How localized is an extended quantum system?

G. Ortiz\textsuperscript{a} and A.A. Aligia\textsuperscript{b}

\textsuperscript{a}Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545
\textsuperscript{b}Comisión Nacional de Energía Atómica, Centro Atómico Bariloche and Instituto Balseiro,
\hspace{1em}8400 S.C. de Bariloche, Argentina

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We elaborate on a geometric characterization of the electromagnetic properties of matter. A fundamental complex quantity, \(z_L\), is introduced to study the localization properties of extended quantum systems. \(z_L\), which allows us to discriminate between conducting and non-conducting thermodynamic phases, has an illuminating physical (and geometric) interpretation. Its phase can be related to the expectation value of the position operator (and a Berry phase), while its modulus is associated with quantum electric polarization fluctuations (and a quantum metric). We also study the scaling behavior of \(z_L\) in the one-dimensional repulsive Hubbard model.

Introduction. The continued cross-fertilization between topology and physics has generated simple ideas that allow one to clarify many subtle issues in condensed matter and quantum field theories. Several problems in distinct areas of physics can be phrased in geometrical terms resulting in a clearer understanding of its structure and a more elegant expression of its solution. A purpose of this paper is to show that the concept of localization and the field of quantum phase transitions belong to that class of problems. Physically, what distinguishes an insulator from a metal, or superconductor, is the way the system responds to external electromagnetic probes, e.g., in an insulator a steady current cannot flow at zero temperature. That macroscopic characterization of matter translates microscopically into a study of the localization properties of their quantum states, which differ in a fundamental way. How localized is an extended quantum system? What are the topological differences between the states defining a conductor and an insulator? Can one establish a criterion for localization? Are some of the questions we want to address. The ultimate goal is to establish the foundations that will allow one to study and predict the electromagnetic properties of generic models of interacting quantum particles from general principles.

The seminal work of Kohn on the nature of the insulating state is a landmark in the quantum theory of matter\textsuperscript{1}. Kohn was apparently the first to point out that the sensitivity of the ground-state energy, \(E_0\), to changes in the boundary conditions is a measure of the electric static conductivity of the system, i.e., its Drude weight \(D_c\). In fact, in the thermodynamic limit (TL), he argued that \(D_c\) is finite for a non-disordered conductor (metal or superconductor), while it vanishes for an insulator. Physically, this last result is a consequence of the localization properties of the many-electron wave function, which is exponentially localized in the insulating case. Almost thirty years later, Scalapino and co-workers\textsuperscript{2} suggested a complementary criteria to Kohn’s. They proposed to study the limiting behavior of the paramagnetic current-current correlation function \(\Lambda_{xx}\). The appropriate long-wavelength and low-frequency limits of \(\Lambda_{xx}\) should distinguish between an ideal metal, superconductor and insulator. Moreover, they speculated that if the system supports a gap one would expect that \(D_c\) equals the superfluid weight.

Recently, Resta\textsuperscript{3} and the present authors\textsuperscript{4} have introduced a complex quantity \(z_L\) that allowed one to discriminate between conducting and non-conducting thermodynamic phases; \(|z_L| \to 0 \text{ or } 1 \text{ in the large system size limit, depending upon the system being conducting or insulating, respectively.}\) \(z_L\) has an enlightening physical interpretation: its phase is related to the macroscopic electric polarization of matter (Berry phase) while its modulus provides information on the polarization fluctuations (related to a quantum metric\textsuperscript{4}).

It is evident that these different indicators are fundamentally inter-related so, in a sense, they are conceptually complementary to each other. Then, why another criteria for localization. Apart from helping one to understand the nature of metal(superconducting)-insulator transitions better, some of the motivations are the following\textsuperscript{4}: a) physical connection to the modern theory of macroscopic polarization\textsuperscript{5}; b) appealing geometric content; c) sharper distinction between conductors and non-conductors (a two value criteria); d) numerically more convenient.

We have also identified and used geometric concepts to characterize the internal topology of stable phases of models of interacting quantum particles. Each topological quantum number (related to a Berry phase) labels a thermodynamic state, and transitions between them determine the boundaries of the quantum phase diagram\textsuperscript{6}. We have examined phase stability and the electromagnetic properties of various strongly correlated fermion systems. Here, the study of superconducting and Mott phase transitions are among the most fundamental issues. In a few cases, exact results have helped to elucidate the nature of these transitions, but in general one has to rely on numerical calculations of finite sys-
tems for which quantities like $D_c$ or any other correlation function, vary smoothly at the transition. Consequently, for example, the boundaries between charge-density-wave (CDW) or spin-density-wave (SDW) insulators and metallic phases are difficult to establish using localization indicators, while the boundaries are extremely sharp when using topological quantum numbers.

