

Quantum Geometry of Correlated Many-Body State

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SRH, RS, AC, PRB 98 (23), 235134 (2018)
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What is an insulator?

Is an insulator a property of low lying excited states or just the ground state property?

Conventional way: the gap between the ground state and the first excited state. Ex: Band Insulator

Mott insulator, Anderson Insulator, or any other kind of insulator(except many body localisation) can be characterized by one definition?

Walter Kohn's view on the insulating state

- The insulating behaviour is a property of the ground state.
- Electrons organise themselves in the ground state as to satisfy a many electrons localisation.
- The insulating state emerges whenever the ground state of the extended system breaks up into sum of function

$$\psi_M (\Psi(r_1, r_2, \dots, r_n) = \sum_M \phi_M(r_1, r_2, \dots, r_n)$$
 which are localized in disconnected region of \mathcal{R}_M of the high dimensional configuration space. Hence electronic localization in an insulator occurs in the configuration space not in the position space
- Kohn argued that such disconnectedness is in fact a signature of the insulating wave function.

Resta prescription for Many electrons localization

- Resta and Sorrela proposed how to measure the electronic localization length to address the shape of the ground state wavefunction.
- They define the localization tensor $\langle r_\alpha r_\beta \rangle_c$. It has dimension of square of length; it is an intensive quantity that characterizes the ground state.
- It is related with Quantum geometric tensor $\eta_{\alpha\beta}$.

Non-interacting fermions

- Consider N_B tight binding model.

$$H = \sum_{i\alpha, j\beta} t_{ij}^{\alpha\beta} c_{i\alpha}^\dagger c_{j\beta} + h.c$$

- In momentum space \mathbf{k} (where \mathbf{k} takes values in BZ) H is:

$$H = \sum_{\mathbf{k}\alpha\beta} h(\mathbf{k})_{\alpha\beta} c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k}\beta}$$

The single particle Hamiltonian $h(\mathbf{k})$ in the quasi momentum space \mathbf{k} is $N_B \times N_B$ matrix.

- Its spectrum is denoted by, $h(\mathbf{k})u^n(\mathbf{k}) = \epsilon_n(\mathbf{k})\mathbf{u}^n(\mathbf{k})$
- The single-particle states in the n^{th} band are denoted by $\rho^n(\mathbf{k}) = \mathbf{u}^n(\mathbf{k})(\mathbf{u}^n(\mathbf{k})^\dagger)$
- Basically, the single particle states, $u^n(\mathbf{k})$ define mapping from the BZ to the projective hilbert space, $\mathbf{k} \rightarrow \rho^n(\mathbf{k})$. The projective hilbert space is the space of physical states.

Space of the physical states

- Quantum theory represents the physical states by rays in a Hilbert space.
- A ray in Hilbert space is the following. Consider a vector $|u^n(\mathbf{k})\rangle$. Take it to be normalized $\langle u^n(\mathbf{k})|u^n(\mathbf{k})\rangle = 1$.
- $|u^n(\mathbf{k})\rangle$ and $e^{i\phi(\mathbf{k})}|u^n(\mathbf{k})\rangle$ represents the same states. So the phase is not detectable. Each state has a direction. These what we call rays.
- Correspondence between normalized vectors in a Hilbert space and the physical states is many to one.

Non-interacting fermions: Bargmann invariant

- Each band of states, we associate a n th Bargmann invariant with every ordered sequence of n point in the BZ, $\mathbf{k} = (\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_n)$.
 $B^n(\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_n) = \text{Tr}(\rho^n(\mathbf{k}_1)\rho^n(\mathbf{k}_2)\rho^n(\mathbf{k}_3) \cdots \rho^n(\mathbf{k}_n))$
- The quantum distances and geometric phases in the BZ come from this map.
- Quantum distance:

$$d^2(\mathbf{k}_1, \mathbf{k}_2) = 1 - B^{(2)}(\mathbf{k}_1, \mathbf{k}_2)$$

- Geometric phase:

$$\Omega(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) = \frac{B^{(3)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3)}{|B^{(3)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3)|}$$

Quantum geometry of Interacting Fermions

- Just we have seen the single particle state is parametrized by quasi momentum \mathbf{k} .
- But in the case of many body states there is no such parametrization. Let us consider a many body state $|\psi\rangle$:

$$|\psi\rangle = \sum_{\mathbf{k}} c_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \dots, \mathbf{k}_n} |\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_n, \dots, \mathbf{k}_n\rangle$$

- We can see there is no parametrization as $|\psi(\mathbf{k})\rangle$ for many body state $|\psi\rangle$.
- Then there is a natural question to ask how to generalize a concept of quantum distance in a physical parameter space such as BZ wave space.

