Quantum Mechanical Position Operator and Localization in Extended Systems

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We introduce a fundamental complex quantity, z_L, which allows us to discriminate between conducting and nonconducting thermodynamic phases in extended quantum systems. Its phase can be related to the expectation value of the position operator, while its modulus provides an appropriate definition of a localization length. The expressions are valid for *any* fractional particle filling. As an illustration we use z_L to characterize insulator to "superconducting" and Mott transitions in one-dimensional lattice models with infinite on-site Coulomb repulsion at quarter filling. [S0031-9007(99)08740-2]

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Macroscopically, the fundamental property that distinguishes an insulator from a conductor is that a steady current cannot flow at zero temperature. Understanding the quantum nature of the insulating state and possible phase transitions to a conducting state is a significant endeavor which started with the seminal work of Kohn [1]. Localization of the electronic wave function and the existence of a dielectric polarization density field are two related features of the insulating ground state (GS). Accordingly, one would expect that wisdom developed from the recent microscopic theory of polarization [2] could be exploited to establish a criterion for localization. Important advances have been made recently [3,4], and a criterion of localization based on a GS expectation value has been proposed [4]. However, as shown below, this criterion is valid only at integer particle filling in translationally invariant systems, and its utility to identify a metal-insulator transition has not been demonstrated.

In this Letter we introduce a complex quantity, z_L, which enables us to distinguish between conducting (metal, superconductor) and nonconducting (band, Peierls, Anderson, and Mott insulators) states of matter. Its phase corresponds to the GS expectation value of the position operator, intrinsically connected to macroscopic polarization [3], while its modulus provides an unambiguous definition of a localization length which can be described entirely in terms of the properties of the many-body GS. We show the usefulness of these ideas to characterize metal(superconducting)-insulator quantum phase transitions in strongly correlated lattice models.

To describe the intrinsic bulk properties of extended quantum systems it is almost mandatory to assume N interacting particles enclosed in a box subjected to periodic Born–von Kármán (BvK) boundary conditions (BC). On the other hand, the fact that the quantum state is defined in a nonsimply connected manifold makes the center of mass of its wave function an ill-defined concept. In recent interesting papers [3,4], the appropriate definition of the GS expectation value of the position operator $\langle\hat{X}\rangle$ [3] and the localization length λ [4] in one-dimensional (1D) systems satisfying BvK BC were discussed. The primary quantity was $z_N = \langle g|e^{i\frac{2\pi}{L}\hat{X}}|g\rangle$, where $|g\rangle$ is the GS of the system ($\langle g|g\rangle = 1$), $\hat{X} = \sum_{j=1}^{N} x_j$ is the sum of particle positions ($\hat{X}/N$ is the center of mass coordinate), and L is the number of unit cells. $\langle\hat{X}\rangle$ was defined from the phase of z_N, while λ was specified from the modulus of z_N, taking the thermodynamic limit ($N, L \to \infty$, keeping the density $n_0 = N/L$ constant).

Translational invariance and BvK (or twisted) BC are convenient, and in most cases imperative, since the Hamiltonian can be diagonalized separately in each Hilbert subspace of the many-body states which belong to the same irreducible representation of the space group. For systems which do not possess translational invariance, BvK (or twisted) BC are not always an advantage over open BC, and for the latter, the traditional definition of the expectation value of the position operator (i.e., the first moment of the modulus squared of the many-body wave function, $|g|^2$, or "dipole") is a well-defined concept. Thus, in the following we concentrate on translational invariant systems, although the localization citerion derived below is valid in general. For these systems, excluding accidental degeneracies, $|g\rangle$ belongs to a well-defined irreducible representation of the space group. If the GS is nondegenerate (as assumed in Refs. [3,4]), calling $\hat{T}$ the operator which translates one unit cell (taken as the unit of length) to the right, one has $\hat{T}|g\rangle = e^{iK}|g\rangle$, where K is the total momentum of the GS. Degeneracies of states which differ in K or any other conserved quantum number do not affect our arguments (energy level crossings are allowed whenever the states involved belong to different symmetry sectors).

