & p_3 & \dots & p_N \end{pmatrix} \quad (0.3)$$

which means that 1 goes to p_1 , 2 goes to p_2 , and so on. The odd or even nature of permutations are determined by comparing a particular permutation with the zeroth permutation of the set. For this set S_N , the zeroth permutation is chosen to be $1, 2, \dots, N$. Even (odd) permutations will then be those which can be reached from the zeroth permutation via an even (odd) number of permutations. The sign factor $(-1)^p$ will be $+1$ for all even permutations and -1 for the odd ones. For brevity, we can drop the index i that labels the particle by defining the following notation: the first ket in the product denotes the state of the first particle, the second that of the second particle and so on. For three particles, it looks like

$$|k_1, k_2, k_3\rangle = \frac{1}{\sqrt{3!}} [|k_1\rangle |k_2\rangle |k_3\rangle + |k_3\rangle |k_1\rangle |k_2\rangle + |k_2\rangle |k_3\rangle |k_1\rangle - |k_2\rangle |k_1\rangle |k_3\rangle - |k_1\rangle |k_3\rangle |k_2\rangle - |k_3\rangle |k_2\rangle |k_1\rangle] \quad (0.4)$$

0.2 Entanglement entropy of two-particle Fermi sea

The ground state wavefunction for a two-particle Fermi sea (with momenta k_{\pm} is

$$|\Psi\rangle_{12} = \frac{1}{\sqrt{2}} (|k_+\rangle_1 |k_-\rangle_2 - |k_-\rangle_1 |k_+\rangle_2) \quad (0.5)$$

The notation $|k_{\pm}\rangle_i$ means it is a state of the i^{th} particle, in a momentum k_{\pm} . The total two-particle density matrix is

$$\rho_{12} = |\Psi\rangle_{12} \langle\Psi|_{12} \quad (0.6)$$

The reduced density matrix for the first particle is obtained by tracing over all states of the second particle:

$$\rho_1 = \sum_{j=\pm} \langle k_j|_2 \rho_{12} |k_j\rangle_2 = \sum_{j=\pm} \langle k_j|_2 |\Psi\rangle_{12} \langle\Psi|_{12} |k_j\rangle_2 \quad (0.7)$$

The inner product evaluates as follows:

$$\langle k_{\pm}|_2 |\Psi\rangle_{12} = \frac{1}{\sqrt{2}} \mp |k_{\mp}\rangle_1 \quad (0.8)$$

such that

$$\langle k_j|_2 |\Psi\rangle_{12} \langle\Psi|_{12} |k_j\rangle_2 = \frac{1}{2} |k_{\mp}\rangle_1 \langle k_{\mp}|_1 \quad (0.9)$$

and

$$\rho_1 = \frac{1}{2} (|k_{+}\rangle_1 \langle k_{+}|_1 + |k_{-}\rangle_1 \langle k_{-}|_1) = \begin{pmatrix} \frac{1}{2} & \\ & \frac{1}{2} \end{pmatrix} \quad (0.10)$$

The von-Neumann entropy of ρ_1 is obtained by finally tracing $-\rho_1 \ln \rho_1$ over all the momentum states of particle 1.

$$S_1 = - \sum_{j=\pm} \langle k_j|_1 \rho_1 \ln \rho_1 |k_j\rangle_1 = \ln 2 \quad (0.11)$$

0.3 von-Neumann entropy of intermediate reduced state

If we trace out m particles from the total density matrix ρ^N , the von-Neumann entropy S_m of the remaining density matrix ρ^{N-m} is

$$S_m = \ln \frac{N(N-1)\dots(N-m+1)}{m!} = \ln {}^N C_m \quad (0.12)$$

This has the property $S_{N-m} = \ln {}^N C_{N-m} = \ln {}^N C_m = S_m$

0.4 von-Neumann entropy of final reduced state

If we trace out $N-1$ particles from the total density matrix ρ^N , the von-Neumann entropy S_{N-1} of the remaining density matrix ρ^{N-1} is

$$S_m = \ln N \quad (0.13)$$

0.5 Large system approximation

For a total number N , let N_0 be the number of momentum states on the Fermi surface and $N_{<}$ the number of momentum states inside. Then, $N_0 \sim L^{d-1}$ and $N_{<} \sim L^d$, so

$$\frac{N_0}{N_{<}} \sim \frac{1}{L} \rightarrow 0 \text{ as } L \rightarrow \infty \quad (0.14)$$

