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On the Localization Index of One–Electron Eigenstates

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Abstract. We show that the localization index or the inverse participation ratio (IPR) can be derived using the square modulus of the one–electron Green's function in site representation. Hence it is shown that the site and energy representations are unitary equivalent for the description of the localization properties of one–electron eigenstates. A natural generalization of the IPR is also given in connection to the spatial separation of the eigenstates. Furthermore, based on the relation between the IPR and the information entropy, we propose new limits for the cutoff value of the IPR separating localized states from extended ones in finite systems. These limits depend on the dimension of the embedding system and the decay form of the states.

1. The definition of the localization index and its cutoff value

The localization characteristics of the one–electron eigenstates of a system seems to be of fundamental theoretical importance in many aspects. In condensed matter physics the identification of localization induced by disorder (Anderson–transition), by electron–electron interaction (Mott–transition) or by other kinds of phenomena has been extensively studied by several analytical and numerical means [1,2]. In quantum chemistry, on the other hand, the main problem is the maximum localization of the one–electron orbitals, thus minimizing the number of Coulomb integrals to be calculated. In both cases practical computations need an exact definition for the localization properties of the eigenstates.

In a majority of numerical calculations the localization index or inverse participation ratio (IPR) of a one–electron eigenstate $|\mu\rangle$ is defined on the basis of reference [3] as

$$L_\mu = \sum_i |c_{i\mu}|^4, \tag{1}$$

where $|\mu\rangle$ is expanded over the set of site states $\{|i\rangle\}$ as $|\mu\rangle = \sum_i c_{i\mu}|i\rangle$. We have assumed an orthonormal site representation.

In quantum chemistry a generalized version of equation (1) has been recently introduced by Pipek [4] based on the Mulliken–charge, which reduces to equation (1) in the case of a non–overlapping atomic basis set. Pipek and Mezey [5] have successfully adopted this definition in the localization procedure of the canonical Hartree–Fock orbitals.

The sum in definition (1) practically enhances the coefficients close to unity and suppresses the ones close to zero. Thus $L_\mu \approx n^{-1}$ for a state distributed nearly uniformly over n sites, or in other words, the inverse of L_μ gives the number of sites the state extends to. In most cases the authors do not give any further explanation for their application of the IPR except the above arguments. In the next section we will present a simple justification for the usage of the IPRs.

The range of L_μ is $0 \leq L_\mu \leq 1$, where $L_\mu = 0$ for an extended state on an infinite lattice and $L_\mu = 1$ for a state localized on one single site. Furthermore, since localized and extended states cannot coexist at the same energy [2], the distribution of L_μ over the energy spectrum defines the mobility edge: the upper and lower ends of the energy interval where L_μ is zero are called the mobility edges. These properties are rigorously valid only for an infinite system. For a finite system, however, L_μ is always larger then zero, in fact $L_\mu \geq N^{-1}$ if N is the system size, and it is difficult to sharply separate localized and extended states from each other and thus to locate the mobility edges. This is the reason why various attempts have been performed [6–9] in order to give a reasonable estimate for the cutoff value of the localization index $L_c = \alpha/N$ above which the states are supposed to be localized, and the same way, to define also the mobility edges in numerical simulations.

This task has been performed up to now by means of computer simulations on finite size systems, which suffered from the limiting value of the system size, depending on the model and on the numerical method applied. In our approach, on the other hand, in Section 3 we will present results resting on mainly analytical grounds that, by definition, do not depend on the choice of N and the model.

Therefore the problem is to find an adequate value of parameter α so that wave functions extending to less than the N/α portion of the total system, can be considered as localized. There is no assumption that α would be independent of N. In fact an $L_c \approx N^{-1/2}$ relation would also be reasonable stating that fluctuations of the order of the system size could be a limit separating localized states from extended ones. In this paper we remain with the interpretation of α as described above and in the following. In Table 1 we have listed the values of parameter α obtained by several authors with the respective system sizes under consideration.

reference	α	N	Δ
Ching and Huber[6]	6	1006	2.0×10^{-1}
Elyutin[7]	64	–	7.4×10^{-4}
Blumen *et al.*[8]	20	100	2.4×10^{-2}
Gibbon *et al.*[9]	80	500	3.1×10^{-4}
present work	237.15	–	1.0×10^{-6}

Table 1. Comparision of parameter α related to the cutoff localization index $L_c = \alpha/N$ for exponential localization in dimension $d = 3$. The respective value of the system size N is also given where it is relevant, as well as the relative deviation of the structural entropy from the one of the extremely localized ($\alpha \to \infty$) case ($S^0_{str} = 3(1 - \ln 2) = 0.9205588$).

