PHYSICAL REVIEW B **99**, 205144 (2019)

A simple position operator for periodic systems

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(Received 13 November 2018; revised manuscript received 11 February 2019; published 24 May 2019)

We present a position operator that is compatible with periodic boundary conditions (PBCs). It is a one-body operator that can be applied in calculations of correlated materials by simply replacing the traditional position vector by the new definition. We show that it satisfies important fundamental as well as practical constraints. To illustrate the usefulness of the PBC position operator, we apply it to the localization tensor, a key quantity that is able to differentiate metallic from insulating states. In particular, we show that the localization tensor given in terms of the PBC position operator yields the correct expression in the thermodynamic limit. Moreover, we show that it correctly distinguishes between finite precursors of metals and insulators.

DOI: 10.1103/PhysRevB.99.205144

I. INTRODUCTION

Expectation values that involve the position operator $\hat{\mathbf{r}}$ play a prominent role in both molecular and condensed-matter physics. Many important quantities are expressed in terms of $\hat{\mathbf{r}}$, e.g., the multipole moments and the localization tensor. The latter quantity was introduced by Resta *et al.* [1–3], following an idea of Kohn [4] that information about electron localization could be obtained from the ground-state wave function (see also Ref. [5]). The localization tensor is able to distinguish between conductors and insulators. When the number of electrons tends to infinity, it diverges in the case of a conductor, while it remains finite in the case of an insulator. It has been applied to study the metallic behavior of clusters [6–14] and has recently also been used to investigate Wigner localization [15].

In its standard definition, the position operator $\hat{\mathbf{r}}$ is simply defined as the multiplication with the position vector $\mathbf{r}$. However, this definition is not compatible with periodic boundary conditions (PBCs), since $\mathbf{r}$ is not a periodic function. This is a problem, since many quantities of interest are related to the solid state, which are conveniently described using PBC. Therefore, it is of great interest to search for a position operator that is compatible with PBC while reducing to the position vector $\mathbf{r}$ in the appropriate limit. We will provide such a definition of the position operator in this paper. For notational convenience, we will mainly focus on one dimension in the remainder of this paper. All our findings can be generalized to higher dimensions. In particular, our main results, i.e., Eqs. (2) and (7), can be generalized to three dimensions by replacing x with $\mathbf{r}$. We use Hartree atomic units ($\hbar = 1$, $e = 1$, $m_e = 1$, $4\pi\epsilon_0 = 1$).

We study a system of length L whose electronic many-body wave function Ψ satisfies PBC, i.e., for each x_i the following condition holds:

$$\Psi(x_1, \cdots, x_i, \cdots, x_N) = \Psi(x_1, \cdots, x_i + L, \cdots, x_N), \quad (1)$$

where N is the number of electrons. We are looking for a position operator that is compatible with PBC. We denote such an operator as $\hat{q}$.

Let us summarize important criteria that $\hat{q}$ should satisfy: (1) $\hat{q}$ should be invariant with respect to a translation L. (2) $\hat{q}$ should reduce to the standard position operator $\hat{x} = x$ for finite systems described within PBC, i.e., in a supercell approach ($L \to \infty$ for fixed N) [16] one should obtain results that coincide with those obtained within open-boundary conditions (OBC). (3) The distance defined in terms of $\hat{q}$ should be real and gauge-invariant, i.e., it should be independent of the choice of the origin. This criterium is important since the main purpose of a position operator is to yield the correct distance between two spatial coordinates. Finally, we add a fourth criterium: (4) For a system of many particles, $\hat{q}$ should be a one-body operator, as is $\hat{x}$. Although the last criterium is not a fundamental one, it is crucial if we want to apply the new operator to realistic systems.

In a seminal work, Resta proposed a definition for the *expectation value* of the total position operator $\hat{X} = \sum_{i=1}^{N} x_i$ that is compatible with PBC [17]. Following a similar strategy, Resta *et al.* also proposed an expression for the localization tensor that is compatible with PBC [1,2]. Despite the important progress made in these works, there are also several shortcomings to this approach. (1) They provide definitions for expectation values *but not a definition for the position operator itself*. (2) the operators are N-body, which make them unpractical for the calculation of expectation values of real correlated systems with many electrons. Finally, we note that their approach can yield diverging localization tensors for

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systems with a finite number of electrons; namely, for those systems that become metallic in the thermodynamic limit.

Instead, in this paper we propose a definition for the *position operator itself*. We will demonstrate that it satisfies the four criteria mentioned above. Moreover, we will explicitly show that it yields a useful expression for the localization tensor. The latter gives finite values at finite N and L while yielding the correct values in the thermodynamic limit.

The paper is organized as follows. We start by giving an introduction in Sec. I. In Sec. II, we present a position operator that is compatible with PBC and we show how it can be used to define a PBC localization tensor. We also briefly discuss the polarizability. In Sec. III, we report results obtained for uncorrelated and correlated model systems. Finally, in Sec. IV we draw our conclusions.