The entanglement entropy on tracing out N_0 states will be given by

$$\begin{aligned}
S &= \ln \frac{N!}{N_{<}!N_0!} \\
&\approx N \ln N - N - N_{<} \ln N_{<} + N_{<} - N_0 \ln N_0 + N_0 \quad [\ln N! \approx N \ln N - N] \\
&= N_{<} \ln \frac{N_0 + N_{<}}{N_{<}} + N_0 \ln \frac{N_0 + N_{<}}{N_0} \quad [N = N_0 + N_{<}] \\
&= N_{<} \ln \left(1 + \frac{N_0}{N_{<}} \right) + N_0 \ln \left(\frac{N_{<}}{N_0} + 1 \right) \\
&\approx N_{<} \frac{N_0}{N_{<}} + N_0 \ln \left(\frac{N_{<}}{N_0} + 1 \right) \quad [\ln(1+x) \approx x \text{ for } x \rightarrow 0] \quad (0.15) \\
&\approx N_{<} \frac{N_0}{N_{<}} + N_0 \ln \left(\frac{N_{<}}{N_0} \right) \quad \left[\frac{N_{<}}{N_0} \rightarrow \infty \right] \\
&= N_0 \left[1 + \ln \left(\frac{N_{<}}{N_0} \right) \right] \\
&\approx N_0 \ln \left(\frac{N_{<}}{N_0} \right) \quad \left[\frac{N_{<}}{N_0} \rightarrow \infty \right] \\
&\sim cL^{d-1} \ln L
\end{aligned}$$

0.6 Fermi gases and Fermi liquids

$$\begin{aligned}
N_0 &= \text{number of particles on Fermi surface} \\
N_{<} &= \text{number of particles inside Fermi surface} \\
N &= N_0 + N_{<}
\end{aligned} \quad (0.16)$$

Trace out all particles *on and above* Fermi surface.

$$S_{FL} = \ln [{}^N C_{N_0}] = \ln [{}^N C_{N_{<}}] = \ln \frac{(N_0 + N_{<})!}{N_{<}!} \quad (0.17)$$

Both the numbers N_0 and $N_{<}$ have topological stability. The entanglement entropy S_{FL} is thus a topological quantity.

Using the previous approximations, this turns out to be

$$S_{FL} = N_0 \ln \left(\frac{N_{<}}{N_0} \right) \sim cL^{d-1} \ln L \quad (0.18)$$

0.7 Marginal Fermi liquid

$$\begin{aligned}
N_{>} &= \text{number of particles outside Fermi surface} \\
N_0 &= \text{number of particles on Fermi surface} \\
N_{<} &= \text{number of particles inside Fermi surface} \\
N &= N_0 + N_{<} + N_{>}
\end{aligned} \quad (0.19)$$

Trace out all particles *on and above* Fermi surface.

$$S_{MFL} = \ln [{}^N C_{N_0+N_{>}}] = \ln [{}^N C_{N_{<}}] \quad (0.20)$$

The change from FL is

$$S_{FL} - S_{MFL} = \ln \frac{{}^N C_{N_{<}^{FL}}}{{}^N C_{N_{<}^{MFL}}} \quad (0.21)$$

Assuming $N^{FL} = N^{MFL}$, the fraction simplifies to

$$\frac{{}^N C_{N_{<}^{FL}}}{{}^N C_{N_{<}^{MFL}}} = \frac{N_{<}^{MFL}! (N_0^{MFL} + N_{>}^{MFL})!}{N_{<}^{FL}! N_0^{FL}!} \quad (0.22)$$

