An approach to the quantum geometry of correlated states

R. Shankar
The Institute of Mathematical Sciences, Chennai

Novel Phases of Quantum Matter
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Collaborators

- S. R. Hassan
- Ankita Chakraborty

Outline

Motivation

Quantum geometry

Mean field states

Correlated states

Motivation

Why study the quantum geometry of correlated many-particle states ?

- "Because its there".
- It underlies the topological invariants.
- It has been useful in understanding insulating states

QHE: The Berry curvature

- The Hall conductivity identified with topological invariant, the Chern number.
- For mean field states, the Chern number could be written as an integral over the Brillioun zone of a geometric quantity, the Berry curvature, constructed from the single particle wavefunctions.
- The Berry curvature identified as the “anomalous velocty”, the component of the velocity perpendicular to the electric field.

Insulators

PHYSICAL REVIEW VOLUME 133, NUMBER 1A 6 JANUARY 1964

Theory of the Insulating State*

WALTER KOHN
University of California, San Diego, La Jolla, California
(Received 30 August 1963)

In this paper a new and more comprehensive characterization of the insulating state of matter is developed. This characterization includes the conventional insulators with energy gap as well as systems discussed by

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The insulating state of matter: a geometrical theory

R. Resta[1,2,a]

[1] Dipartimento di Fisica, Università di Trieste, Strada Costiera 11, 34151 Trieste, Italy
[2] DEMOCRITOS National Simulation Center, Istituto Officina dei Materiali (CNR), Trieste, Italy

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Abstract. In 1964 Kohn published the milestone paper "Theory of the insulating state", according to which insulators and metals differ in their *ground state*. Even before the system is excited by any probe, a different organization of the electrons is present in the ground state and this is the key feature discriminating between insulators and metals. However, the theory of the insulating state remained somewhat incomplete

Insulators: The quantum metric

- Kohn's idea the "Insulators can be distinguished by the organisation of the electrons in the ground state" interpreted as "Insulators can be distinguished by the quantum geometry of the ground state" (Resta, Sorrella,...).
- The geometric object identified was the "localization tensor" which is finite in the insulating phase and diverges in the metallic phase.
- For mean field states, the localization tensor can be written as an integral over the Brillioun zone, of the quantum metric constructed from the single particle wavefunctions.

Our Objectives

- Topological invariants are theoretically well defined for abritrary many-particle states, in terms of response to twisted boundary conditions.
- The Berry curvature and quantum metric have been defined in terms of the interacting Green's functions. We do not find the definition "satisfactory".

Our aim is to:

- Provide a "satisfactory definition" of the quantum geometry of arbitrary many-partcle states. I will present our approach in this talk.
- Use the definition to study and analyse the geometry of a variety of correlated many-fermion states and try to get some feeling for what are the physically relevant quantities in different situations. Hassan will present our first attempt in the next talk.

Motivation

Quantum geometry

Mean field states

Correlated states

Quantum Kinematics

ANNALS OF PHYSICS **228**, 205–268 (1993)

Quantum Kinematic Approach to the Geometric Phase. I. General Formalism

N. MUKUNDA*

Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore 560 012, India

AND

R. SIMON

The Institute of Mathematical Sciences, C.I.T. Campus, Madras 600 113, India

Received July 22, 1992; revised April 9, 1993

Physical states

- Physical states are in one-to-one correspondence with rays in Hilbert space.
- Ray in the Hilbert space = Point in the projective Hilbert space

$$|\psi\rangle \ \sim \ \lambda|\psi\rangle, \quad \lambda \in \mathcal{C}$$

  For N level systems, CP_{N-1}. For $N = 2$, CP_1 =the Bloch sphere.
- Physical state = Pure state density matrix

$$\rho(\psi) = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle}$$

- The inner-product defines a geometry of the space or rays.

Observables

$$O = \sum_n |n\rangle O_n \langle n| \equiv \sum_n O_n \rho_n$$

Consider the “transition probability",

$$|\langle\chi|O|\psi\rangle|^2 = \sum_n O_n \mathrm{tr}\left(\rho_\chi \rho_n \rho_\psi\right)$$

Bargmann invariants:

$$\begin{aligned}
B_2(\psi_1, \psi_2) &\equiv \mathrm{tr}\rho(\psi_1)\rho(\psi_2) \\
&= |\langle\psi_1|\psi_2\rangle|^2 \\
B_3(\psi_1, \psi_2, \psi_3) &\equiv \mathrm{tr}\rho(\psi_1)\rho(\psi_2)\rho(\psi_3) \\
&= \langle\psi_1|\psi_2\rangle\langle\psi_2|\psi_3\rangle\langle\psi_3|\psi_1\rangle \\
\ldots &\equiv \ldots
\end{aligned}$$

Distance and Geometric Phase

Distance:

$$(d_{12})^2 = 1 - (\mathrm{Tr}\ (\rho_1 \rho_2))^{\frac{\alpha}{2}} = 1 - |\langle \psi_1 | \psi_2 \rangle|^{\alpha}$$

Triangle inequalities satisfied for $\alpha \geq 1$.