Generalized IPRs have also been extensively used [10–12] where other moments $L^{(p)}_\mu = \sum_i |c_{i\mu}|^{2p}$ of the charge distribution of the eigenstates were used, forming the basis of multifractal analysis [12]. The energy averaged $L^{(p)}_\mu$ quantities have already been related to the p–particle Green's functions in energy representation [10], forming the basis of a field theoretical treatment. In this work we show that the individual IPRs ($L_\mu \equiv L^{(2)}_\mu$) themselves are associated to the one–electron Green's function in site representation via a unitary transformation.

2. Description of localization in site and energy representations

For the description of localization in site representation, one of the most important quantities is P_{ij}, the longtime average probability that an electron created on site i at $t = 0$ is on site j at $t = \infty$, which is defined using the time–dependent one–electron Green's function

$$G_{ij}(t) = \langle j| \exp(-iHt/\hbar)|i\rangle, \tag{2}$$

where H is the Hamiltonian of the system under consideration. Hence P_{ij} is the following [13, 14]

$$P_{ij} = \lim_{T\to\infty} \frac{1}{T} \int_0^T |G_{ij}(t)|^2 dt. \tag{3}$$

Inserting the complete set of eigenstates into equation (2) with the help of their expansion over the basis set $\{|i\rangle\}$ this probability reads as

$$P_{ij} = \sum_\mu |c_{i\mu}|^2 |c_{j\mu}|^2, \tag{4}$$

where for sake of simplicity we have already assumed nondegeneracy [13,14]. The diagonal elements P_{ii} are the so–called return probabilities of the electrons which have been studied extensively both analytically [1,2,15] and numerically [9].

The integrand in equation (3) is in fact the Fourier transform of a special matrix element of the 2–particle Green's function $\mathcal{G}_{ii,jj}(E)$, which is fundamentally responsible for the description of quantum transport processes (see e.g. ref [16]). As we have mentioned earlier the energy averaged IPR is connected to $\mathcal{G}_{ii,jj}(E)$, as well, we expect a close relation between the IPRs and matrix P_{ij}.

Let us now introduce a non–negative real matrix $\mathbf{A}$ with matrix elements defined as $A_{i\mu} = |c_{i\mu}|^2$, that may be called the charge distribution matrix giving the charge density of eigenstate $|\mu\rangle$ on site i. Using matrix $\mathbf{A}$ we can rewrite equation (7) in a more compact form

$$\mathbf{P} = \mathbf{A}\mathbf{A}^\dagger, \tag{5}$$

where $\mathbf{A}^\dagger$ denotes the transposed form of $\mathbf{A}$.

It is possible to associate matrix $\mathbf{P}$ describing the propagation of electrons in site representation to a new matrix $\mathbf{Q}$ giving the charge overlap of the eigenstates of the system with the definition

$$\mathbf{Q} = \mathbf{A}^\dagger\mathbf{A}. \tag{6}$$

The matrix elements of $\mathbf{Q}$ according to equation (6) read as

$$Q_{\mu\nu} = \sum_i |c_{i\mu}|^2 |c_{i\nu}|^2. \tag{7}$$

As a consquence of ref [17] finite matrices of the form of $\mathbf{P}$ and $\mathbf{Q}$ (see equations 5 and 6) are unitary equivalent, i.e. there exists a unitary matrix $\mathbf{U}$ that

$$\mathbf{Q} = \mathbf{U}\mathbf{P}\mathbf{U}^\dagger. \tag{8}$$

Due to normalization both $\mathbf{P}$ and $\mathbf{Q}$ are so-called stochastic matrices with eigenvalues ranging in the $[0, 1]$ interval. Such property may ensure the existence of a unitary equivalence even in the infinite case, but we have not been able to show that. However, in practical calculations one always uses finite matrices for which equation (8) holds. Furthermore, using matrix $\mathbf{A}$, we may establish some other relations: $\mathbf{P}^n = \mathbf{A}\mathbf{Q}^{n-1}\mathbf{A}^\dagger$ and $\mathbf{Q}^n = \mathbf{A}^\dagger\mathbf{P}^{n-1}\mathbf{A}$ if $n = 2, 3, \ldots$. Therefore $\mathbf{P}^n$ commutes with $\mathbf{AU}$ and $\mathbf{Q}^n$ with $\mathbf{UA}$, and $\mathbf{P}^n\mathbf{A} = \mathbf{A}\mathbf{Q}^n$ if $n \geq 2$.

