Unitary Renormalization Group Approach to Single-Impurity Anderson Model

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April 16, 2021

Contents

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

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

$$|k_1, k_2, ..., k_N\rangle \tag{0.1}$$

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 $|k_a\rangle_1 |k_b\rangle_2 ... |k_q\rangle_N$ 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

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

S_N is the set of all permutations of the set $\{1, 2, ..., N\}$. p is a string of numbers $p_1 p_2 ... p_N$, 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

$$\begin{pmatrix} 1 & 2 & 3 & ... & N \\ p_1 & p_2 & p_3 & ... & p_N \end{pmatrix} \tag{0.3}$$

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 $1, 2, ..., N$. 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

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

0.1 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

$$S_m = \ln \frac{N(N-1)...(N-m+1)}{m!} = \ln {}^N C_m \tag{0.5}$$

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

0.2 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

$$S_m = \ln N \tag{0.6}$$

0.3 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

$$\frac{N_0}{N_<} \sim \frac{1}{L} \to 0 \text{ as } L \to \infty \tag{0.7}$$

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

$$\begin{aligned}
S &= \ln \frac{N!}{N_<! N_0!} \\
&\approx N \ln N - N - N_< \ln N_< + N_< - N_0 \ln N_0 + N_0 && [\ln N! \approx N \ln N - N] \\
&= N_< \ln \frac{N_0 + N_<}{N_<} + N_0 \ln \frac{N_0 + N_<}{N_0} && [N = N_0 + N_<] \\
&= N_< \ln \left(1 + \frac{N_0}{N_<}\right) + N_0 \ln \left(\frac{N_<}{N_0} + 1\right) \\
&\approx N_< \frac{N_0}{N_<} + N_0 \ln \left(\frac{N_<}{N_0} + 1\right) && [\ln(1+x) \approx x \text{ for } x \to 0] \\
&\approx N_< \frac{N_0}{N_<} + N_0 \ln \left(\frac{N_<}{N_0}\right) && \left[\frac{N_<}{N_0} \to \infty\right] \\
&= N_0 \left[1 + \ln \left(\frac{N_<}{N_0}\right)\right] \\
&\approx N_0 \ln \left(\frac{N_<}{N_0}\right) && \left[\frac{N_<}{N_0} \to \infty\right] \\
&\sim c L^{d-1} \ln L
\end{aligned} \tag{0.8}$$

0.4 Fermi gases and Fermi liquids

$$\begin{aligned}
N_0 &= \text{number of particles on Fermi surface} \\
N_< &= \text{number of particles inside Fermi surface} \\
N &= N_0 + N_<
\end{aligned} \tag{0.9}$$

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

$$S_{FL} = \ln \left[{}^N C_{N_0}\right] = \ln \left[{}^N C_{N_<}\right] \tag{0.10}$$

0.5 Marginal Fermi liquid

$$\begin{aligned} N_> &= \text{number of particles outside Fermi surface} \\ N_0 &= \text{number of particles on Fermi surface} \\ N_< &= \text{number of particles inside Fermi surface} \\ N &= N_0 + N_< + N_> \end{aligned} \tag{0.11}$$

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

$$S_{MFL} = \ln \left[{}^N C_{N_0+N_>} \right] = \ln \left[{}^N C_{N_<} \right] \tag{0.12}$$

The change from FL is

$$S_{FL} - S_{MFL} = \ln \frac{{}^N C_{N_<^{FL}}}{{}^N C_{N_<^{MFL}}} \approx \ln \frac{N_<^{MFL}!}{N_<^{FL}!} \quad [\text{ using } N - m \approx N] \tag{0.13}$$

0.6 Derivations-I

The goal is to calculate the von-Newman 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.