In order for z_N to be different from zero, the operator $\mathcal{U}_L = e^{i\frac{2\pi}{L}\hat{X}}$, when decomposed into irreducible representations, should contain the trivial representation of the space group. *This is not the case if n_0 is not an integer*. It is straightforward to check that $\hat{T}\mathcal{U}_L\hat{T}^\dagger = e^{-i2\pi n_0}\mathcal{U}_L$. Then $\langle g|\mathcal{U}_L|g\rangle = \langle g|\hat{T}^\dagger\hat{T}\mathcal{U}_L\hat{T}^\dagger\hat{T}|g\rangle = e^{-i2\pi n_0}\langle g|\mathcal{U}_L|g\rangle$, and the matrix element should vanish unless n_0 is an integer. This restriction is too severe. For example, in 1D a Mott transition can take place for any

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filling, particularly if n_0 is given by a simple fraction [5]. For noninteger fillings, the definitions of Refs. [3,4] lead to an undefined $\langle \hat{X} \rangle$ and infinite λ *for any* system which is *incorrect*.

The correct definition for arbitrary fillings $n_0 = n/l$, where n/l is an irreducible fraction, is

$$z_L[n/l] = \langle g | e^{i\frac{2\pi}{L} l \hat{X}} | g \rangle = \langle g | \mathcal{U}_L^l | g \rangle . \quad (1)$$

Then, the GS expectation value of the position operator is defined [mod(L/l)] as

$$\langle \hat{X}[n/l] \rangle = \frac{L}{2\pi l} \, \mathrm{Im} \, \ln z_L[n/l] , \quad (2)$$

and similarly to Ref. [4] one can introduce a localization length λ. The first important point in these definitions is that the operator $\mathcal{U}_L^l$ is invariant under translations and has no definite parity under space inversion. This ensures that z_L is not zero in finite systems, except for very particular cases in which hidden quantum numbers exist, like for free electrons, in which not only the total wave vector K but also the one-particle wave vectors are conserved by the Hamiltonian, while the latter are shifted by the operator $\mathcal{U}_L^l$ [6,7]. The second important remark is that, for noninteger n_0, when a family of Hamiltonians is introduced in which the one-particle wave vectors are shifted by a parameter α [Eq. (5) of Ref. [3]], there is a crossing of levels as a function of α between states of different K's. Crossings of this type were found previously when calculating Berry's phases in systems which show the so-called anomalous flux quantization characteristic of superconductors [6,8] and are *harmless*, since the states involved have different quantum numbers and, therefore, are not mixed by the Hamiltonian. However, as a consequence of this crossing, Eq. (7) of Ref. [3], stating that $\mathcal{U}_L |g\rangle = e^{i\gamma_L} |g\rangle + \mathcal{O}(1/L)$ (where γ_L is a geometric phase), is *incorrect*, since both members have different K's for noninteger n_0. Finally, the behavior of z_L in the thermodynamic limit provides us with a universal criterion to distinguish between a conductor (metal or superconductor, as we will see below) and an insulator: z_L vanishes in the first case, while $|z_L| \to 1$ in the second.

In the general case (except for the above mentioned particular cases with hidden symmetries) one has $\mathcal{U}_L^l |g\rangle = e^{i\gamma_L} |g\rangle + \mathcal{O}(1/L)$, and the rest of the demonstration leading to Eq. (2) can be done following Ref. [3] with simple and straightforward changes. As shown elsewhere [6], the Berry's phase $\gamma_L = 2\pi l \langle \hat{X} \rangle / L$ is

$$\gamma_L = i \int_0^{2\pi l} d\Phi \left\langle g_K(\Phi) \left| \frac{\partial}{\partial \Phi} g_K(\Phi) \right. \right\rangle , \quad (3)$$

where $|g_K(\Phi)\rangle$ is the state obtained by adiabatic continuation of the GS $|g\rangle$, when a flux Φ is threaded through the ring [9] (a 1D system with BvK BC is topologically equivalent to a ring).