We can see that the diagonal elements of matrix $\mathbf{Q}$ are nothing else but the IPRs given in equation (1) $Q_{\mu\mu} = L_\mu$. Thus, starting from the time–dependent one–electron Green's function $G_{ij}(t)$ in site representation, we have arrived at the localization index or inverse participation ratio (IPR). Moreover, equation (8) shows that apart from the unitary equivalence of the site and energy representations of the wave functions, there exists a further unitary equivalence for the description of localization in these representations.

Matrix $\mathbf{Q}$ is an important quantity for the description of localized states in energy representation. Since the overlap matrix in the energy representation is a unit matrix it is $\mathbf{Q}$ that plays the role describing the spatial separation of localized eigenstates in phenomena like the hopping conduction. Using $\mathbf{Q}$ we do not have to assume any specific decay form for the wave functions. A variant form of $\mathbf{Q}$ has already been introduced earlier

by Pipek [18] for the treatment of two–electron integrals and the long–range behavior of the Fock matrix elements of molecular orbitals in connection to their spatial separation. Recently Milovanović *et al.* [19] have used a quantity called the cross IPR in order to detect independent (i.e. well separated) local–moment states in the investigation of the metallic state of a disordered interacting Fermi–liquid. The cross IPR can be derived from our $Q_{\mu\nu}$ the same way as Root *et al.* [13] have calculated the so–called quantum connectivity from the matrix P_{ij}. In both of the above applications [18, 19] the off–diagonal elements $Q_{\mu\nu}$ are used in terms of the spatial separation of localized states. The diagonal elements, on the other hand, are naturally related to the localization length of the states.

Until this point we have shown the existence of a connection between the IPR and the Green's function $G_{ij}(t)$. This general relation, however, does not provide a clear definition for the cutoff value of the IPR L_c. In the next section with the use of the information entropy we propose such a definition.

3. The role of the Shannon–entropy: the definition of the cutoff localization index

It is well–known that the complexity of a general distribution can be characterized by the so–called Shannon–entropy S. This quantity can be calculated for the eigenstates as

$$S_\mu = -\sum_i |c_{i\mu}|^2 \ln |c_{i\mu}|^2. \tag{9}$$

The entropy S has already been used exploiting its property that for increasing system size N one obtains that $S \propto \ln N$ for extended states and it saturates to a constant for localized states [20].

Recently we have shown [21] that assuming a definite decay form of the eigenstates embedded in a d–dimensional atomic network, the entropy S and the IPR L are related to each other (referring to one eigenstate we may drop index μ). First we have split S into a sum of two contributions: the extension entropy S_{ext} and the structural entropy S_{str}. The first part is simply $S_{ext} = -\ln L$, therefore only the remaining S_{str} is important for us. Next we have calculated $q = L^{-1}/N$, the quantity describing the spatial extension of the state compared to the system size N.

It has been shown that for a given decay form $|c_i|^2 \approx Af(|\mathrm{r}_i - \mathrm{r}_0|/\xi)$ the filling factor and the structural entropy arise as $q = q(\xi/N)$, $S_{str} = S_{str}(\xi/N)$, where the functions $q(z)$ and $S_{str}(z)$ themselves are independent of A, r_0, ξ, and N. They are completely determined by the decay form $f(\rho)$ of the wave functions and the dimensionality of the system. In Figure 1 we have plotted some important reference curves S_{str} vs q for ideal exponential $f(\rho) = \exp(-\rho)$ and Gaussian $f(\rho) = \exp(-\rho^2)$ charge distributions.