Geometric phase (Pancharathnam-Berry Phase):

$$e^{i\Omega_{123}} = \frac{\mathrm{Tr}\ (\rho_{12}\rho_{23}\rho_{31})}{|\mathrm{Tr}\ (\rho_{12}\rho_{23}\rho_{31})|} = \frac{\langle \psi_1 | \psi_2 \rangle \langle \psi_2 | \psi_3 \rangle \langle \psi_3 | \psi_1 \rangle}{|\langle \psi_1 | \psi_2 \rangle \langle \psi_2 | \psi_3 \rangle \langle \psi_3 | \psi_1 \rangle|}$$

Quantum metric

Consider a subspace of the ray-space parameterised by local coordinates, $\rho(\xi),\ \xi_i,\ i = 1, \ldots, N$,

$$d^2(\xi + d\xi, \xi) = \frac{\alpha}{4}\,\mathrm{tr}\left(\partial_a\rho(\xi)\partial_b\rho(\xi)\right) d\xi^a d\xi^b$$

$$g_{ab}(\xi) = \frac{\alpha}{4}\,\mathrm{tr}\left(\partial_a\rho(\xi)\partial_b\rho(\xi)\right)$$

Berry curvature

$$\Omega(\xi, \xi + d\xi_1, \xi + d\xi_2) = \mathcal{F}_{ab}(\xi)\ d\xi^a \wedge d\xi^b$$

$$\mathcal{F}_{ab}(\xi) \equiv \frac{1}{2i} \mathrm{tr}\left(\rho(\xi)\left[\partial_a \rho(\xi), \partial_b \rho(\xi)\right]\right)$$

Notation

- Single particle hamiltonian:

$$h_{\alpha\beta}(k),\ \alpha,\beta = 1,\dots,N_B,\ k \in BZ$$

- Single particle spectrum:

$$h_{\alpha\beta}(k)u^n_\beta(k) = \epsilon^n(k)u^n_\alpha(k)$$

$$\rho^n_{\alpha\beta}(k) = u^n_\alpha(k)\,(u^n(k)_\beta)*$$

- Fermion operators:

$$C_n(k) \equiv \sum_\alpha u^n_\alpha(k)C_\alpha(k)$$

- Mean field states:

$$|MF\rangle = \prod_{k_{occ}} C^\dagger_1(k)|0\rangle$$

Distances and Geometric phases in the Brillioun zone

$$d_n^2(k_1,k_2) \equiv 1 - \mathrm{tr}\rho_n(k_1)\rho_n(k_2)$$
$$e^{i\Omega(k_1,k_2,k_3)} \equiv \frac{\mathrm{tr}\rho_n(k_1)\rho_n(k_2)\rho_n(k_3)}{|\mathrm{tr}\rho_n(k_1)\rho_n(k_2)\rho_n(k_3)|}$$

Visualising the geometry:

- Each band defines a mapping from the BZ to the single particle space of rays, CP_{N_B-1}:

$$k \to \rho_n(k)$$

- So the Fermi sea of occupied states is represented by a surface in CP_{N_B-1}
- The distances and geometric phases on the embedding space, CP_{N_B-1} induce distances and phases on the embedded surface defined by the Fermi sea

Our strategy

- For mean field states, express the distances and geometric phases in terms of the expectation values of many-particle hermitian operators. i.e. operators constructed from $(C, C^\dagger)$.
- Hypothesize that these operators represent observables corresponding to distances and geometric phases.
- prove/disprove that expectation values of these operators for abritrary states satisfy the geometric requirements:
  - Triangle inequalities for the distances.
  - Additivity law for the geometric phases.

Exchange operators and mean field states

Define the hermitian "exchange operators"

$$E(k_1,k_2)C^\dagger_{k_1,\alpha}C^\dagger_{k_2\beta}E^\dagger(k_1,k_2) \equiv -C^\dagger_{k_2,\alpha}C^\dagger_{k_1\beta}$$

$$E(k_1,k_2)\left(u^n_\alpha(k_1)C^\dagger_\alpha(k_1)\right)\left(u^n_\beta(k_2)C^\dagger_\beta(k_2)\right)|0\rangle = -\left(u^n_\alpha(k_1)C^\dagger_\alpha(k_2)\right)\left(u^n_\beta(k_2)C^\dagger_\beta(k_1)\right)|0\rangle$$

$$\langle MF|E(k_1,k_2)|MF\rangle = \left|\left(u^n(k_1)\right)^\dagger u^n(k_2)\right|^2$$