In the present manuscript we plan to review these fundamental ideas from a general perspective, illustrating main concepts in the context of Hubbard-like models.

General Framework. We will be concerned with generic quantum $N$-body systems (in a.u. $\hbar = m = e = c = 1$) in the Schrödinger picture, described by the non-relativistic Hamiltonian

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2} + V(\{x_i\}),$$

(1)

where, for simplicity (unless otherwise stated), we will assume a one-dimensional ($1d$) system with particle position and momentum labeled by $x_i$ and $p_i$, respectively. The generalization to higher dimensions is straightforward. In condensed matter physics we are interested in the behavior of extended systems, i.e., their large-$N$ limit ($N \to \infty$ and volume $L \to \infty$, such that $N/L = n_0$ is finite). The boundary conditions on the state $\Psi$ in $L$ then become an essential ingredient. It turns out that the generalized Bloch boundary conditions provides the system’s configuration space $\mathcal{M}$ (of volume $L$) with a non-simply-connected structure. Therefore, the state $\Psi$ ($\in \mathcal{L}_2(\mathcal{M}, N)$) becomes a section of a $U(1)$ fiber-bundle whose base space is $\mathcal{M}$. In this way, the topologically interesting properties of the bundle will be related to the localization properties of the physical system.

Consider a finite $N$-particle system and define the complex quantity

$$z_L = \langle \Psi_0 | \Psi_0(\alpha) \rangle, \quad |\Psi_0(\alpha)\rangle = e^{i\alpha \hat{X}} |\Psi_0\rangle,$$

(2)

where $\alpha = \frac{2\pi \ell}{L} \ (n_0 = N/L = n, \ (n, \ell) \ \text{are integers with} \ n/\ell \ \text{an irreducible fraction}), \ \hat{X} = \sum_{j=1}^{N} \hat{x}_j$, and $|\Psi_0\rangle$ is the ground state ($H |\Psi_0\rangle = E_0 |\Psi_0\rangle, \ <\Psi_0 |\Psi_0\rangle = 1$). Considered as a continuous function of $\alpha$, $z_L$ plays the role of a characteristic function generating all moments of the operator $\hat{X}$, and trivially satisfies $z_L[0] = 1, \ |z_L[\alpha]| \leq 1, \ z_L[\alpha] = z_L[-\alpha]$. Note, however, that the operator $\hat{X}$ is not a genuine operator in the Hilbert space bundle defined above, although its exponential is a legitimate one. Therefore, expectation values of arbitrary powers of $\hat{X}$ have only meaning in terms of $z_L$. Assuming analyticity in the neighborhood of $\alpha = 0$, $z_L$ can be written in terms of cumulants $C_j(\hat{X})$

$$z_L = \exp \left[ \sum_{j=1}^{\infty} \frac{(i\alpha)^j}{j!} C_j(\hat{X}) \right].$$

(3)

It turns out that

$$\alpha^{-1} \text{Im} \ln z_L[\alpha] = \langle \hat{X} \rangle + \mathcal{O}(\alpha^2),$$

$$-\alpha^{-2} \ln |z_L[\alpha]|^2 = \langle \hat{X}^2 \rangle - \langle \hat{X} \rangle^2 + \mathcal{O}(\alpha^2).$$

(4)

so that the phase of $z_L$ is related to the macroscopic electric polarization $\mathcal{P}$ while its modulus provides information on the quantum polarization fluctuations $\mathcal{E}$ [14]. Kudinov using the fluctuation-dissipation theorem showed that, in the TL, $\alpha(\langle \hat{X}^2 \rangle - \langle \hat{X} \rangle^2)$ is finite for an insulator while it diverges in a conductor [15].

The analyticity assumption of $z_L$ about $\alpha = 0$ in the TL is equivalent to saying that the system has a gap (see below). In general, this is true for finite systems, particularly in 1d. As we will argue now, (barring possible pathologies) $z_L \to 0$ when the system is a conductor. Basically, the operator $e^{i\alpha \hat{X}}$ shifts all one-particle wave vectors by $-\alpha$. Therefore, in Fermi or Luttinger liquids, the Fermi surface is shifted and $z_L$ should vanish for $L \to \infty$. It is also easy to see that $e^{i\alpha \hat{X}}$ applied to the BCS wave function for the superconducting ground state converts it into a current carrying superconducting state orthogonal to the former in the TL, which also leads to $z_L \to 0$. In contrast to the Drude weight, these results are also valid in the presence of disorder.