If the extra states outside the Fermi volume have come solely from the Fermi surface, we can also assume $N_{<}^{MFL} = N_{<}^{FL}$ and $N_0^{FL} = N_0^{MFL} + N_{>}^{MFL}$, such that

$$\frac{{}^N C_{N_{<}^{FL}}}{{}^N C_{N_{<}^{MFL}}} = 1 \quad (0.23)$$

and $S_{FL} = S_{MFL}$, which essentially means that since the particle exchanges have happened completely inside the subsystem we are tracing out (Fermi surface and beyond), the connectivities between the two subsystems haven't changed and so the entanglement entropy is unchanged.

If, however, the extra states have come from inside the Fermi volume, then

$$\frac{{}^N C_{N_{<}^{FL}}}{{}^N C_{N_{<}^{MFL}}} = \frac{N_{<}^{MFL}! (N_0^{FL} + N_{>}^{MFL})!}{N_{<}^{FL}! N_0^{FL}!} \approx \frac{N_{<}^{MFL}!}{N_{<}^{FL}!} [N_0^{FL} \gg N_{>}^{MFL}] \quad (0.24)$$

0.8 Gapped states

0.9 Derivations-I

The goal is to calculate the von-Neuman entropy of the reduced density matrix of the general state eq. 0.2. To that end, we try to rewrite it in terms of the Slater determinants of $N - 1$ particles.

$$\begin{aligned} |\Psi^N\rangle &= \frac{1}{\sqrt{N!}} \sum_{p \in S_N} (-1)^p \prod_{i=1}^N |k_{p_i}\rangle_i \\ &= \frac{1}{\sqrt{N!}} \sum_{p_1=1}^N \sum_{\substack{p_2=1 \\ p_2 \neq p_1}}^N \dots \sum_{\substack{p_N=1 \\ p_N \neq p_1, p_2, \dots, p_{N-1}}}^N (-1)^p \prod_{i=1}^N |k_{p_i}\rangle_i \\ &= \frac{1}{\sqrt{N!}} \sum_{p_1=1}^N \sum_{p^1 \in S_N^{p_1}} (-1)^p \prod_{i=1}^N |k_{p_i}\rangle_i \end{aligned} \quad (0.25)$$

$S_N^{p_1}$ is the set of permutations of the set $\{1, 2, \dots, \hat{p}_1, \dots, N\}$, where the hat on p_1 means it is absent. The index which runs over the set $S_N^{p_1}$ is p^1 .

The factor of $(-1)^p$ can be made independent of p_1 , in the following fashion. Consider a particular value of p_1 and hence the unique sequence $s_{\text{unique}} = p_1 p_2 p_3 \dots p_N$, $p_2 > p_3 > \dots > p_N$. There are two possibilities.

- p_1 's value is such that s_{unique} is even and $(-1)^p$ is $+1$
- p_1 's value is such that s_{unique} is odd and $(-1)^p$ is -1

For the first case, we will define the sequence $s_{\text{zeroth}}^1 = p_2 p_3 \dots p_N$, $p_2 > p_3 > \dots > p_N$ as the zeroth sequence of $S_N^{p_1} = \{p^1\}$. Then, all even permutations of s_{unique} (which implies $(-1)^p = +1$) will essentially be even permutations of s_{zeroth}^1 (because p_1 is fixed at the front), and hence will imply

$$(-1)^{p^1} = +1 = (-1)^p \forall p = \text{even and } s_{\text{unique}} = \text{even} \quad (0.26)$$

The odd permutations of s_{unique} will be odd permutations of s_{zeroth}^1 and we will have

$$(-1)^{p^1} = -1 = (-1)^p \forall p = \text{odd and } s_{\text{unique}} = \text{even} \quad (0.27)$$

