Intrinsic and extrinsic geometries of many body state

S. R. Hassan

The Institute of Mathematical Sciences,
CIT Campus, Tharamani, Chennai

ICTS Meeting, Novel Phases of Quantum Matter , Bangalore, 31st Decemeber, 2019

In Collaboration with: Ankita Chakrabarti (AC), R. Shankar (RS)

SRH, RS, AC, PRB 98 (23), 235134 (2018)
AC, SRH, RS, PRB,99 (8), 085138 (2019)
SRH, AC, RS, arxive:1905.13535

Outline

- Recap of 1d t-V model.
- Computing distances for t-V model.
- Analysing properties of distances by **Distance Geometry**.
- Computing statistical metric or distance, the **Wasserstein-Kantrovich-Rubinstein** metric.
- Barycenter
- OIllivier-Ricci Curvature.
- Conclusion

Recap of Id t-V model

- The hamiltonian is

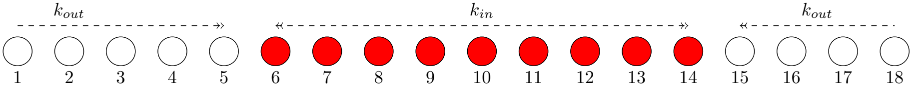
$$H = \sum_{i}^{L} (-t(c_i^\dagger c_{i+1} + h.c) + V n_i n_j)$$

Recap of phases of Id t-V model:

- Fermi Liquid at V=0
- Luttinger liquid at V between 0^+ to 2
- Luttinger liquid to CDW transition at $V = V_c = 2$
- CDW for $V > 2$

Parameter Space (BZ)

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



- $\mathbf{k_{out}}$: represents unoccupied states.
- $\mathbf{k_{in}}$: represents filled states.
- for V=0

$$|GS>= \prod_{k_n \leq k_f} C^{\dagger}_{k_n} |0>$$

Quantum distances for interacting fermions

- Many-body state:

$$|\Psi>=\sum_{\{k\}} C_{k_1,k_2,......k_L}|k_1k_2.....k_L>$$

- Distance between two points k_1 and k_2 on the BZ is computed as :

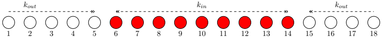
$$d^2(k_1,k_2)=1-|<\Psi|E(k_1,k_2)|\Psi>|^2$$

where

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

- We can arrange these distances in the form of matrix.

Distance Matrix as a function of V



At $V = 0$:

$$D = \begin{bmatrix} & k_{in} & k_{out} \\ \hline k_{in} & 0 & I \\ k_{out} & I & 0 \end{bmatrix}$$

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

$$D_{ij} = \begin{bmatrix} 0 & i = j \\ 1 & i = j + \frac{L}{2} \\ \sqrt{\frac{3}{4}} & i \neq j, i \neq j + \frac{L}{2} \end{bmatrix}$$

At an arbitary V:

$$D = \begin{bmatrix} \Delta & \Delta_e \\ \Delta_e & \Delta \end{bmatrix}$$

What is Distnace Geomtery?

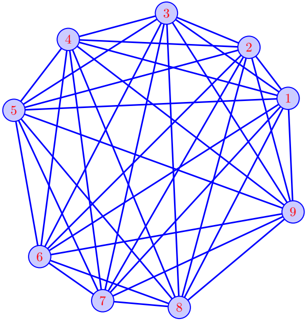
Distance Geometry (DG) is the study of geometry with the basic entity being distance. It all began with the Greeks, specifically Heron, or Hero, of Alexandria sometime between 150BC and 250AD, who showed how to compute the area of a triangle given its side lengths .

We human took almost two thousand years to revisit Hero's Forumula, finally Arthur Cayley's in 1841 asked the relationships between the distances of five points in space. The gist of what he showed is that a tetrahedron can only exist in a plane if it is flat (in fact, he discussed the situation in one more dimension). This yields algebraic relations on the side lengths of the tetrahedron.
Karl Menger and Arthur Cayley started this field.

Geometry: Metric Space (Distance Space)

- We view geometric object as a discrete object.
- This object is defined by set of points and the distances between them.
- We denote all points by set V and all distances by d. Together we represent as $X = (V, d)$
- X is called Metric space or we may call space of distances in a loose sense.

- We may view this geometric objects as a graph or network:



Ptolemaic distance space

- In our case, it is a Ptolemaic metric.
- **The question is what to do with it?**
- **What information one can extract for the physical system?**
- **How to characterize space of distances mathematically?**

Distance Space: Local view

- We can characterise metric by studying distances and triangles.
- We can define scalar or edge dependent curvatures using distances.
- There are many definition of curvature on a distance space: Menger curvature, Haantjes curvature, Forman Ricci curvature, and Ollivier-Ricci curvature. Many More.