In the case of a system which is insulating due to the effect of disorder, with correlations playing a secondary role, one expects that the ground state is a single Slater determinant with the $N$ particles occupying the $N$ energetically more favorable localized wave functions. We calculate $z_L$ in a more general case, in which the ground state is a combination of $M$ Slater determinants

$$|\Psi_0\rangle = \sum_{j=1}^{M} c_j |\Phi_j\rangle,$$

(5)

$$\langle \{x_1\} |\Phi_j\rangle = \sum_p (-1)^p \psi_{j P_1}(x_1) \psi_{j P_2}(x_2) \ldots \psi_{j P_N}(x_N),$$

with $\sum_j |c_j|^2 = 1$, and the single-particle orbital $l$ of the $j^{th}$ Slater determinant satisfies

$$|\psi_{jl}(x)| < A e^{-|x-R_{jl}|/\lambda}.$$  

(6)

Then,

$$z_L = \sum_{ij} c_i^* c_j \sum_p (-1)^p \prod_{l=1}^{N} e^{i\alpha R_{il}} \langle \psi_{il} | e^{i\alpha(x-R_{il})} |\psi_{jl}\rangle.$$  

(7)

Because of the bound $[\psi]$ the exponential in the matrix element can be expanded in powers of $\alpha$ and only the first term survives in the TL $L \gg 2\pi \ell \lambda \ (\alpha \lambda \ll 1)$. Thus, orthonormality of the one-particle orbitals leads to

$$\lim_{L \to \infty} z_L = \sum_{j=1}^{M} |c_j|^2 e^{i\alpha \sum_j R_{jj}}.$$  

(8)
This leads to $|z_L| \rightarrow 1$ in the case of only one Slater determinant, or in the general case provided that $\alpha$ can be chosen in such a way that the exponents in Eq. (8) have the same value for all determinants. For translationally invariant systems, this is the reason for the introduction of the factor $\ell$ in the definition $\alpha = 2\pi \ell / L$.

For insulating systems in the presence of disorder and correlations, we are not able to prove that $|z_L| \rightarrow 1$ without introducing additional hypotheses.

On the other hand, under the assumption that $|\Psi_0(\beta)\rangle$ is non-degenerate in the interval $0 < \beta < \alpha = 2\pi \ell / L$, for any correlated insulator $|z_L| \rightarrow 1$ in the large system size limit. To understand this statement let’s first rewrite $z_L$ in the following manner

$$z_L = \frac{2}{N\alpha} \langle \Psi_0 | \hat{P} \Psi_0(\alpha) \rangle , \quad \hat{P} = \sum_{i=1}^{N} p_i , \quad (9)$$

an expression that is obtained after simple algebraic manipulations, using the fact that the state $|\Psi_0(\alpha)\rangle$ is an eigenstate of the $\alpha$-dependent Hamiltonian

$$\hat{H} = H - \alpha \hat{P} , \quad (10)$$

with eigenvalue $\tilde{E}_0 = E_0 - \alpha^2 N / 2 \left( \hat{H} | \Psi_0(\alpha)\rangle = \tilde{E}_0 | \Psi_0(\alpha)\rangle \right)$. Assuming that this state remains non-degenerate for $0 < \alpha < 2\pi \ell / L$, one can iterate the equation

$$|\Psi_0(\alpha)\rangle = |\Psi_0\rangle - \alpha G \left[ \mathbb{I} - |\Psi_0(\alpha)\rangle \langle \Psi_0 | \right] \hat{P} |\Psi_0(\alpha)\rangle , \quad (11)$$

with $G = (E_0 - H)^{-1}$. This is the starting point of Rayleigh-Schrödinger perturbation theory to any order in $\alpha$. For an insulating state the result is

$$|\Psi_0(\alpha)\rangle = e^{i\gamma} \left\{ |\Psi_0\rangle - \alpha \sum_{i \neq 0} \frac{\hat{P}_{0i}}{E_{0i}} |\Psi_i\rangle + \mathcal{O}(\alpha^2) \right\} , \quad (12)$$

where $|\Psi_i\rangle$ are eigenstates of $H$, $\hat{P}_{ij} = \langle \Psi_i | \hat{P} | \Psi_j \rangle$ and $E_{ij} = E_i - E_j$. Notice that since the parameter $\alpha \sim 1 / L$, the $\mathcal{O}(\alpha^2)$ does not have the usual meaning because the matrix elements themselves depend upon $L$. However, we argue that when $L \gg \xi$ ($\xi$ is a correlation length), in the insulating case, this expansion is well-behaved. Therefore, up to third order in $\alpha$ (including the normalization of $|\Psi_0(\alpha)\rangle$) to the same order)