II. A POSITION OPERATOR COMPATIBLE WITH PERIODIC BOUNDARY CONDITIONS

To treat PBC systems, we associate to the electron position x the *complex position* $q_L(x)$, defined as

$$q_L(x) = \frac{L}{2\pi\mathrm{i}}\left[\exp\left(\frac{2\pi\mathrm{i}}{L}x\right) - 1\right], \tag{2}$$

with i the imaginary unit. The complex position $q_L(x)$ is a continuous and infinitely differentiable function of x. In complete analogy with the quantum treatment of the position operator $\hat{x}$, we define the action of the complex position operator $\hat{q}$ as the multiplication with $q_L(x)$.

Let us review the criteria mentioned above with respect to $q_L(x)$. (1) $q_L(x)$ is trivially invariant under a translation, i.e., $q_L(x+L) = q_L(x)$. Therefore, the complex position $q_L(x)$, unlike the ordinary position x, satisfies the PBC constraint. (2) $q_L(x)$ reduces to the standard position operator x in the limit $L \to \infty$, in the sense of a supercell approach mentioned above. This can be shown by expanding the exponential function: $\exp(\frac{2\pi\mathrm{i}}{L}x) = 1 + \frac{2\pi\mathrm{i}}{L}x + O(1/L^2)$[18]. (3) the distance $|q_L(x_2) - q_L(x_1)|$ is real and gauge independent. By defining the difference $q_{L,x_0}(x_2, x_1) = q_L(x_2 - x_0) - q_L(x_1 - x_0)$, where x_0 is the (arbitrary) origin, it can be verified that

$$q_{L,x_0}(x_2, x_1) = \frac{L}{2\pi\mathrm{i}}e^{-\frac{2\pi\mathrm{i}}{L}x_0}\left[e^{\frac{2\pi\mathrm{i}}{L}x_2} - e^{\frac{2\pi\mathrm{i}}{L}x_1}\right]. \tag{3}$$

Therefore, the distance

$$\begin{aligned}|q_L(x_2) - q_L(x_1)| &= \sqrt{q^*_{L,x_0}(x_2, x_1)q_{L,x_0}(x_2, x_1)}\\ &= \frac{L}{2\pi}\sqrt{2 - 2\cos\left[\frac{2\pi}{L}(x_2 - x_1)\right]}\end{aligned} \tag{4}$$

is real and independent of x_0, as it should be [19]. (4) $q_L(x)$ is a one-body operator.

A. The localization tensor

Let us now demonstrate how the complex position in Eq. (2) yields a useful expression for the localization tensor within PBC using an approach that is completely analogous to the OBC case. The localization tensor λ is defined as the total position spread (TPS) per electron where the TPS is a one-body operator that is defined as the second cumulant moment of the total position operator $\hat{X} = \sum_{i=1}^{N} x_i$[21]:

$$\lambda(N) = \frac{1}{N}[\langle\Psi|\hat{X}^2|\Psi\rangle - \langle\Psi|\hat{X}|\Psi\rangle^2]. \tag{5}$$

The second term in the square brackets ensures gauge invariance with respect to the choice of the origin of the coordinate system. The localization tensor is translationally invariant.

In complete analogy with the OBC definition, within PBC we replace the position of a particle x_i by its complex position $q_L(x_i)$. In such a way, the complex total position operator is still a one-body operator, defined as

$$\hat{Q}_L = \sum_{i=1}^{N} \hat{q}_L(x_i). \tag{6}$$

The localization tensor within PBC λ_L is also a real quantity, like λ. It is defined as the second cumulant moment of the complex total position operator per electron,

$$\lambda_L(N) = \frac{1}{N}[\langle\Psi|\hat{Q}_L^\dagger\hat{Q}_L|\Psi\rangle - \langle\Psi|\hat{Q}_L^\dagger|\Psi\rangle\langle\Psi|\hat{Q}_L|\Psi\rangle], \tag{7}$$

in complete analogy with the OBC definition in Eq. (5). Equation (7), together with Eq. (2), is the main result of this paper. The simple expression is completely general, it can be applied to correlated many-body wave functions and is valid for both finite systems and infinite systems, e.g., by taking the thermodynamic limit. In the special case of a single-determinant wave function, it can be shown that the expression in Eq. (7) coincides with the result obtained in Ref. [2] in the thermodynamic limit. The proof is given in the Appendix.

B. The polarizability

The polarization has been related to the position operator [17,22]. However, since the current operator is compatible with PBC, variations of the polarization can also be calculated as a time integral of the current density. Instead, the expression for the polarization itself proposed in Ref. [23] is not gauge invariant and cannot be written as an expectation value of any operator; it requires the calculation of a Berry-phase expression [22–25].