Generalization of concept of distance on a physical parameter space for MBS

- Let us first investigate for the mean field state. The mean field state for a multiband system is written as:

$$|n\rangle = \prod_{\mathbf{k}, \alpha} (u_{\alpha}^n(\mathbf{k}) c_{\mathbf{k}, \alpha}^{\dagger}) |0\rangle$$

- The density matrix at \mathbf{k}_1 and \mathbf{k}_2 are $\rho^n(\mathbf{k}_1) = \mathbf{u}^n(\mathbf{k}_1)(\mathbf{u}^n(\mathbf{k}_1))^{\dagger}$ and $\rho^n(\mathbf{k}_2) = \mathbf{u}^n(\mathbf{k}_2)(\mathbf{u}^n(\mathbf{k}_2))^{\dagger}$
- The second Bargmann invariant:

$$B^{(2)}(\mathbf{k}_1, \mathbf{k}_2) = \text{Tr}(\rho^n(\mathbf{k}_1)\rho^n(\mathbf{k}_2))$$

Mean-field states

$$\begin{aligned}
 B^{(2)}(\mathbf{k}_1, \mathbf{k}_2) &= (u^{n\dagger}(\mathbf{k}_1)u^n(\mathbf{k}_2)(u^{n\dagger}(\mathbf{k}_2)u^n(\mathbf{k}_1))) \\
 &= - \langle 0 | (u^{n\dagger}(\mathbf{k}_1)c_{\mathbf{k}_1})(u^{n\dagger}(\mathbf{k}_2)c_{\mathbf{k}_2})(u^{n\dagger}(\mathbf{k}_2)c_{\mathbf{k}_2}^\dagger)(u^{n\dagger}(\mathbf{k}_1)c_{\mathbf{k}_1}^\dagger) | 0 \rangle \\
 &= - \langle \mathbf{k}_1, \mathbf{k}_2 | (u^{n\dagger}(\mathbf{k}_2)c_{\mathbf{k}_2}^\dagger)(u^{n\dagger}(\mathbf{k}_1)c_{\mathbf{k}_1}^\dagger) | 0 \rangle \\
 &= \langle \mathbf{k}_1, \mathbf{k}_2 | E(\mathbf{k}_1, \mathbf{k}_2)c_{\mathbf{k}_1}^\dagger c_{\mathbf{k}_2}^\dagger E(\mathbf{k}_1, \mathbf{k}_2) | 0 \rangle
 \end{aligned}$$

$E(\mathbf{k}_1, \mathbf{k}_2)$ is a unitary operator, which we may call a certain type of exchange operator, such that

$$\begin{aligned}
 E(\mathbf{k}_1, \mathbf{k}_2)|0 \rangle &= |0 \rangle \\
 E(\mathbf{k}_1, \mathbf{k}_2)|0 \rangle &= |\mathbf{k}_1, \mathbf{k}_2 \rangle \\
 E(\mathbf{k}_1, \mathbf{k}_2)c_{\mathbf{k}_1}^\dagger c_{\mathbf{k}_2}^\dagger E(\mathbf{k}_1, \mathbf{k}_2) &= -c_{\mathbf{k}_2}^\dagger c_{\mathbf{k}_1}^\dagger
 \end{aligned}$$

Exchange operator

- $B^{(2)}(\mathbf{k}_1, \mathbf{k}_2) = \langle n | E(\mathbf{k}_1, \mathbf{k}_2) | n \rangle$
- The Bargmann invariant $B^{(2)}$ can be written as expectation value of E over many body state $|n\rangle$.
- $E(\mathbf{k}_1, \mathbf{k}_2) = e^{\frac{\pi}{2} \sum_{\alpha} (c_{\mathbf{k}_1\alpha}^{\dagger} c_{\mathbf{k}_2\alpha} - h.c.)}$

Distance and Geometric phase

The second Bargmann invariant has been used to define a distance between two states $|\psi_1\rangle$ and $|\psi_2\rangle$

$$d(\mathbf{k}_1, \mathbf{k}_2) = \sqrt{1 - B^2(\mathbf{k}_1, \mathbf{k}_2)^{\frac{\lambda}{2}}}$$

- λ is a real number ≥ 1
- maximum distance is 1 when states are orthogonal to each other.
- minimum distance is 0.
- satisfies the triangle inequality
- The phase of Bargmann invariant as a geometric phase is related with 3-vertex Bargmann invariant.