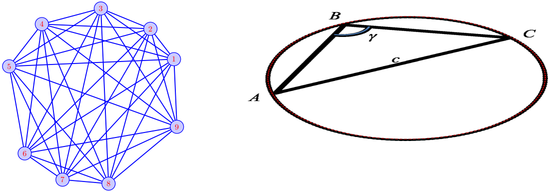


Figure: Menger Curvature at B, $C(B) = \frac{4A}{d(AB)d(BC)d(AC)}$

Distance Space: Global structure

- How does a distance space look in Euclidean space ?
- How do we determine the shape of this distance space using only distances? Embedding.
- This can be answered using Distance Geometry. What is distance geometry?
- We can arrange the distances as a matrix D.

$$\begin{bmatrix} 0 & d_{12} & d_{13} & ..... & d_{iN} \\ d_{21} & 0 & d_{23} & ...... & d_{2N} \\ ... & ... & .... & .... & ... \\ ... & ... & .... & .... & ... \\ ... & ... & .... & .... & ... \\ d_{N1} & d_{N2} & d_{N3} & ..... & d_{NN} \end{bmatrix}$$

Distance Geometry:Embedding

- We consider Euclidean Space R^n. Each nodes we represent by coordinate $x_i, \cdot\cdot x_n$. We ask the following equation:

$$|x_i - x_j|^2 = d_{ij}$$

- Gramian Matrix $G_{ij} = x_i.x_j$

$$G = X^T X$$

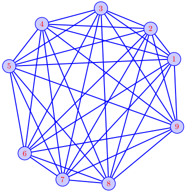
- We assume x_i are mean centered $(\sum_i x_i = 0)$
- Matrix G can be expressed in terms of D as

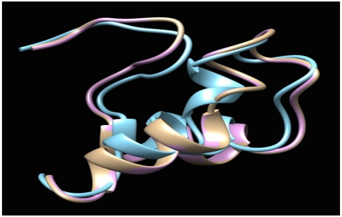
$$G = -\frac{1}{2} J D^2 J, J = (I - \frac{ee^T}{n}), e^T = (1, 1, 1, 1 \cdot 1)$$

Embedding

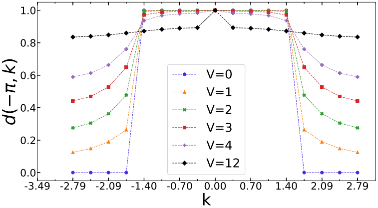
- If D can be embedded in the Euclidean space then G must be positive semi definte. Its all eigen values must be positive.
- The rank of G is a dimensionality of the embedding space.
- In most of the cases embedding dimension is very large, so we may emebed approximatley.
- Non-interacting or Mean field state can be alwayse mbedded in finite dimesnion, but strongly correlated system is embedded in very high dimension.
- Near the phase transition embedding dimension may change.

Distance Geometry





Distance Matrix



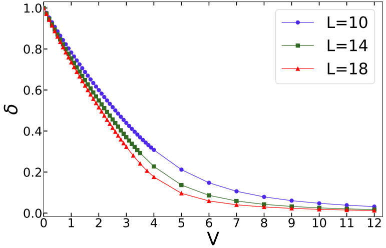


Figure: Distance $d(-\pi, k)$ between $k = -\pi$ and the other k modes in the Brillouin zone (BZ) for different values of the interaction strength V.

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

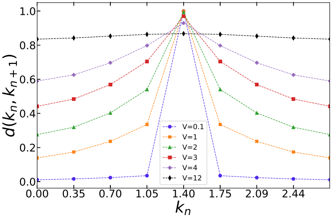
Quantum metric g(k)

- The Quantum metric g(k) is defined as:

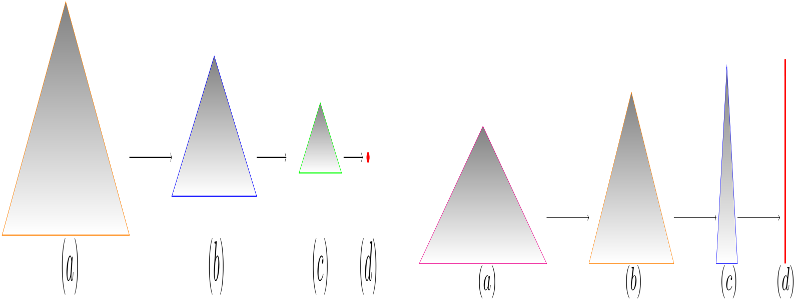
$$lim_{\Delta k \rightarrow 0} d^2(k, k+\Delta k) = g(k)\Delta^2 k$$

- In this model the distance between two quasi-momentum does not decrease monotonically with the separation.
- The $V = \infty$ all distances are the same.
- At even small V there is an optimal value of distance irrespective of the system size. The metric g(k) is not well defined in this model.