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

Exchange operators and mean field states

Define the unitary "cyclic operators"

$$\mathcal{C}(k_1, k_2, k_3) C^\dagger_{k_1,\alpha} C^\dagger_{k_2\beta} C^\dagger_{k_3\gamma} \mathcal{C}^\dagger(k_1, k_2, k_3) \equiv C^\dagger_{k_2,\alpha} C^\dagger_{k_3\beta} C^\dagger_{k_1\gamma}$$

$$\mathcal{C}(k_1, k_2, k_3) = E(k_1, k_2) E(k_1, k_3)$$

$$e^{i\Omega(k_1,k_2,k_3)} = \frac{\langle MF|\mathcal{C}(k_1, k_2, k_3)|MF\rangle}{|\langle MF|\mathcal{C}(k_1, k_2, k_3)|MF\rangle|}$$

Quantum distances for correlated states

Question:
Do

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

satisfy the triangle inequalities ?

$$d(k_1, k_2) + d(k_2, k_3) \geq d(k_3, k_1)....$$

for abritrary $|\psi\rangle$?
Answer:
Yay ! They do! Proof using “Ptolemy inequalities”.

Geometric phases for correlated states

Question:
Do

$$e^{i\Omega(k_1,k_2,k_3)} \equiv \frac{\langle\psi|\mathcal{C}(k_1,k_2,k_3)|\psi\rangle}{|\langle\psi|\mathcal{C}(k_1,k_2,k_3)|\psi\rangle|}$$

Satisfy the additive law ?

$$\Omega(k_1,k_2,k_3)+\Omega(k_1,k_3,k_4)=\Omega(k_1,k_2,k_4)+\Omega(k_3,k_4,k_2)$$

Answer:
Sadly, they do not ! Many numerically generated counter examples.

The Green's function approach

- Use the Green's function of the interacting theory to define "an effective single particle hamiltonian"

$$G^{-1}_{\alpha\beta}(i\omega, k) = \left(G^{-1}_{\beta\alpha}(-i\omega, k)\right)^* \Rightarrow \left(G^{-1}(0,k)\right)^\dagger = G^{-1}(0,k)$$

$$h^{eff}(k) \equiv G^{-1}(0,k)$$

  Use the eigenfunctions to construct quantum distances and geometric phases.
- "Unsatisfactory" in our opinion because,
  - It implies that the geometry of all correlated states is the same as that of some mean field state.
  - Consequently, the quantum geometry partially filled interacting one-band models are trivial.

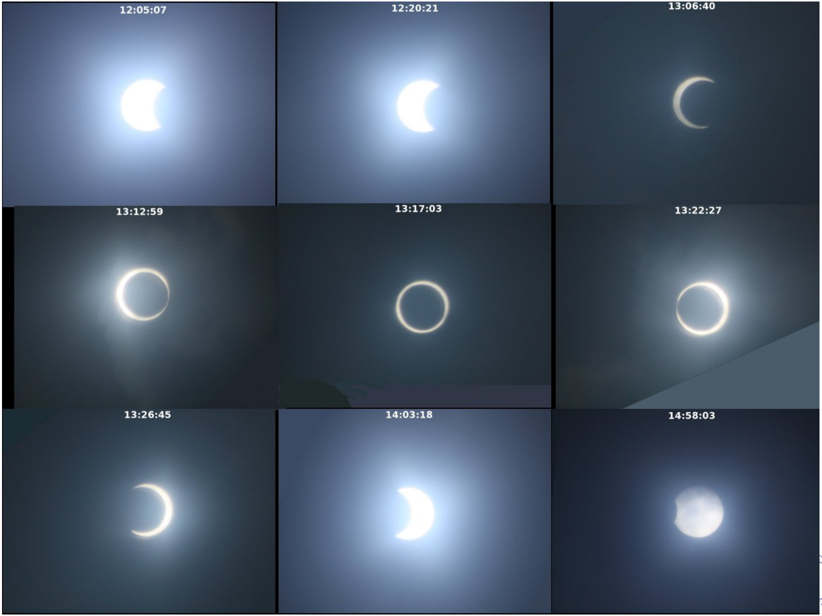
1-band models

- Our approach gives non-trivial results for partially filled, one-band models.
- In the context of the 1-dimensional $t - V$ model, we are able correlate the geometry with the known metal-insulator transition in the model (Luttinger liquid - CDW). Our analysis in the next talk.
- For translationally invariant 1-band models:

$$d^2(k_1, k_2) = \langle (n_{k_1} - n_{k_2})^2 \rangle$$

where $n_k = C_k^\dagger C_k$.
So far, we have analysed the geometry using exact diagonalisation of small systems. But other techniques can be used for larger systems.

Thank You !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