Instead of the current density, we focus here on a related quantity, namely the polarizability, i.e., the variation of the current due to a perturbing field. For one-dimensional chains, the polarizability can also be related to the macroscopic polarization in the thermodynamic limit [26].

The static polarizability α for OBC can be written as

$$\alpha(N) = 2\langle\Psi_0|x(\hat{H} - E_0)^{-1}_{\perp}x|\Psi_0\rangle, \tag{8}$$

where Ψ_0 is the ground-state wave function and $(\hat{H} - E_0)^{-1}_{\perp}$ is the reduced resolvent of the Hamiltonian in the orthogonal complement to Ψ_0 [27]. Therefore, in complete analogy with the OBC definition above, we define the PBC polarizability $\alpha_L(N)$ as

$$\alpha_L(N) = 2\langle\Psi_0|q_L^\dagger(x)(\hat{H} - E_0)^{-1}_{\perp}q_L(x)|\Psi_0\rangle, \tag{9}$$

III. RESULTS

We will now demonstrate that the PBC localization tensor given by Eq. (7) can differentiate between metals and insulators and that it can be applied to both finite and infinite systems. To do so, we will apply it to model systems.

A. Noninteracting electrons

First, we will treat the simple case of N noninteracting electrons in a one-dimensional box of length L. This model system can be seen as a prototype of a conductor. For this reason, it is particularly important that the formalism we propose in this paper can be applied to such a system. In analogy to the OBC case [3], one expects that the localization tensor $\lambda_L(N)$, diverges in the thermodynamic limit.

We consider $N = 2m + 1$ noninteracting electrons where m is a non-negative integer. For the sake of simplicity, we assume that the particles are spinless. In the case of particles with spin, the final result can be trivially obtained by multiplying the spinless-particle result by the spin multiplicity of a single particle. The eigenfunctions of the Hamiltonian of this system are periodic orbitals given by

$$\phi_n(x) = \frac{1}{\sqrt{L}} \exp\left(\mathrm{i}\frac{2\pi n}{L}x\right), \tag{10}$$

where n is an integer. Since the particles do not interact, the ground-state wave function is a single Slater determinant of the occupied orbitals, given by $|\Phi_0\rangle = |\phi_{-m}\cdots\phi_m\rangle$. The corresponding localization tensor reads

$$\lambda_L(N) = \frac{L^2}{4\pi^2 N}\left[\langle\Phi_0|\sum_{i=1}^{N} e^{-\frac{2\pi\mathrm{i}}{L}x_i}\sum_{j=1}^{N} e^{\frac{2\pi\mathrm{i}}{L}x_j}|\Phi_0\rangle - \langle\Phi_0|\sum_{i=1}^{N} e^{-\frac{2\pi\mathrm{i}}{L}x_i}|\Phi_0\rangle\langle\Phi_0|\sum_{j=1}^{N} e^{\frac{2\pi\mathrm{i}}{L}x_j}|\Phi_0\rangle\right]. \tag{11}$$

Inserting a complete set of states in the first term in the square brackets yields

$$\lambda_L(N) = \frac{L^2}{4\pi^2 N}\sum_{I\neq 0}\sum_{i,j=1}^{N}\langle\Phi_0|e^{-\mathrm{i}\frac{2\pi}{L}x_i}|\Phi_I\rangle\langle\Phi_I|e^{\mathrm{i}\frac{2\pi}{L}x_j}|\Phi_0\rangle \tag{12}$$

$$= \frac{L^2}{4\pi^2 N}\sum_{|p|\leqslant m}\sum_{|l|>m}\langle\phi_p|e^{-\mathrm{i}\frac{2\pi}{L}x}|\phi_l\rangle\langle\phi_l|e^{\mathrm{i}\frac{2\pi}{L}x}|\phi_p\rangle, \tag{13}$$

where in the last step we used the Slater-Condon rules for one-electron operators [28]. Inserting Eq. (10) into the above expression leads to the following expression for the matrix element $\langle\phi_p|e^{-\mathrm{i}\frac{2\pi}{L}x}|\phi_l\rangle$:

$$\frac{1}{L}\int_L \exp\left(\mathrm{i}\frac{2\pi(l-p-1)}{L}x\right)dx = \delta_{l-p-1}. \tag{14}$$

Therefore, there is only one nonzero contribution in the double summation over p and l in Eq. (13), namely when $p = m$ and $l = m + 1$. We can write the final result as

$$\lambda_L(N) = \frac{L^2}{N^2}\frac{N}{4\pi^2}, \tag{15}$$

from which we can deduce the behavior of the localization tensor in the thermodynamic limit. Since, in this limit, N/L remains constant, the localization tensor diverges linearly with N, as one would expect for a measure of conductivity applied to a perfect conductor.