Nearest Neighbour distance



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



Particle triangles: It starts shrinking and shrink to points at $V = 0$:
Particle-Hole triangles: It changes shape at $V \sim 2$ and become isosceles traingle, they then shrink to segment at $V = 0$

Emebedding D

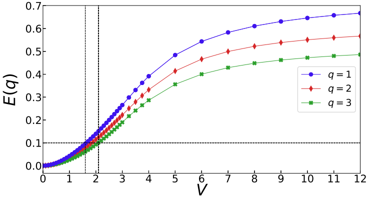


Figure: Truncation error for $E(q) = 1.0 - \sqrt{\frac{\sum_{i=0}^{q} \lambda_i}{\sum_i \lambda_i}}$ keeping first few (1-3) eigenvalues for embedding D.The truncation error for approximate embedding is less than 12% in case of embedding in one dimension $E(q = 1)$ up to $V \approx 1.5$ and for embedding in three dimension $E(q = 3)$ up to $V \approx 2$

Statistical Distance from Quantum Distances

The statistical distance between any two nodes is defined with respect to Π_{ij} as

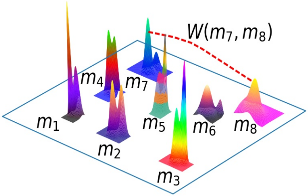
$$W(i,j) = \sum_{l,m} d(l,m)\Pi_{i,j}(l,m)$$

This distance is known as **Wasserstein-Kantrovich-Rubinstein** distance or only **Wasserstien** among Mathematicians.

Distance distribution on Metric Space (Distance Space)

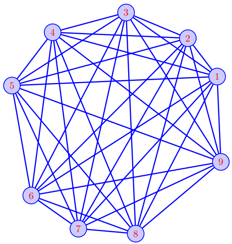
We define the distance disribution at point i in the distance sapce M as a random walk on M:

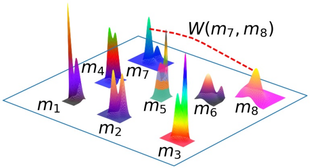
$$m_i(j) = \frac{d_{ij}}{\sum_j d_{ij}}$$



Probability distribution space

Distance space to
Probability space of Distance distributions:





Kantorovich Formulation

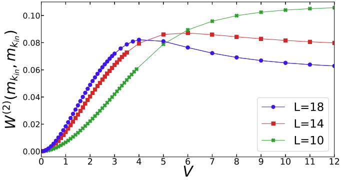
$$W(m_i, m_j) = Inf_{\{\pi \in \Pi\}} \sum_{i,j} d(i,j)\pi(i,j)$$

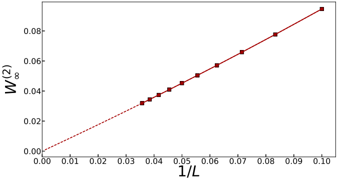
$$\sum_j \pi(i,j) = m_i$$

$$\sum_i \pi(i,j) = m_j$$

- $W(m_i, m_j)$ is distance between distrbutions m_i and m_j.
- $W(m_i, m_j)$ is also known as Earth's Mover Distance (in computer science) and Kantorovich-Wasserstein distance (or metric) among mathematicians. However, Wasserstein has not invented this distance. But it is commonly known wasserstein distance. Strange world!

Fields Medalist, Cedric Villani's book: Optimal Transport, old and new, Springer, 2003



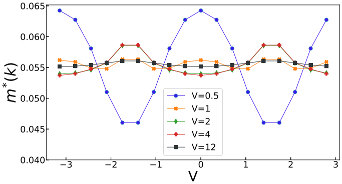


- We can expect W to indicate the critical interaction strength for the LL to CDW transition, by occurance of a peak in the Thermodynamic limit.
- We found W_∞ vanishes in the thermodynamic limit. It vanishes as $1/L$.