Quantum distance for strongly interacting fermions

- How to define the quantum distance for the correlated systems?
- We define induced distance between two points on the BZ as distance between $|\Psi\rangle$ and $E(k_1, k_2)|\Psi\rangle$

$$d^2(k_1, k_2) = 1 - |\langle \Psi | E(k_1, k_2) | \Psi \rangle|^2$$

where

$$E(k_1, k_2) = e^{\frac{\pi}{2}(c_{k_1}^\dagger c_{k_2} - h.c.)}$$

$$|\Psi\rangle = \sum_{\{k\}} C_{k_1, k_2, \dots, k_L} |k_1 \otimes k_2 \otimes \dots \otimes k_L\rangle$$

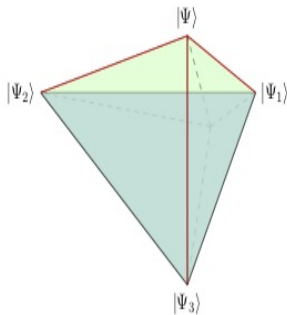
Quantum distance

- $d(k, k) = 0$, $d(k_1, k_2) = d(k_2, k_1)$
- Triangle inequality $d(k_1, k_2) + d(k_2, k_3) \geq d(k_3, k_1)$ is also satisfied.
Can be proven by Ptolemy inequality.
- $|1 \rangle = E(k_2, k_3)|GS \rangle$, $|2 \rangle = E(K_3, k_1)|GS \rangle$,
 $|3 \rangle = E(k_1, K_2)|GS \rangle$
- It can be shown that $\langle 1|2 \rangle = \langle 2|3 \rangle = \langle 3|1 \rangle$. This condition helps to prove triangle inequality.

Ptolemy inequality

Four normalized Hilbert space vectors $|\Psi\rangle$, $|1\rangle$, $|2\rangle$, and $|3\rangle$ can be constructed. Six distances d_{ij} between any four distinct points $i, j = 1, 2, 3, 4$ satisfy the following Ptolemy inequality

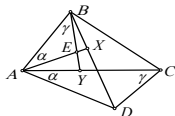
$$d_{ij}d_{kl} + d_{ik}d_{jl} \geq d_{il}d_{jk}$$



Theorem (Ptolemy's Inequality) Let $ABCD$ be a quadrilateral. We have

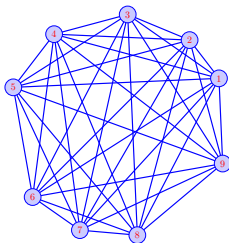
$$AB \times CD + DA \times BC \geq AC \times BD$$

with equality if and only if $ABCD$ is a cyclic quadrilateral.



Ptolemaic distance space

- All these distances induced on the pair of physical parameter space is a metric space. It is also called Ptolemaic metric or we can call it distance space.
- We have distance space. The question is what to do with it. What information we can extract for the physical system?
- How to characterize distance space mathematically?
- we can view this distance space as a network or a graph:



Geometric Phase

- Our exchange operator generated states
 $|GS\rangle = |\Psi_1\rangle, |\Psi_2\rangle = E(12)|GS\rangle, |\Psi_3\rangle = E(13)|GS\rangle, \dots$
- The third order Bargmann Invariant:
 $B^3(|\Psi_1\rangle, |\Psi_2\rangle, |\Psi_3\rangle) = \text{Tr}(\rho(\Psi_1)\rho(\Psi_2)\rho(\Psi_3))$

- This satisfies additive properties of phases.
- Total geometric phase can be computed.
- The question is how to express the third order Bargmann invariant as $B^{(3)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3)$?
- Can it be written as expectation value of some operator $C(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3)$ where C is:

$$C(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) = E(\mathbf{k}_1, \mathbf{k}_2)E(\mathbf{k}_2, \mathbf{k}_3)$$

- This form works for mean-field state but not the correlated states.

Application: Quantum distance in the t-V modle

- The hamiltonian is

$$H = \sum_i^L (-t(c_i^\dagger c_{i+1} + h.c.) + V n_i n_j)$$

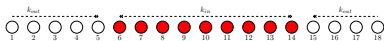
- for $V=0$

$$|FS\rangle = \prod_{k_n \leq k_f} C_{k_n}^\dagger |0\rangle$$

- $c_{k_n} = \sum_i c_i e^{-ik_n i}$ and $k_n = \frac{2\pi n}{L}$



Distance Matrix at $V = 0, \infty$



At $V = 0$:

$$D = \left[\begin{array}{cc|cc} & & k_{in} & k_{out} \\ \hline k_{in} & & 0 & I \\ k_{out} & & I & 0 \end{array} \right]$$

Distance Matrix at $V = \infty$ (CDW state):

$$D_{ij} = \left[\begin{array}{cc} 0 & i = j \\ 1 & i = j + \frac{L}{2} \\ \sqrt{\frac{3}{4}} & i \neq j, i \neq j + \frac{L}{2} \end{array} \right]$$

At an arbitrary V :

$$D = \left[\begin{array}{cc} \Delta & \Delta_e \\ \Delta_e & \Delta \end{array} \right]$$

Distance Matrix

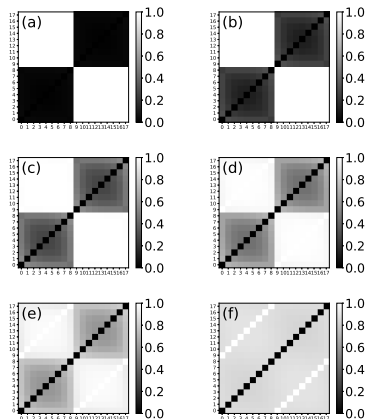


Figure: (a)-(f) Distance matrices obtained from numerical computation for interaction strengths $V = 0.1$ (a), $V = 1$ (b), $V = 2$ (c), $V = 3$ (d), $V = 4$ (e) and $V = 12$ (f).