Using z_L to distinguish between a conducting and a nonconducting system is more stringent than the criterion introduced by Kohn [1]. Kohn's criterion, universally used in actual calculations, is based on the value of the charge stiffness D_c (i.e., sensitivity of the curvature of the total energy to phase changes in the BC): in the thermodynamic limit D_c is zero in the insulating phase, while it can attain any positive value in a conducting system. Instead, $\lim_{L\to\infty} |z_L| = 0$ for conducting systems, and $\lim_{L\to\infty} |z_L| = 1$ for noncorrelated insulators, or systems in which all particles are localized in nonoverlapping sectors [7]. To prove that this last limit can be achieved for *any* correlated insulator is rather involved, but one can prove, for a generic insulating state, that, for large L, $|z_L| \simeq 1 - D_c/n_0$, and then $\lim_{L\to\infty} |z_L| = 1$.

To illustrate the main concepts described above, we consider an extended Hubbard model (EHM) with arbitrary nearest-neighbor interaction V and infinite on-site repulsion U in 1D, at quarter filling ($n_0 = 1/2$). By a straightforward extension of the methods used in similar models [10], it can be shown that this is mapped onto a simple model of spinless interacting fermions [11], for which some analytical results can be obtained in the thermodynamic limit. We explore the possibility of quantum phase transitions using our generalizations z_L and $\langle \hat{X} \rangle$. Finally, we discuss two generalizations of this model.

The Hamiltonian which describes the charge dynamics of the model in a ring of $L = 2N$ sites with BvK BC ($c_{j+L}^\dagger = c_j^\dagger$) threaded by a flux Φ is

$$H(\Phi) = \sum_j -t(e^{i\frac{\Phi}{L}} c_{j+1}^\dagger c_j + \mathrm{H.c.}) + V n_{j+1} n_j . \quad (4)$$

The gauge transformation $\bar{c}_j^\dagger = e^{ij\Phi/L} c_j^\dagger$ transforms $H(\Phi)$ into a Hamiltonian $\bar{H}(\Phi)$ in which the phase factors disappear at the cost of introducing twisted BC $\bar{c}_{j+L}^\dagger = e^{i\Phi} \bar{c}_j^\dagger$ except for fluxes $\Phi = 2\pi \times$ integer [11].

For $V \gg t$, the GS can be obtained by perturbation theory. For $t = 0$ it is twofold degenerate between the charge-density-wave (CDW) states $|1\rangle$ and $|2\rangle$, with the particles occupying every second site: $|1\rangle = \prod_{j=0}^{N-1} \times c_{2j+1}^\dagger |0\rangle$; $|2\rangle = \prod_{j=1}^{N} c_{2j}^\dagger |0\rangle$. These states are mixed in Nth order perturbation theory by $2N!$ processes in which all particles hop either to the left or to the right in some order. For odd N [12], the effective matrix element is $-r(N)\,(t/V)^N \cos(\Phi/2)$, where $r(N)$ is a real positive number with $1 < r(N)/2 < N!$. Thus, the eigenstates are $|g_0(\Phi)\rangle = (|1\rangle + |2\rangle)/\sqrt{2}$ and $|g_\pi(\Phi)\rangle = (|1\rangle - |2\rangle)/\sqrt{2}$. The former (latter) is the GS for $\Phi = 0$ ($\Phi = 2\pi$). It is interesting to note what happens if Φ is varied adiabatically from 0 to 2π: the wave vector $K = 0$ of the GS of $H(\Phi)$ remains the same, while the wave vector $\bar{K}$ in the representation of $\bar{H}(\Phi)$ varies as $\bar{K} = K + \Phi n_0$ in general [6]. Since $\bar{H}(2\pi) = \bar{H}(0)$, after completing this cycle, $|g_0(\Phi)\rangle$ has evolved from the GS of $\bar{H}(0)$ with $\bar{K} = 0$ to its first excited state with $\bar{K} = \pi$. After another cycle $|g_0(4\pi)\rangle$ returns to the GS of $\bar{H}(0)$ except for the geometrical phase Eq. (3). It is easy to see that $\hat{X}|2\rangle = \sum_{j=1}^{N} (2j)\,|2\rangle = N(N+1)\,|2\rangle$, $\hat{X}|1\rangle = N^2 |1\rangle$. Then, $\mathcal{U}_L |g_0(\Phi)\rangle = \pm |g_\pi(\Phi)\rangle$ [the sign depends on the parity

of $(N + 1)/2]$ and $\mathcal{U}_L^2|g_0(\Phi)\rangle = |g_0(\Phi)\rangle$. This leads to $z_N = 0$ but to $z_L[1/2] = 1$.