Barycenter

- In Euclidean case, for a collection of points $(x_1 ... x_p)$, the barycenter x^* is obatained by minimsing the function $\sum_i^p \lambda_i |x - x_i|^2$, $\sum_i \lambda_i = 1$
- In the present case, the barycenter $m^*(k)$ is defined as a single function on the BZ as:

$$J(m^*) = inf_m \frac{1}{L} \sum_i^L W^2(m_i, m)$$

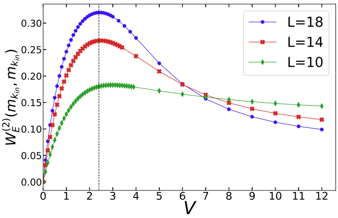


Quadratic Cost

$$W(m_i, m_j) = Inf_{\{\pi \in \Pi\}} \sum_{i,j} |i-j|^2 \pi(i,j)$$

$$\sum_j \pi(i,j) = m_i$$

$$\sum_i \pi(i,j) = m_j$$



Ollivier-Ricci curvature on a distance space

We compute distance between two distributions at i and j as:

$$W(m_i, m_j) = inf_\pi \sum_{l,m} d_{lm} \pi_{ij}(l,m)$$

$$\sum_l \pi_{ij}(l,m) = m_j(m), \sum_j \pi_{ij}(l,m) = m_i(l)$$

Ricci-curvature $K(i,j)$ is defines as:

$$K(i,j) = 1.0 - \frac{W(i,j)}{d_{ij}}$$

Y. Ollivier, C. R. Acad. Sci. Paris, Ser. I 345 (2007).
(Comptes rendus de l'Academie des Sciences)

Ricci-curvature for the nearest neighbour edges

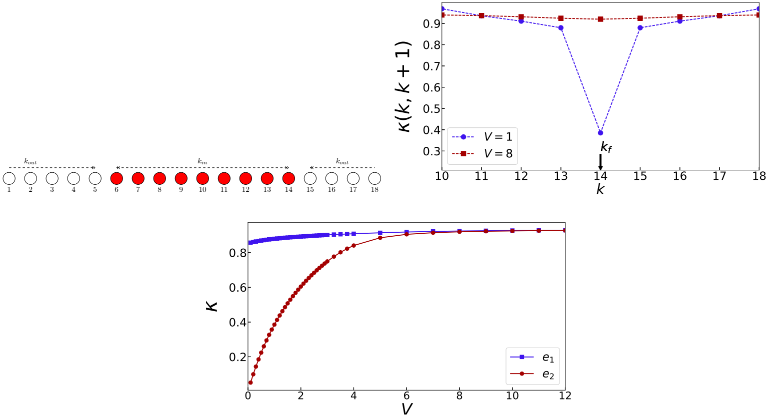


Figure: Curvatures for the nearest neighbour edges $(k, k+1)$ over half the BZ for different interaction strengths. The metallic regime is characterised by a discontinuity at the Fermi point k_f.
Curvatures for both type of edges e_1 and e_2 as function of interaction strength V.

Scalar curvature

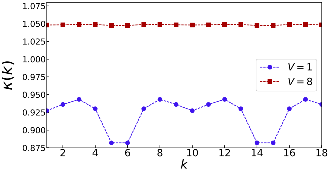
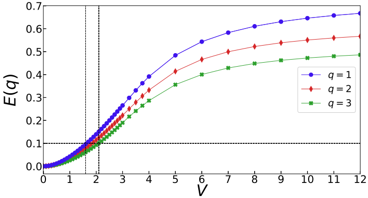


Figure: Scalar Curvature as a function of the quasi-momenta modes representing vertices of the graph. In insulating regime the scalar curvature is uniform over all the vertices.

Emebedding D and W



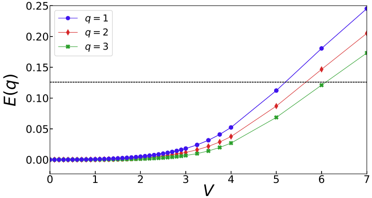


Figure: Truncation error for keeping first few (1-3) eigenvalues for embedding D. The truncation error for approximate embedding is less that 12% in case of embedding in one dimension $E(q=1)$ up to $V \approx 1.5$ and for embedding in three dimension $E(q=3)$ up to $V \approx 2$.
Truncation error for keeping first few $(1-3)$ eigenvalues of G as a function of the interaction strength, for approximate embedding of W.

Conclusion

- We have studied properties of distances and tried to extract from it possible cross over transition.
- We also showed using quantum distance and the statistical distance we can probe the shape of the ground state wave function.
- Our expresssion of the Quantum distance is very general. *can be applied even in one band Hubbard model, which is not possible to study geomtery by any other approach such as the Greens function method.*
- *This can be applied to spin system. Work is in progress for MG Model.*
- *Topology can be studied by computing betti numbers of graph of a state or using concept of* **magnitude function** *of metric space recently developed in enriched category theory. Work in progress.*

Thank you very much.