For the second case, we will define the other unique sequence $s_{\text{zeroth}}^{1'} = p_2 p_3 \dots p_N$, $p_2 < p_3 < \dots < p_N$ as the zeroth sequence of $S_N^{p_1} = \{p^1\}$, such that s_{unique} would be an odd permutation. Using similar arguments in the previous case, we can again show that the odd(even) permutations of this zeroth sequence would be the odd(even) permutations of s_{unique} . Combining both cases, we can write

$$(-1)^{p^1} = (-1)^p \forall p \quad (0.28)$$

With this observation, we can write

$$\begin{aligned} |\Psi^N\rangle &= \frac{1}{\sqrt{N!}} \sum_{p_1=1}^N |k_{p_1}\rangle \sum_{p^1 \in S_N^{p_1}} (-1)^{p^1} \prod_{i=2}^N |k_{p_i^1}\rangle \\ &= \frac{1}{\sqrt{N}} \sum_{p_1=1}^N |k_{p_1}\rangle |\Psi^{N-1}(\hat{p}_1)\rangle \end{aligned} \quad (0.29)$$

The ket

$$|\Psi^{N-1}(\hat{p}_1)\rangle = \frac{1}{\sqrt{(N-1)!}} \sum_{p^1 \in S_N^{p_1}} (-1)^{p^1} \prod_{i=2}^N |k_{p_i^1}\rangle \quad (0.30)$$

is the antisymmetrised state of $N - 1$ particles, with momenta ranging from 1 to N excluding k_{p_1} . The set $S_N^{p_1}$ has a zeroth sequence determined by the value of p_1 , hence it is a function of p_1 .

Equation 0.29, when expanded, looks like

$$|\Psi^N\rangle = \frac{1}{\sqrt{N!}} \left[|k_1\rangle |\Psi^{N-1}(\hat{k}_1)\rangle + |k_2\rangle |\Psi^{N-1}(\hat{k}_2)\rangle + |k_3\rangle |\Psi^{N-1}(\hat{k}_3)\rangle + \dots + |k_N\rangle |\Psi^{N-1}(\hat{k}_N)\rangle \right] \quad (0.31)$$

We can now trace out the 1st particle from the density matrix $\rho^N = |\Psi^N\rangle \langle \Psi^N|$.

$$\rho^{N-1} = \sum_i \langle k_i | \Psi^N \rangle \langle \Psi^N | k_i \rangle = \frac{1}{N} \sum_{p_1=1}^N |\Psi^{N-1}(\hat{p}_1)\rangle \langle \Psi^{N-1}(\hat{p}_1)| \quad (0.32)$$

We can again write the states $|\Psi^{N-1}(\hat{p}_1)\rangle$ in terms of the smaller kets.

$$|\Psi^{N-1}(\hat{p}_1)\rangle = \frac{1}{\sqrt{N-1}} \sum_{\substack{p_2=1 \\ p_2 \neq p_1}}^N |k_{p_2}\rangle |\Psi^{N-2}(\hat{p}_1 \hat{p}_2)\rangle \quad (0.33)$$

so that the next reduced density matrix would be

$$\rho^{N-2} = \sum_{j \neq p_1} \langle k_j | \rho^{N-1} | k_j \rangle = \frac{1}{N(N-1)} \sum_{p_1=1}^N \sum_{\substack{p_2=1 \\ p_2 \neq p_1}}^N |\Psi^{N-2}(\hat{p}_1 \hat{p}_2)\rangle \langle \Psi^{N-2}(\hat{p}_1 \hat{p}_2)| \quad (0.34)$$

If we trace out m particles from the total density matrix ρ^N , we will end up with (extrapolating from eq. 0.34)

$$\rho^{N-m} = \frac{1}{N(N-1)\dots(N-m+1)} \sum_{\substack{p_1, p_2, \dots, p_m=1 \\ p_2 \neq p_1, \dots, p_m \neq p_1, p_2, \dots, p_{m-1}}}^N |\Psi^{N-m}(\hat{p}_1 \hat{p}_2 \dots \hat{p}_m)\rangle \langle \Psi^{N-m}(\hat{p}_1 \hat{p}_2 \dots \hat{p}_m)| \quad (0.35)$$