For attractive V and $|V| \gg t$, all particles group together. For $t = 0$ the GS is any of the states $|\mathrm{PS}\rangle_j = \hat{T}^j|\mathrm{PS}\rangle$ $(0 \le j \le N - 1)$, $|\mathrm{PS}\rangle = \prod_{j=1}^{N} c_j^\dagger|0\rangle$. Then, $\mathcal{U}_L^2|\mathrm{PS}\rangle_j = (-1)^{N+1}|\mathrm{PS}\rangle_j$, and $z_L[1/2] = (-1)^{N+1}$.

For arbitrary values of V and t, the spinless model is equivalent (via a Jordan-Wigner transformation) to an XXZ model $\sum_{\langle ij\rangle\alpha} J_\alpha S_i^\alpha S_j^\alpha$ with N spins up, and $J_x = J_y = 2t$, $J_z = V$. This model was solved by the Bethe ansatz [13]. From the solution one knows that there is a Mott transition at $V = 2t$ and a transition to the phase segregated (PS) state at $V = -2t$. We have calculated the correlation exponent K_ρ of the EHM in the conducting phase $(-2t < V < 2t)$, solving the Bethe-ansatz integral equations for the energy per site $e(n_0)$ of the equivalent XXZ model [13] and using the expression $K_\rho = \pi\sqrt{D_c/(2\partial^2 e/\partial n_0^2)}$, where the Drude weight (or charge stiffness) is given by the Bethe-ansatz result $D_c = 2\pi t \sin\mu/[8\mu(\pi - \mu)]$ with $\mu = \arccos(V/2t)$ [14]. We obtain that $K_\rho > 1$ (superconducting correlations dominate at large distances) for $-2t < V < V_c$, with $V_c = -\sqrt{2}\,t$ within our accuracy (10^{-3}). It is clear that this model provides a rich zero temperature phase diagram and an interesting laboratory to study localization and transitions to superconducting (SC) states.

Unfortunately the Bethe-ansatz wave function is quite difficult to handle. Therefore, we obtained the GS $|g\rangle$ for finite systems with up to $L = 16$ sites by the Lanczos method. As usual, $|g\rangle$ was taken at the value of Φ which minimizes the GS energy $E_g(\Phi)$. In the spinless model, this corresponds to $\Phi = 0$ (BvK BC) for odd N and $\Phi = \pi$ (antiperiodic BC) for even N, and in both cases $\bar{K} = 0$ [11]. This choice reduces the dependence of the GS energy and z_L with size and also leads to a slightly more abrupt change in $|z_L|$ near the transitions. The resulting $|z_L|$ calculated with Eq. (1) is represented in Fig. 1 for various sizes, together with the corresponding numerical results for $D_c = (L/2)\partial^2 E_g(\Phi)/\partial\Phi^2$ and the Bethe-ansatz result for D_c in the thermodynamic limit. From the latter, the conductor-insulator transitions at $|V| = 2t$ are evident. However, the finite-size results always lead to a nonzero D_c and, except perhaps for the change in curvature near $V \sim -2.5t$, there are no clear indications of any transition. The situation improves if the finite-size results are extrapolated using a polynomial in $1/L$. The extrapolation agrees very well with the exact result in the conducting phase, and suggests a transition near $V = -2t$. However, from the extrapolated D_c no conclusions concerning the Mott transition at $V = 2t$ can be drawn. Only the large size dependence near $V \sim 3t$ is indicative of a charge gap.