B. A tight-binding model

We now consider a dimerized chain containing $4m + 2$ atoms at half filling, i.e., $N = 4m + 2$, in a tight-binding model. The Hamiltonian is given by, for OBC and PBC, respectively,

$$\hat{H}_{\mathrm{OBC}} = \sum_{i=1}^{N-1} -t_i(\hat{a}_i^\dagger\hat{a}_{i+1} + \hat{a}_{i+1}^\dagger\hat{a}_i), \tag{16}$$

$$\hat{H}_{\mathrm{PBC}} = \sum_{i=1}^{N-1} -t_i(\hat{a}_i^\dagger\hat{a}_{i+1} + \hat{a}_{i+1}^\dagger\hat{a}_i) - t_N(\hat{a}_N^\dagger\hat{a}_1 + \hat{a}_1^\dagger\hat{a}_N), \tag{17}$$

where $\hat{a}_i^\dagger$ ($\hat{a}_i$) is a creation (annihilation) operator and the hopping parameter $t_i = 1 - (-1)^i\delta$ with $0 \leqslant \delta \leqslant 1$. This means that the dimerization is at its maximum when $\delta = 1$ while there is no dimerization when $\delta = 0$. The latter system can be interpreted as a precursor of a metal since in the thermodynamic limit this system becomes metallic. It is convenient to express the Hamiltonian in the site basis. Upon diagonalization, we thus obtain the eigenfunctions which, when inserted in Eqs. (5) and (7), yield the OBC and PBC localization tensors of the dimerized chain.

In Fig. 1, we report $\lambda(N)$, as defined in Eq. (5) for OBC, as well as $\lambda_L(N)$, as defined in Eq. (7) for PBC, as a function of the number of electrons for various values of δ. The length of the unit cell has been set to unity and we have set $L = N$ such that the density $N/L = 1$. First of all, we see that the PBC localization tensor is well-defined for finite N also for the

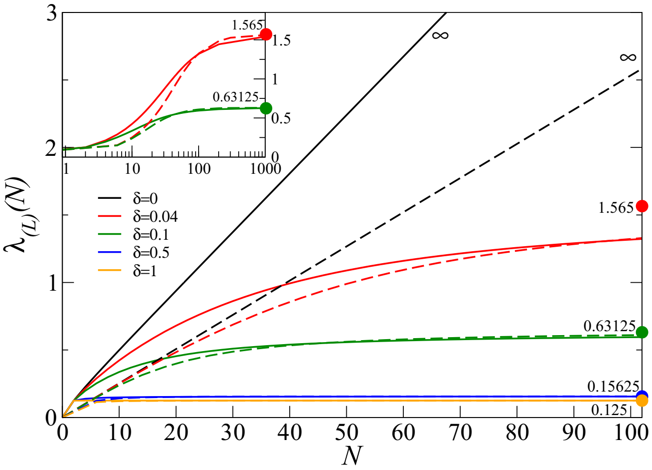

FIG. 1. The OBC localization tensor $\lambda(N)$ (solid lines) and the PBC localization tensor $\lambda_L(N)$ (dashed lines) as a function of the number of electrons N for various values of the dimerization parameter δ in a tight-binding model [see Eqs. (16) and (17)]. The dots and numbers next to each curve are the values of the PBC localization tensor in the thermodynamic limit. They were obtained from Eq. (22). Inset: $\lambda_{(L)}(N)$ for $\delta = 0.04$ and $\delta = 0.1$ for large N.

"metallic" chain ($\delta = 0$). Second, as expected, the OBC and PBC localization tensors, $\lambda(N)$ and $\lambda_L(N)$, respectively, differ for finite N, since they describe different systems. Instead, in the thermodynamic limit, both localization tensors describe the same system and indeed we obtain the same values in that limit.

The advantage of the PBC localization tensor is that the thermodynamic limit can be obtained without extrapolating results for finite N and L. Instead, at least for single-particle Hamiltonians, one can obtain an expression involving information of a single unit cell.

In the case of the dimerized chain, one can derive an analytical expression for the localization tensor in the thermodynamic limit. The unit cell of length d contains two sites separated by $d/2$ with one electron per site. In the site basis, the Hamiltonian $\hat{H}_\kappa$, which corresponds to the periodic part of the wave function, is then given by ($d = 1$)

$$H_{\kappa,11} = H_{\kappa,22} = 0, \tag{18}$$

$$H_{\kappa,12} = H^*_{\kappa,21} = -(1+\delta)e^{\frac{-\pi i}{\kappa n}} + (1-\delta)e^{\frac{\pi i}{\kappa n}}, \tag{19}$$

where $\kappa = 0, 1, 2, \ldots, n-1$ is an integer and n is the number of cells. The eigenvectors of the matrix H_κ are the periodic part of the Bloch functions ϕ_{ik}. There is one occupied valence state ϕ_{vk} and one unoccupied conduction state ϕ_{ck}. They are given by