$$\begin{aligned} |\Psi^N\rangle &= \frac{1}{\sqrt{N!}} \sum_{p \in S_N} (-1)^p \prod_{i=1}^{N} |k_{p_i}\rangle_i \\ &= \frac{1}{\sqrt{N!}} \sum_{p_1=1}^{N} \sum_{\substack{p_2=1 \\ p_2 \neq p_1}}^{N} \cdots \sum_{\substack{p_N=1 \\ p_N \neq p_1, p_2, \cdots, p_{N-1}}}^{N} (-1)^p \prod_{i=1}^{N} |k_{p_i}\rangle_i \\ &= \frac{1}{\sqrt{N!}} \sum_{p_1=1}^{N} \sum_{p^1 \in S_N^{p_1}} (-1)^p \prod_{i=1}^{N} |k_{p_i}\rangle_i \end{aligned} \tag{0.14}$$

$S_N^{p_1}$ is the set of permutations of the set $\{1, 2, ..., \hat{p}_1, ..., N\}$, 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 $s_{\text{unique}} = p_1 p_2 p_3 ... p_N,\ p_2 > p_3 > ... > p_N$. 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 $s^1_{\text{zeroth}} = p_2 p_3 ... p_N,\ p_2 > p_3 > ... > p_N$ 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^1_{zeroth} (because p_1 is fixed at the front), and hence will imply

$$(-1)^{p^1} = +1 = (-1)^p \,\forall\, p = \text{even and } s_{\text{unique}} = \text{even} \tag{0.15}$$

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

$$(-1)^{p^1} = -1 = (-1)^p \,\forall\, p = \text{odd and } s_{\text{unique}} = \text{even} \tag{0.16}$$

For the second case, we will define the other unique sequence $s^{1'}_{\text{zeroth}} = p_2 p_3 ... p_N,\ p_2 < p_3 < ... < p_N$ 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

$$(-1)^{p^1} = (-1)^p \,\forall\, p \tag{0.17}$$

With this observation, we can write

$$\begin{aligned} |\Psi^N\rangle &= \frac{1}{\sqrt{N!}} \sum_{p_1=1}^{N} |k_{p_1}\rangle \sum_{p^1 \in S_N^{p_1}} (-1)^{p^1} \prod_{i=2}^{N} |k_{p_i^1}\rangle \\ &= \frac{1}{\sqrt{N}} \sum_{p_1=1}^{N} |k_{p_1}\rangle \, |\Psi^{N-1}(\hat{p}_1)\rangle \end{aligned} \tag{0.18}$$

The ket

$$|\Psi^{N-1}(\hat{p}_1)\rangle = \frac{1}{\sqrt{(N-1)!}} \sum_{p^1 \in S_N^{p_1}} (-1)^{p^1} \prod_{i=2}^{N} |k_{p_i^1}\rangle \tag{0.19}$$

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 0.18, when expanded, looks like

$$|\Psi^N\rangle = \frac{1}{\sqrt{N!}} \Big[|k_1\rangle \, |\Psi^{N-1}(\hat{k}_1)\rangle + |k_2\rangle \, |\Psi^{N-1}(\hat{k}_2)\rangle + |k_3\rangle \, |\Psi^{N-1}(\hat{k}_3)\rangle + ... + |k_N\rangle \, |\Psi^{N-1}(\hat{k}_N)\rangle \Big] \tag{0.20}$$

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

$$\rho^{N-1} = \sum_i \langle k_i| \, |\Psi^N\rangle \langle\Psi^N| \, |k_i\rangle = \frac{1}{N} \sum_{p_1=1}^{N} |\Psi^{N-1}(\hat{p}_1)\rangle \langle\Psi^{N-1}(\hat{p}_1)| \tag{0.21}$$

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

$$|\Psi^{N-1}(\hat{p}_1)\rangle = \frac{1}{\sqrt{N-1}} \sum_{\substack{p_2=1 \\ p_2 \neq p_1}}^{N} |k_{p_2}\rangle \, |\Psi^{N-2}(\hat{p}_1 \hat{p}_2)\rangle \tag{0.22}$$

so that the next reduced density matrix would be

$$\rho^{N-2} = \sum_{j \neq p_1} \langle k_j | \, \rho^{N-1} \, | k_j \rangle = \frac{1}{N(N-1)} \sum_{p_1=1}^{N} \sum_{\substack{p_2=1 \\ p_2 \neq p_1}}^{N} |\Psi^{N-2}(\hat{p}_1 \hat{p}_2)\rangle \, \langle \Psi^{N-2}(\hat{p}_1 \hat{p}_2)| \tag{0.23}$$