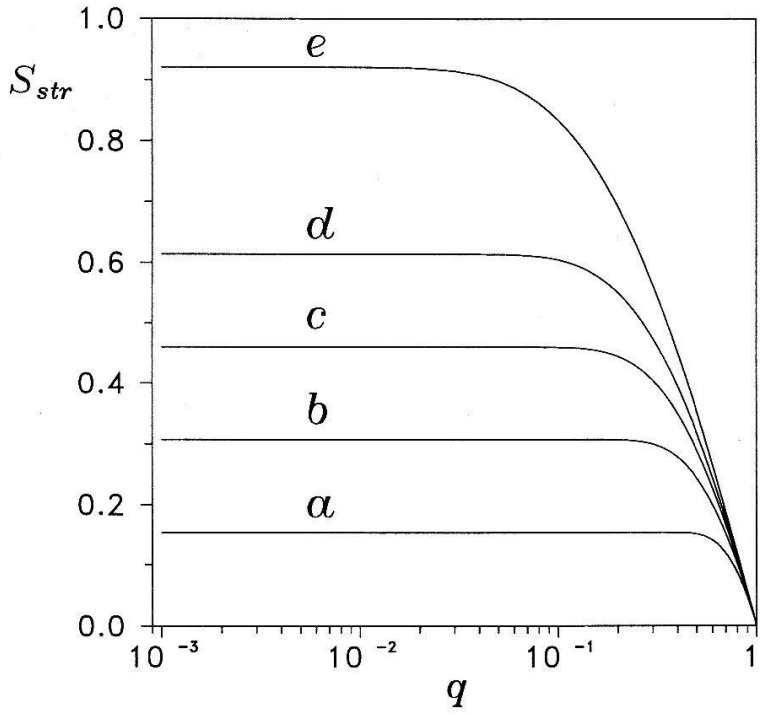

Figure 1. Structural entropy S_{str} vs spatial filling factor $q = L^{-1}/N$ for ideal decay forms. Curves labelled a, b, c are for Gaussian localization and the ones labelled b, d, e are for exponential localization in $d = 1, 2, 3$, respectively

The case of extreme localization corresponds to $q \to 0$ ($\xi/N \to 0$) which for exponential localization yields $S^0_{str} = d(1 - \ln 2)$ and for Gaussian localization $S^0_{str} = d(1 - \ln 2)/2$. The curves in Figure 1 are clearly separated and show that S_{str} is constant over a wide range of q in the regime $0 < q \ll 1$, i.e. with increasing system size N, localized wave functions do not change their characteristics when they occupy less then a certain amount of the system.

Therefore the value of q at which S_{str} approaches S^0_{str} with a desired tolerance Δ can be considered as a cutoff value q_c so that

$$S^0_{str} - S_{str}(q) \leq \Delta, \qquad \text{if} \qquad 0 < q \leq q_c, \tag{10}$$

where equality holds for $q = q_c$, from which by setting $\alpha = q_c^{-1}$ we obtain $L_c = \alpha/N$. Such a definition will provide different L_c values depending on the decay form and dimension d as long as the curves are different. Thus any state with IPR $L > L_c$ can be considered localized since then $q < q_c$ with $S_{str}(q) \approx S^0_{str}$.

decay form	$d=1$	$d=2$	$d=3$
exponential	9	51	237
Gaussian	3	9	22

Table 2. Parameter $\alpha = q_c^{-1}$ related to the cutoff localization index $L_c = \alpha/N$ for different kinds of localization in dimensions $d = 1$, 2, and 3 ($\Delta = 10^{-6}$).