Distance Matrix

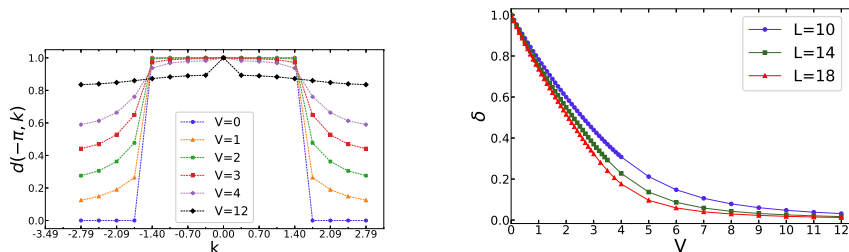
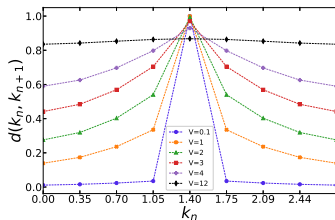


Figure: Distance $d(-\pi, k)$ between $k = -\pi$ and the other k modes in the Brillouin zone (BZ) for different values of the interaction strength V .

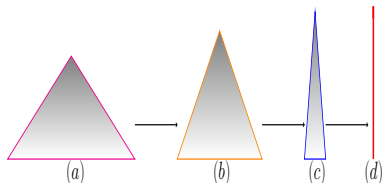
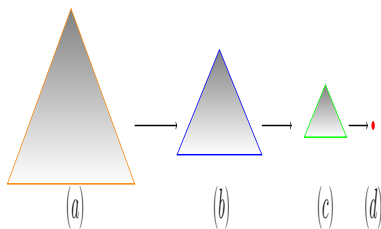
$\delta = d(-\pi, -\pi/2) - d(-\pi, -\pi/2 - 2\pi/L)$, gives a measure of the discontinuity across the Fermi points. It is studied as a function of interaction strength V for different system sizes.

Properties of NN distances



- $V=0$: all zero except fermi point (delta function singularity at k_f)
- intermediate V : this singularity remains but smoothen out.
- $V = \infty$: all NN distances are equal.

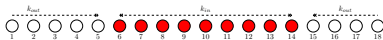
Behaviour of triangles



Particle triangles:

Particle-Hole triangles:

Understanding Distances



Define

a radius R in terms sum of NN dist :

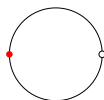
$$2\pi R = \sum_i d(k_i, k_{i+1})$$

NN distance represented by an angle:

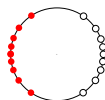
$$\theta_{i,i+1} = \frac{d(k_i, k_{i+1})}{R}$$

Each quasi momentum by an angle:

$$\theta_k = \sum_j^k \theta_{j,j+1}$$



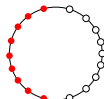
$V=0$



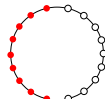
$V=1$



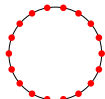
$V=2$



$V=3$

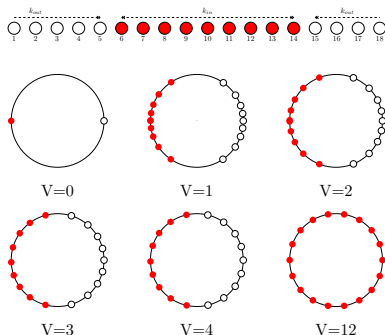


$V=4$



$V=12$

Unit Circle representation



- $V = 0$ all the points collapse into $\theta = 0, \pi$.
- Small V : they spread out but points in the Fermi sea and those outside it are well separated
- In the crossover regions ($2 \leq V \leq 3$): the separation starts closing.
- In the insulating state: the separation is indistinguishable.
- $V = \infty$: they are equally spaced.

Summary

- We presented an approach how to construct distance space for the many body state.
- We have studied properties of distances and tried to extract from it possible cross over transition.
- The Quantum distance probes the shape of the ground state wave function
- Our expression of the Quantum distance is very general and can be applied in one band Hubbard model. Other approaches fail to study geometry for such cases.
- We can apply in spin systems/bose system
- We are unable to parametrize the third order Bargmann invariant in terms of BZ vectors.