$$\phi_{ik}(x) = \frac{1}{\sqrt{n}} e^{ikx} u_{ik}(x) \quad (i = v, c), \tag{20}$$

where x is the coordinate along the chain, $k = 2\pi\kappa/L$ is the wave vector and $u_{ik}(x)$ is a periodic function that is normalized over a single cell. To obtain the localization tensor, we use a similar strategy to that used for the system of noninteracting electrons, i.e., we insert a complete set of states in Eq. (7) and use the Slater-Condon rules. This yields the following expression [9]:

$$\lambda_L(N) = \frac{L^2}{4\pi^2} \sum_{\kappa=0}^{n-1} \langle \phi_{vk} | e^{-i\frac{2\pi}{L}x} | \phi_{ck'} \rangle \langle \phi_{ck'} | e^{i\frac{2\pi}{L}x} | \phi_{vk} \rangle, \tag{21}$$

with $k' = k + 2\pi/L$. In the thermodynamic limit, the variable κ becomes continuous and the summation over κ can be replaced with an integral over k. We finally obtain

$$\lambda_\infty \equiv \lim_{N,L\to\infty} \lambda_L(N) = \frac{1+\delta^2}{16|\delta|}. \tag{22}$$

As expected, for a periodic system, λ_∞ is an even function of δ. We note that λ_∞ goes to infinity as $1/|\delta|$ when δ tends to zero, i.e., when we go from an insulator ($\delta \neq 0$) to a metal ($\delta = 0$). We reported the limiting values obtained with Eq. (22) in Fig. 1.

Finally, in Fig. 2 we report the static polarizability per electron $\bar{\alpha}(N) = \alpha(N)/N$ and $\bar{\alpha}_L(N) = \alpha_L(N)/N$ as a function of the number of electrons for various values of δ. As before, the length of the unit cell has been set to unity and we have set $L = N$ such that the density $N/L = 1$. As was the case for the PBC localization tensor, the PBC polarizability is well-defined for finite N for the "metallic" chain ($\delta = 0$). We note that, while the localization tensor diverges linearly for this chain, the polarizability per electron diverges quadratically. Most importantly, in the thermodynamic limit, $\bar{\alpha}(N)$ and $\bar{\alpha}_L(N)$ tend to the same values, as they should.

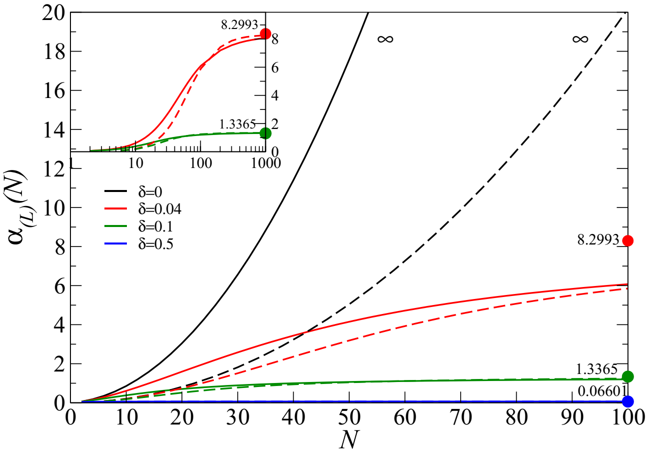

FIG. 2. The OBC polarizability $\bar{\alpha}(N)$ (solid lines) and the PBC polarizability $\bar{\alpha}_L(N)$ (dashed lines) as a function of the number of electrons N for various values of the dimerization parameter δ in a tight-binding model. The dots and numbers next to each curve are the values of the PBC localization tensor in the thermodynamic limit. They were obtained from Eq. (24). Inset: $\bar{\alpha}(N)$ and $\bar{\alpha}_{(L)}(N)$ for $\delta = 0.04$ and $\delta = 0.1$ for large N.

In the thermodynamic limit, we can obtain an analytical expression for the PBC polarizability $\bar{\alpha}_L$ of the tight-binding model in a similar way as that employed for the localization tensor, which is described in the paper. The PBC polarizability $\bar{\alpha}_L$ can be rewritten as

$$\bar{\alpha}_L(N) = \frac{L^2}{4\pi^2} \sum_{\kappa=0}^{n-1} \frac{\langle \phi_{vk} | e^{-i\frac{2\pi}{L}x} | \phi_{ck'} \rangle \langle \phi_{ck'} | e^{i\frac{2\pi}{L}x} | \phi_{vk} \rangle}{\epsilon_{ck'} - \epsilon_{vk}}, \tag{23}$$

where ϵ_{vk} ($\epsilon_{ck'}$) is the orbital energy of a valence (conduction) state. In the thermodynamic limit, the variable κ becomes continuous and the summation over κ can be replaced with