Near $V = -2t$, as V increases, $|z_L|$ decreases abruptly from values near one, to very small values, as expected for an insulator-conductor transition. For $V \sim 2t$, the change in $|z_L|$ is rather smooth and the size dependence is small, but also the change of behavior becomes more abrupt with

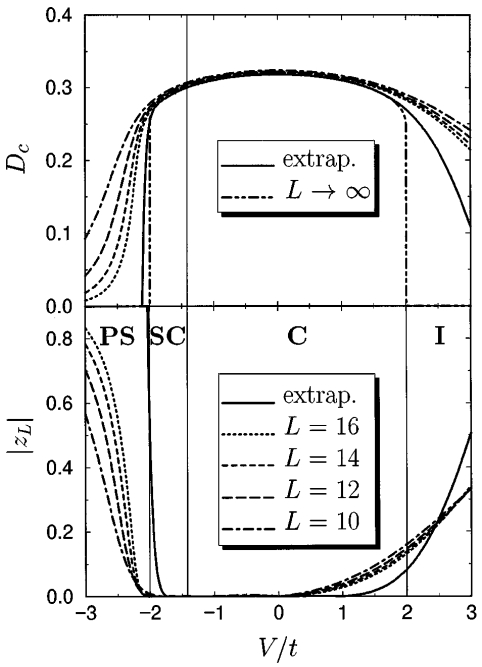

FIG. 1. Drude weight D_c (top) and modulus of z_L defined by Eq. (1) (bottom) for the $U \to +\infty$ EHM at filling $n_0 = 1/2$ for rings of various lengths L. Also shown are the corresponding quantities extrapolated to the thermodynamic limit using a cubic polynomial in $1/L$ and the exact result for D_c in the thermodynamic limit. The vertical lines separate the regions of phase segregation, Luttinger liquid with $K_\rho > 1$ (SC) or $K_\rho < 1$ (C), and a new insulating phase at large V/t (I).

increasing size. The extrapolated values of $|z_L|$ clearly show an abrupt transition near $V = -2t$, indicating that the system is a conductor (very small $|z_L|$) for $-1.8t < V < 1.2t$, and suggesting that it is an insulator for $V \sim 3t$. Notice that the convergence to the thermodynamic limit for D_c and $|z_L|$ is, in absolute value, about the same. However, for any value of V, D_c decreases with system size while, in general, $|z_L|$ decreases well inside the metallic phases $(|V| < 1.5t)$ and increases well inside the insulating phases $(|V| \sim 3t)$. Thus, the results for $|z_L|$ are complementary to Kohn's D_c criterion [1], $|z_L|$ providing a more useful measure.

We have also studied the behavior of γ_L [Eq. (3)] near the transitions. Because of inversion symmetry, $\gamma_L = 0$ or π $[\mathrm{mod}(2\pi)]$. In contrast to previous cases [6,8], we do not find a jump in γ_L at the transition from the SC to the PS regime $(V = -2t)$, or at the opening of the charge gap $(V = 2t)$. However, as in the case of attractive U [6], there is a jump from $\gamma_L = \pi$ to $\gamma_L = 0$ as the dominant correlation functions at large distances change from the superconducting to the CDW ones. For $8 \le L \le 16$ we obtain with four digits accuracy $V_c = -\sqrt{2}\,t$ in perfect agreement with the value obtained from the numerical solution of the Bethe-ansatz integral equations. Instead, the corresponding jump in the phase of z_L takes place for $V_c \sim -1.55t$. This suggests that using $\langle\hat{X}\rangle = L\gamma_L/(2\pi l)$ and Eq. (3) one obtains a faster convergence for $\langle\hat{X}\rangle$ to the

thermodynamic limit than using Eq. (2). In addition, since in the gapless metallic phases $\lim_{L\to\infty}|z_L| = 0$, it might be difficult to identify V_c from the corresponding zero of z_L for sufficiently large L. As in Ref. [6], we also find jumps in γ_L for other values of V, in particular for $V = 0$ and $V = t$, without an obvious physical meaning.