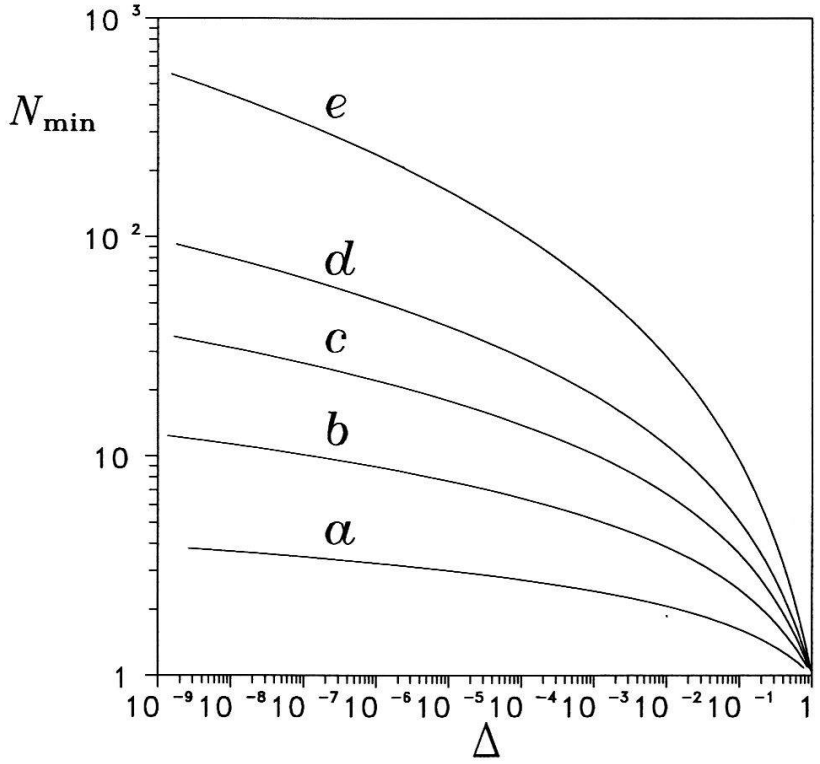

Figure 2. Minimum system size $N_{min} = \alpha$ versus the tolerance in the structural entropy $\Delta = 1 - S_{str}/S^0_{str}$, with $S^0_{str} = d(1 - \ln 2)/2$ for Gaussian localization and $S^0_{str} = d(1 - \ln 2)$ for exponential localization in dimensions $d = 1$, 2, and 3. Curves are labelled the same way as for Figure 1.

The results for $\Delta = 10^{-6}$ are listed in Table 2, and the comparison with former results is given in Table 1 for the case of three dimensional exponential localization. In addition, we have listed in Table 1 the relative deviation of the structural entropy compared to the $q \ll 1$ case $S^0_{str} = 3(1 - \ln 2)$. Note, that the desired tolerance Δ may be *a priori* set, which makes it possible to check the accuracy of numerical methods, for example. Previous results were obtained mainly based on numerical simulations, whereas our result is free of the choice of the model and numerical methods.

We have to mention, however, that the $L \leq L_c$ relation for a given eigenstate may hold for different kinds of localization, i.e. it does not *guarantee* the detection of, for example, exponential or Gaussian localization. The values given in Table 2 may serve as guides for the minimum size of the system one has to consider in order to be able to detect

states localized with a very short localization length. Our calculations show that the cutoff values listed in Table 2 correspond to localization lengths $\xi = N/4$ and $N/20$ for Gaussian and exponential localization, respectively.

Using our cutoff limits, a state extending over D sites can be safely identified as localized (with tolerance Δ) by considering a system of the minimum size $N = \alpha D$. It is true that the flatness of the $S_{str}(q)$ curves for $q \ll 1$ (Figure 1) indicates that a high accuracy in S_{str} requires a very large system to be considered. In Figure 2 we have plotted the minimum system size $N_{min} = \alpha$ one has to consider in order to detect wave functions extending over $D = 1$ sites with exponential and Gaussian localization with tolerance Δ.

4. Conclusions

As a summary we may conclude that the localization properties of the one–electron eigenstates may be described by matrix P_{ij} in site representation and by matrix $Q_{\mu\nu}$ in energy representation. These descriptions are unitary equivalent and may be used in various contexts emphasizing different features of the localized electronic systems. P_{ij}, in close relation to the Green's function $|G_{ij}(t)|^2$, is the essential tool for the phenomenological renormalization group study of these systems, while $Q_{\mu\nu}$ is very useful in connection to the localization index, the localization length and the spatial separation of the eigenstates. Due to this unitary equivalence real–space studies (return probabilities, renormalization, etc. (Refs. [1, 9, and 15])) and energy–dependent studies (localization index, IPR, neighborhood quantity, etc. (Refs. [3–8, 18, 19])) are expected to be mapped onto each other, therefore results obtained in site representation maybe compared with the ones obtained in energy representation and visa versa.

On the other hand, we have made use of the relation between the IPR and another fundamental quantity, the Shannon–entropy [21]. On the basis of this relation we have given different cutoff IPR values L_c for exponential and Gaussian localization in 1, 2, and 3 dimensional systems. These limits imply that in numerical calculations one has to consider very large systems (much larger than expected) in order to detect localization accurately (see Figure 2).

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