Each unordered set $\{p_1, \dots, p_m\}$ occurs $m!$ times, and can be designated by a label s .

$$\rho^{N-m} = \frac{m!}{N(N-1)\dots(N-m+1)} \sum_s |\Psi^{N-m}(s)\rangle \langle \Psi^{N-m}(s)| \quad (0.36)$$

The kets $|\Psi^{N-m}(s)\rangle$ and $|\Psi^{N-m}(s')\rangle$ for $s \neq s'$ are orthogonal, because they will involve atleast one uncommon momentum. These states form a Schmidt basis for the density matrix; the density matrix is diagonal in this basis. Since there are ${}^N C_m$ such states in the summation over s , the dimension d^m of the density matrix is

$$d^m = {}^N C_m \quad (0.37)$$

The Schmidt coefficients (whose squares are the diagonal entries) are given by

$$K_{sm}^2 = \frac{m!}{N(N-1)\dots(N-m+1)} = \frac{1}{{}^N C_m} = \frac{1}{d^m} \quad (0.38)$$

Therefore

$$\rho^{N-m} = \sum_{s=1}^{d^m} K_{sm}^2 |\Psi^{N-m}(s)\rangle \langle \Psi^{N-m}(s)| = \frac{1}{d^m} \sum_{s=1}^{d^m} |\Psi^{N-m}(s)\rangle \langle \Psi^{N-m}(s)| \quad (0.39)$$

The von-Neumann entropy of ρ^{N-m} is thus

$$S^{N-m} = \text{Tr} [\rho^{N-m} \ln \rho^{N-m}] = -\frac{1}{d^m} \ln \frac{1}{d^m} \sum_{s=1}^{d^m} = \ln d^m = \ln {}^N C_m \quad (0.40)$$

0.10 Derivation-III

Each of the product states in eq. 0.2,

$$\prod_{i=1}^N |k_{p_i}\rangle_i \quad (0.41)$$

are orthogonal to each other. That is, if p and q , both members of S_N are two distinct permutations, then

$$\left((-1)^q \prod_{j=1}^N \langle k_{q_j} |_j \right) \left((-1)^p \prod_{i=1}^N |k_{p_i}\rangle_i \right) = 0, \text{ and } \left((-1)^p \prod_{j=1}^N \langle k_{p_j} |_j \right) \left((-1)^p \prod_{i=1}^N |k_{p_i}\rangle_i \right) = 1 \quad (0.42)$$

This is because the two products have atleast one momentum state different. There will be $N!$ such product states and they form a part of a particular basis of the Hilbert space. If we label such product states as

$$|\Phi_p\rangle = (-1)^p \prod_{i=1}^N |k_{p_i}\rangle_i \quad (0.43)$$

then

$$\rho^N = |\Psi^N\rangle \langle \Psi^N| = \frac{1}{N!} \sum_{p,q \in S_N} |\Phi_p\rangle \langle \Phi_q| \quad (0.44)$$

To find the von-Neumann entropy of this state, first note that the density matrix has an eigenstate

$$|\chi\rangle = \sum_{r \in S_N} |\Phi_r\rangle \quad (0.45)$$

because

$$\rho |\chi\rangle = \frac{1}{N!} \sum_{r \in S_N} \sum_{p,q \in S_N} |\Phi_p\rangle \langle \Phi_q| |\Phi_r\rangle = \frac{1}{N!} \sum_{r \in S_N} \sum_{p,q \in S_N} |\Phi_p\rangle \delta_{qr} = |\chi\rangle \quad (0.46)$$

Thus, ρ has an eigenvalue 1, which implies that the other eigenvalues must be 0 because the trace of ρ must be 1, and all the eigenvalues must be positive-semi-definite. Therefore, the von-Neumann entropy is zero:

$$S = \sum_i \rho_i \ln \rho_i = 0 + 1 \times \ln 1 = 0 \quad (0.47)$$

[1]

References

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