If we trace out m particles from the total density matrix ρ^N, we will end up with (extrapolating from eq. 0.23)

$$\rho^{N-m} = \frac{1}{N(N-1)...(N-m+1)} \sum_{\substack{p_1, p_2, ... p_m = 1 \\ p_2 \neq p_1, ... p_m \neq p_1, p_2, ..., p_{m-1}}}^{N} |\Psi^{N-m}(\hat{p}_1 \hat{p}_2 ... \hat{p}_m)\rangle \, \langle \Psi^{N-m}(\hat{p}_1 \hat{p}_2 ... \hat{p}_m)| \tag{0.24}$$

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

$$\rho^{N-m} = \frac{m!}{N(N-1)...(N-m+1)} \sum_{s} |\Psi^{N-m}(s)\rangle \, \langle \Psi^{N-m}(s)| \tag{0.25}$$

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

$$d^m = {}^N C_m \tag{0.26}$$

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

$$K_{sm}^2 = \frac{m!}{N(N-1)...(N-m+1)} = \frac{1}{{}^N C_m} = \frac{1}{d^m} \tag{0.27}$$

Therefore

$$\rho^{N-m} = \sum_{s=1}^{d^m} K_{sm}^2 \, |\Psi^{N-m}(s)\rangle \, \langle \Psi^{N-m}(s)| = \frac{1}{d^m} \sum_{s=1}^{d^m} |\Psi^{N-m}(s)\rangle \, \langle \Psi^{N-m}(s)| \tag{0.28}$$

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

$$S^{N-m} = \text{Tr} \left[\rho^{N-m} \ln \rho^{N-m} \right] = -\frac{1}{d^m} \ln \frac{1}{d^m} \sum_{s=1}^{d^m} = \ln d^m = \ln {}^N C_m \tag{0.29}$$

0.7 Derivation-III

Each of the product states in eq. 0.2,

$$\prod_{i=1}^{N} |k_{p_i}\rangle_i \tag{0.30}$$

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

$$\left((-1)^q \prod_{j=1}^{N} \langle k_{q_j}|_j \right) \left((-1)^p \prod_{i=1}^{N} |k_{p_i}\rangle_i \right) = 0, \text{ and } \left((-1)^p \prod_{j=1}^{N} \langle k_{p_j}|_j \right) \left((-1)^p \prod_{i=1}^{N} |k_{p_i}\rangle_i \right) = 1 \tag{0.31}$$

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

$$|\Phi_p\rangle = (-1)^p \prod_{i=1}^{N} |k_{p_i}\rangle_i \tag{0.32}$$

then

$$\rho^N = |\Psi^N\rangle\,|\Psi^N\rangle = \frac{1}{N!}\sum_{p,q\in S_N} |\Phi_p\rangle\,\langle\Phi_q| \tag{0.33}$$

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

$$|\chi\rangle = \sum_{r\in S_N} |\Phi_r\rangle \tag{0.34}$$

because

$$\rho\,|\chi\rangle = \frac{1}{N!}\sum_{r\in S_N}\sum_{p,q\in S_N} |\Phi_p\rangle\,\langle\Phi_q|\,|\Phi_r\rangle = \frac{1}{N!}\sum_{r\in S_N}\sum_{p,q\in S_N} |\Phi_p\rangle\,\delta_{qr} = |\chi\rangle \tag{0.35}$$

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 positve-semi-definite. Therefore, the von-Neumann entropy is zero:

$$S = \sum_i \rho_i \ln \rho_i = 0 + 1 \times \ln 1 = 0 \tag{0.36}$$

[1]

References

[1] P W Anderson. A poor man's derivation of scaling laws for the kondo problem. *Journal of Physics C: Solid State Physics*, 3(12):2436–2441, dec 1970.