In the rest of this Letter, we discuss Eq. (2) in more detail and illustrate its physical meaning using two other simple examples. First, note that if $|g\rangle$ is replaced by one of the CDW states $|1\rangle$ or $|2\rangle$ discussed above, the result is $\langle\hat{X}\rangle = 0$ in both cases. This is reasonable, since $|1\rangle$ and $|2\rangle$ differ in a translation and are thus physically equivalent in translationally invariant systems. This is, in general, the reason why $\langle\hat{X}\rangle$ is defined mod(L/l). Assume now that in the model Eq. (4) one considers an attractive V and adds a next-nearest-neighbor repulsion V' such that $V' \gg |V| \gg t$. For even $N = L/2$, $|g\rangle$ consists of a sequence of two nearest-neighbor sites occupied, the next two empty, and so on. Specifically $|g_{\pm\pi/2}(\Phi)\rangle = (|A\rangle \pm i\hat{T}|A\rangle)/\sqrt{2}$, with $|A\rangle = \prod_{j=0}^{N/2-1} c_{4j+1}^{\dagger} c_{4j+2}^{\dagger}|0\rangle$. Then, $\mathcal{U}_L^2|g_{\pm\pi/2}\rangle = -|g_{\pm\pi/2}\rangle$, and $\langle\hat{X}\rangle = L/4$ [mod$(L/2)$] [$\hat{X}|A\rangle = \sum_{j=0}^{N/2-1}(8j+3)|A\rangle = N(N-1/2)|A\rangle$]. This is consistent with the transfer of half of the particles of the system, either to the left or to the right, necessary to build the state $(|A\rangle \pm i\hat{T}|A\rangle)/\sqrt{2}$ from $(|1\rangle \pm i\hat{T}|1\rangle)/\sqrt{2}$.

In the examples discussed above, the Hamiltonian had inversion symmetry. Under those circumstances the phase of z_L can attain only the values 0 or π (z_L is real). This statement implies that well-defined values of $\langle\hat{X}\rangle$ different from 0 and $L/(2l)$ [mod(L/l)] can be achieved only in the absence of inversion symmetry. A simple example in which this symmetry is explicitly broken is obtained replacing each site in Eq. (4) by a heteronuclear molecule. Specifically, in the spinless case consider a system described by the Hamiltonian

$$H(0) = \Delta\sum_j d_j^{\dagger} d_j - \sum_j (t' d_j^{\dagger} c_j + t c_{j+1}^{\dagger} d_j + \text{H.c.}) + \sum_j (V' c_j^{\dagger} c_j d_j^{\dagger} d_j + V c_{j+1}^{\dagger} c_{j+1} d_j^{\dagger} d_j). \quad (5)$$

It is easy to see that for $V, V', t' \gg t$, and $n_0 = 1/2$ (one particle each two unit cells), $|g\rangle$ is a CDW with every second molecule singly occupied in the GS of the first two terms of Eq. (5). For this $|g\rangle$, Eq. (2) gives $\langle\hat{X}\rangle = NP$ where P is the polarizability of each molecule and varies continuously as a function of t'/Δ [2].

In conclusion, we have introduced a complex quantity z_L which is shown to display a qualitatively different behavior for conductors than for insulators, thereby providing a valuable criterion to distinguish between those states of matter. The criterion, which is valid for any fractional particle filling and for both ordered and disordered systems, is complementary and in a sense sharper than that based on the value of D_c [1]. We have shown how to use z_L to characterize Mott and superconducting transitions in models of strongly correlated quantum particles. z_L involves *only* the computation of the GS of the system, which for time-reversal symmetric Hamiltonians is real valued, whereas D_c needs at least two GS calculations for different BC, and in one of them time-reversal symmetry is broken. This seems innocuous for Lanczos studies, but it is not for stochastic approaches where the study of non-time-reversal symmetric states adds an additional complication to the already infamous fermion sign problem. In addition, z_L can be computed using the powerful density-matrix renormalization group method [15], while so far it does not seem possible to calculate D_c using this method.

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