$$z_L = e^{i\gamma} \left\{ \left( 1 - \frac{D_c}{n_0} \right) \left( 1 - \frac{3}{2} \alpha^2 \sum_{i \neq 0} \frac{|\hat{P}_{0i}|^2}{E_{0i}^2} \right) + \frac{\alpha^2}{\pi n} \sum_{i,j \neq 0} \frac{\hat{P}_{0i} \hat{P}_{ij} \hat{P}_{0j}}{E_{0i} E_{0j}} - \frac{\alpha^3}{\pi n} \sum_{i,i,j \neq 0} \frac{\hat{P}_{0i} \hat{P}_{0j} \hat{P}_{ij} \hat{P}_{0j}}{E_{0i} E_{0j} E_{0j}} + \mathcal{O}(\alpha^4) \right\} , \quad (13)$$

where the Drude weight (or charge stiffness) is defined as

$$D_c = \frac{1}{L} \frac{\partial^2 E_0}{\partial \alpha^2} = n_0 + \frac{\alpha}{\pi \ell} \sum_{i \neq 0} \frac{|\hat{P}_{0i}|^2}{E_{0i}} . \quad (14)$$

According to Kohn’s criteria $\lim_{L \rightarrow \infty} z_L = 0$ in the insulating state, thus, Eq. (13) is telling us that $\lim_{L \rightarrow \infty} |z_L| = 1$. It is useful to bear in mind that Eq. (12) is only valid if the ground state never becomes degenerate with any other state. This is an important physical assumption.

In order to understand the geometric content of the localization indicator $z_L$, we need to understand the Riemannian structure of our Hilbert space bundle. Consider a set of normalized states $\{|\Psi_0(\alpha)\rangle\}$. Let’s assume that this manifold of quantum states is generated by the action of the group of Galilean transformations, i.e.,

$$|\Psi_0(\alpha)\rangle = e^{i\alpha \hat{X}} |\Psi_0(0)\rangle , \quad \alpha \equiv \{ \alpha_{\mu} \}_{\mu=1, d} , \quad (15)$$

where $\alpha$ is a vector and $d$ represents the number of generators $\hat{X}$ (usually the dimension). What is the “distance” between two of these quantum states? To answer this question, we have to define a (gauge invariant) metric tensor in such a manifold.

The problem of establishing a Riemannian structure on an arbitrary differentiable manifold of quantum states has been addressed in the eighties. It turns out that a meaningful definition for the metric is

$$g_{\mu\nu}(\alpha) = \text{Re} \langle \partial_\mu \Psi_0(\alpha) | \partial_\nu \Psi_0(\alpha) \rangle - \gamma_\mu(\alpha) \gamma_\nu(\alpha) , \quad (16)$$

where $\gamma_\mu(\alpha) = -i \langle \Psi_0(\alpha) | \partial_\mu \Psi_0(\alpha) \rangle$ is the Berry connection and $\partial_\mu = \partial / \partial \alpha_\mu$. It can be shown that $g_{\mu\nu}$ is a symmetric and positive definite second rank tensor. Moreover, what is of interest to us is the fact that the infinitesimal distance is related to the quantum fluctuations of the generator $\hat{X}$, i.e., the polarization fluctuations

$$g_{\mu\nu}(0) = \langle \hat{X}_\mu \hat{X}_\nu \rangle - \langle \hat{X}_\mu \rangle \langle \hat{X}_\nu \rangle , \quad (17)$$

and the expectation values are evaluated over $|\Psi_0(0)\rangle \equiv |\Psi_0\rangle$. In a sense, the metric structure on the manifold is fixed by the quantum fluctuations which determine the modulus of $z_L$ in the TL. On the other hand, the antisymmetric tensor $\Omega_{\mu\nu} = \text{Im} \langle \partial_\mu \Psi_0(\alpha) | \partial_\nu \Psi_0(\alpha) \rangle$ plays the role of a curvature. $\Omega_{\mu\nu}$ is a quantity connected to the non-dissipative part of the conductance in adiabatic charge transport.