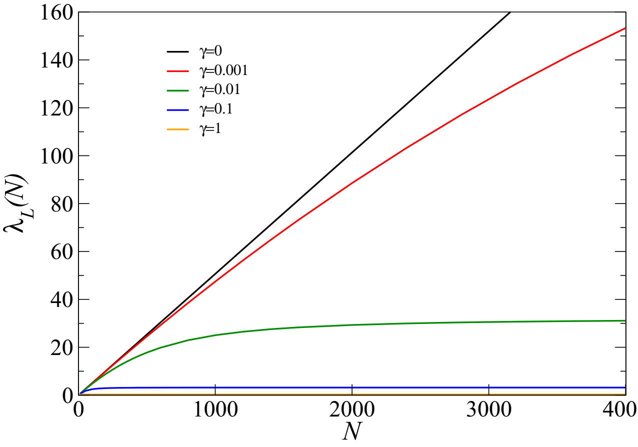

FIG. 3. The PBC localization tensor $\lambda_L(N)$ as a function of the number of electrons N for various values of the electronegativity difference γ for a square lattice in a tight-binding model.

an integral over k. We finally obtain

$$\bar{\alpha}_\infty \equiv \lim_{N,L\to\infty} \alpha_L(N) = \frac{2(1+\delta^2)E(1-\delta^2) - \delta^2 K(1-\delta^2)}{48\pi\delta^2}, \tag{24}$$

where K and E are the complete elliptic integrals of the first and second kinds, respectively:

$$K(x) = \int_0^{\pi/2} (1 - x\,\sin^2\theta)^{-1/2} d\theta, \tag{25}$$

$$E(x) = \int_0^{\pi/2} (1 - x\,\sin^2\theta)^{1/2} d\theta. \tag{26}$$

We reported the limiting values obtained with Eq. (24) in Fig. 2.

C. Square lattice

To demonstrate that our approach is not limited to one dimension, we consider a two-dimensional square lattice with the following tight-binding Hamiltonian,

$$\hat{H} = -\sum_{\langle i,k\rangle}\sum_j a_{i,j}^\dagger a_{k,j} - \sum_i \sum_{\langle j,k\rangle} a_{i,j}^\dagger a_{i,k} + \frac{\gamma}{2}\sum_{i,j}(-1)^{i+j} a_{i,j}^+ a_{i,j}, \tag{27}$$

where the notation $\langle i,k\rangle$ indicates that i and k are nearest neighbors. The Hamiltonian in Eq. (27) describes a nondimerized bipartite lattice with nearest-neighbor hopping $t = 1$. We can obtain the band structure that corresponds to this Hamiltonian in the thermodynamic limit. It is given by

$$\epsilon_\pm(k_x, k_y) = \tfrac{1}{2}[\gamma \pm \gamma^2 + 16(1 + \cos(k_x) + \cos(k_y) + \cos(k_x)\cos(k_y)]^{1/2}. \tag{28}$$

The minimum gap between the two eigenvalues is γ, and it is reached for either $k_x = \pm\pi$ or $k_y = \pm\pi$ (or both). This means that the system is an insulator when it is bipartite, i.e., if $\gamma \neq 0$, while it becomes a metal when all the sites are equivalent, i.e., $\gamma = 0$. The parameter γ can be interpreted as the difference in electronegativity between neighboring sites. Therefore, the Hamiltonian in Eq. (27) represents a model for a single layer of NaCl when $\gamma \neq 0$ and a single layer of the simple-cubic polonium crystal for $\gamma = 0$. We computed the eigenvalues of the localization tensor and the polarizability of this system for various values of γ. Because of the symmetry, the diagonal components are identical, while the off-diagonal components vanish. For this reason, we report only the xx component in the following.

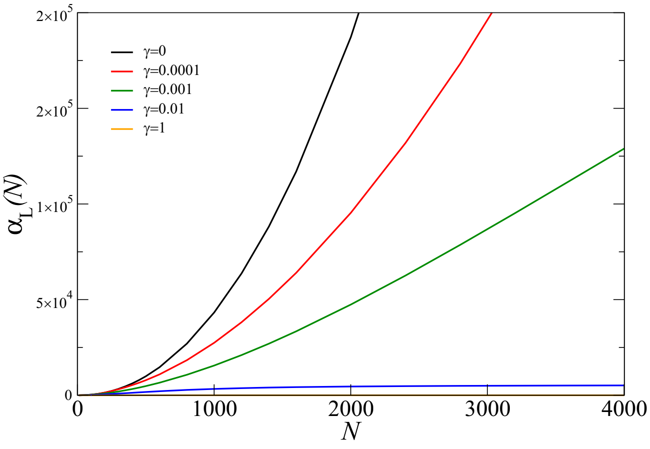

FIG. 4. The PBC polarizability $\bar{\alpha}_L(N)$ as a function of the number of electrons N for various values of the electronegativity difference γ for a square lattice in a tight-binding model.

In Fig. 3, we report the localization tensor as a function of N for various values of γ. For $\gamma \neq 0$, the localization tensor is a monotonous increasing function that saturates to a constant in the limit $N \to \infty$. On the other hand, for $\gamma = 0$, the localization tensor is linear in N, so it diverges linearly for $N \to \infty$. In Fig. 4, the corresponding polarizability per electron are reported. The behavior is very similar to that of the localization tensor. The main difference is that for $\gamma = 0$, the polarizability diverges quadratically as a function of N for large N.

D. A Heisenberg model

Finally, we calculate the spin localization tensor for a correlated Heisenberg model. We study the following Hamiltonians, for OBC and PBC, respectively:

$$\hat{H}_{\text{OBC}} = 2J\sum_{i=1}^{N-1}(1 - (-1)^i\delta)\hat{\vec{S}}_i\hat{\vec{S}}_{i+1}, \tag{29}$$

$$\hat{H}_{\text{PBC}} = 2J\sum_{i=1}^{N-1}\{(1 - (-1)^i\delta)\hat{\vec{S}}_i\hat{\vec{S}}_{i+1}\} + 2J(1-\delta)\hat{\vec{S}}_1\hat{\vec{S}}_N, \tag{30}$$

where $\hat{\vec{S}}_i$ is the spin vector of site i, J is the coupling constant, and $0 \leqslant \delta \leqslant 1$ is the dimerization parameter, i.e., the dimerization is at its maximum when $\delta = 1$ while there is no dimerization when $\delta = 0$. Furthermore, we assume that $N \geqslant 4$ and N is even.

Since the electron positions are fixed in this model, the localization tensor vanishes for all N. However, the localization tensor can be split into four spin contributions [13,14,29],

$$\lambda(N) = \lambda^{\uparrow\uparrow}(N) + \lambda^{\downarrow\downarrow}(N) + \lambda^{\uparrow\downarrow}(N) + \lambda^{\downarrow\uparrow}(N), \tag{31}$$

where $\lambda^{\uparrow\uparrow}(N)$ [$\lambda^{\downarrow\downarrow}(N)$] is a measure of the localization of ↑ (↓) spins, and $\lambda^{\uparrow\downarrow}(N)$ and $\lambda^{\downarrow\uparrow}(N)$ are the couplings between ↑ and ↓ spins. In the following, we will focus on the spin localization tensor $\lambda^S(N) = \lambda^{\uparrow\uparrow}(N) + \lambda^{\downarrow\downarrow}(N)$ obtained from the ground state for an antiferromagnetic ordering ($J = -1$).

In Fig. 5, we report the OBC spin localization tensor $\lambda^S(N)$ as well as the PBC spin localization tensor $\lambda_L^S(N)$ as a function of the number of electrons for various values of δ. The length of the unit cell has been set to unity and we have set $L = N$ such that the density $N/L = 1$. Because of the correlation, the numerical solution of the problem is much more computationally demanding than the uncorrelated calculations discussed in the paper. For this reason, the largest number of electrons we were able to treat is $N = 16$.

Nevertheless, the same conclusions drawn for the uncorrelated tight-binding model discussed in the paper also apply to the correlated Heisenberg model: (1) for the metallic chain ($\delta = 0$), the PBC localization tensor is well-defined for finite N and it diverges linearly with N as does the OBC localization

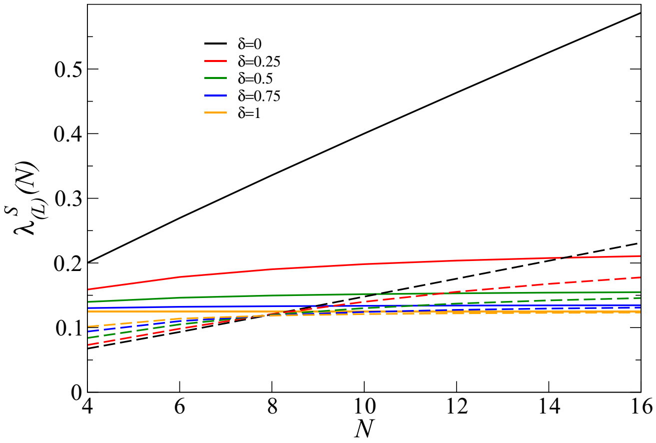

FIG. 5. The OBC spin localization tensor $\lambda^S(N)$ (solid lines) and the PBC spin localization tensor $\lambda^S_L(N)$ (dashed lines) as a function of the number of electrons N for various values of the dimerization parameter δ in a Heisenberg model.

tensor; (2) the OBC and PBC localization tensors, $\lambda(N)$ and $\lambda_L(N)$, respectively, differ for finite N, since they describe different systems; (3) in the thermodynamic limit, both localization tensors describe the same system and the localization tensors tend to the same value in that limit. The last conclusion can only be verified numerically for $\delta \simeq 1$ since, for smaller values of δ, the convergence with respect to N is not fast enough to be visible in the range $4 \leqslant N \leqslant 16$.