The Berry phase is an example of a general geometric concept which finds realization in several physical problems. It is the anholonomy associated with the parallel transport of a vector state in a certain parameter space.
Anholonomy is a geometric concept related to the failure of certain variables to return to their original values after others, driving them, are cyclically changed. In condensed matter, the charge Berry phase $\gamma_c$ is a measure of the macroscopic electric polarization in band or Mott insulators while the spin Berry phase $\gamma_s$ represents the difference between the electric polarization per spin up and down. $\gamma_c$ is determined by the phase of $z_L$, through the relation $\gamma_c = \alpha \langle \hat{\chi} \rangle$. In systems with inversion symmetry $\gamma_c$ and $\gamma_s$ can attain only two values: 0 or $\pi$ (modulo $(2\pi)$). Thus, if two thermodynamic phases differ in the topological vector $\vec{\gamma} = (\gamma_c, \gamma_s)$ this sharp difference allows us to unambiguously identify the transition point even in finite systems. This topological “order parameter” was recently used by us to detect metallic (superconductor), insulator and conductor-insulator transitions in 1d lattice fermion models (1).

Application to Lattice models. To illustrate the concepts developed in previous section, we will study the localization properties of the well-known 1d Hubbard model at half-filling ($n_0 = 1$) (3), whose ground state is always insulating. We concentrate on the analysis of the scaling properties of $z_L$ as a function of the on-site repulsion $U/t$. For the Drude weight, the scaling $D_c \sim \sqrt{\text{Tr} e^{-L/\xi(U)}}$ has been established by Stafford and Millis (3). Using Eq. (13), the fact that odd terms in $\alpha$ in perturbation theory vanish due to the inversion symmetry of the model ($\lim_{L \to \infty} z_L = \pm 1$), and the additional dependence on $L$ (independent of $\alpha = 2\pi \ell / L$) of the sums entering Eq. (13), one finds that for large $L$, $|z_L|$ scales as $1 - \xi / L$, where for large $U$, $\xi \sim U^{-2}$.

![Scaling behavior of $z_L$ and $D_c$. (a) For the exponential(parabolic) scaling: $\xi(4) = 3.93583(4.00134)$ and $\xi(8) = 0.842294(0.797996)$. (b) $\xi(4) = 3.74949(4.0594)$, $\xi(8) = 1.34926(1.4136)$ and $\xi(10) = 1.06704(1.1171)$.](image)

In Fig. 1a, we display $z_L$ for $4 \leq L \leq 24$, calculated with exact diagonalization ($L \leq 12$) and density matrix renormalization group (DMRG) ($L \geq 12$) for $U/t = 4$ and $U/t = 8$. For both values, a parabola in $1/L$ fits very well the results. Moreover, the values of $z_L$ extrapolated to the TL are very close to one ($c(4)=1.00997$ and $c(8)=0.997598$). We also notice that in the scaling regime an exponential of the form $|z_L| = e^{-\xi / L}$ fits the data very well ($c(4)=1.00993$ and $c(8)=0.99968$), but we do not at present have any justification for this functional form. For completeness, Fig. 1b shows $D_c$ for $L \leq 12$.

The ability of $z_L$ to detect Mott metal-insulator transitions as a function of a parameter has been demonstrated in the extended Hubbard model for infinite on-site repulsion $U/t$ at quarter-filling (3) and in the Hubbard model with correlated hopping at half-filling (3). In the latter case, due to the pseudospin $SU(2)$ symmetry, the transition is best determined by the abrupt jump in the charge Berry phase $\gamma_c$. This jump coincides with the change of sign of $z_L$ for $L \to \infty$ (for any finite system, in general $z_L \neq 0$, although $|z_L|$ can be negligible in the metallic phase (3)). In the Hubbard model with correlated hopping, to extrapolate $z_L$ to the TL, it is better to take $U - U_c(L)$ fixed rather than $U$ fixed, where $U_c(L)$ is the value of $U$ for which $z_L(U_c) = 0$.

Summary. Over thirty years ago, Kohn (1) recognized that the essential microscopic property that distinguishes the insulating state of matter is the disconnectedness of its ground-state wave function. In the present paper, we have shown that one can quantify this property using concepts borrowed from topology. In this way, we have seen that the phase of $z_L$ (that is a Berry phase) provides information on the macroscopic electric polarization of matter, while its modulus (connected to a quantum metric) measures the degree of localization in terms of the electric polarization fluctuations. $z_L$ displays a qualitatively different behavior for conductors than for insulators, thereby providing a two-value criterion to distinguish between those states of matter. Moreover, we have seen that $z_L$ can be computed in a simple and very efficient way, using standard many-body techniques. In particular, we have studied the scaling behavior of $|z_L|$ for the 1d repulsive Hubbard model in the insulating phase, and concluded that it is power law in $1/L$. We have also briefly mentioned the use of topological quantum numbers (the phase of $z_L$ being one of them) to determine quantum phase diagrams of interacting particle systems.

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