IV. CONCLUSION

We have presented a simple one-body position operator that is compatible with PBC. We have shown that this operator meets several important fundamental constraints, e.g., it is translationally invariant, it reduces to the common position operator $\hat{\mathbf{r}} = \mathbf{r}$ in the appropriate limit, and the distance expressed in terms of the operator is gauge independent. Moreover, we have demonstrated its usefulness when applied to the localization tensor. In particular, we have shown that it yields the correct expression in the thermodynamic limit and correctly distinguishes between finite precursors of insulators and metals.

Finally, we note that this paper opens the road for the calculation of various other properties of interest for which the corresponding operators involve the position operator. In particular, our definition of position could reconcile the Coulomb potential with PBC since the distance remains well-defined [see Eq. (4)]. Preliminary investigations in this direction, both on the quantum (*ab initio* treatment of the electron gas) and classical level (Madelung sums) are in progress. In the end, this could, for example, enhance the convergence to the thermodynamic limit of Monte Carlo calculations of periodic systems [30].

ACKNOWLEDGMENTS

This work was partly supported by the French Centre National de la Recherche Scientifique (CNRS, also under the PICS Action No. 4263). It has received funding from the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie Grant Agreement No. 642294. This work was also supported by the Programme Investissements d'Avenir under Program No. ANR-11-IDEX-0002-02, Reference No. ANR-10-LABX-0037-NEXT. The calculations of this work have been partly performed by using the resources of the HPC center CALMIP under Grant No. 2016-p1048. Finally, E.V.F.A. acknowledges the support of the Theoretical Chemistry and Computational Modeling(TCCM) Erasmus-Plus Master program.

APPENDIX: PROOF OF EQUIVALENCE WITH THE LOCALIZATION TENSOR OF REF. [2] IN THE THERMODYNAMIC LIMIT FOR A SINGLE SLATER DETERMINANT

In this Appendix, we proof that our definition of the localization tensor in Eq. (7) of the paper reduces to the localization tensor proposed in Ref. [2] in the thermodynamic limit in the special case of a wave function that can be expressed as a single Slater determinant.

For a single Slater determinant, we can rewrite Eq. (7) of the paper according to

$$\lambda_L(N) = \frac{L^2}{4\pi^2} \sum_{v,c} \sum_{\kappa=0}^{n-1} \langle \phi_{vk} | e^{-i\frac{2\pi}{L}x} | \phi_{ck'} \rangle \langle \phi_{ck'} | e^{i\frac{2\pi}{L}x} | \phi_{vk} \rangle, \quad \text{(A1)}$$

$$= \frac{L^2}{4\pi^2} \sum_{v,c} \sum_{\kappa=0}^{n-1} \langle u_{vk} | u_{ck'} \rangle \langle u_{ck'} | u_{vk} \rangle, \quad \text{(A2)}$$

where $k' = k + \frac{2\pi}{L}$ and n is the number of cells. For large L, we can rewrite $u_{ck'}$, which is the periodic part of $\phi_{ck'}$, as

$$u_{ck'}(x) = u_{ck}(x) + \frac{2\pi}{L} \partial_k u_{ck}(x) + O(1/L^2). \quad \text{(A3)}$$

Therefore, the localization tensor in the thermodynamic limit becomes

$$\lim_{N,L\to\infty} \lambda_L(N) = \sum_{v,c} \int dk \langle u_{vk} | \partial_k u_{ck} \rangle \langle \partial_k u_{ck} | u_{vk} \rangle \quad \text{(A4)}$$

$$= \sum_{v,c} \int dk \langle \partial_k u_{vk} | u_{ck} \rangle \langle u_{ck} | \partial_k u_{vk} \rangle. \quad \text{(A5)}$$

Using the completeness relation $\sum_v \langle u_v | u_v \rangle + \sum_c \langle u_c | u_c \rangle = 1$ we can rewrite this as

$$\lim_{N,L\to\infty} \lambda_L(N) = \sum_{v} \int dk \langle \partial_k u_{vk} | \partial_k u_{vk} \rangle \quad \text{(A6)}$$

$$- \sum_{v,v'} \int dk \langle \partial_k u_{vk} | u_{v'k} \rangle \langle u_{v'k} | \partial_k u_{vk} \rangle, \quad \text{(A7)}$$

which is the expression proposed in Ref. [2]. This completes the proof.

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