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Order indices of density matrices for finite systems

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ABSTRACT

The definition of order indices for density matrices is extended to finite systems. This makes it possible to characterize the level of ordering in such finite systems as macromolecules, nanoclusters, quantum dots, or trapped atoms. The general theory is exemplified by explicit calculations of the order index for the first-order density matrix of bosonic atoms confined in a finite box at zero temperature.

1. Introduction

We collaborated with John A. Coleman for 20 years, since 1990 till his death in 2010. Moreover, he was not merely our co-author, but during this time, he became our very close friend, with whom we spent many hours discussing various problems. We are keeping warmest memories of John and his wife Marie Jeanne. With great respect, we devote this paper to the memory of our friend and colleague John Coleman.

One of the interesting ideas, we developed with John Coleman, was the notion of the order indices for density matrices, introduced in Ref. [1]. The properties and applications of the order indices to different types of bulk matter, considered in thermodynamic limit, were studied in Refs. [2–5] and summarized in the book [6]. For infinite systems, however, it is possible to define the standard order parameters (see, e.g., [7,8]), because of which the use of the additional notion of the order indices could seem to be unnecessary. Nevertheless, as has been shown [1–3], the order indices are useful even for infinite systems, where a kind of mid-range order arises.

The principal difference of the order indices from the order parameters is that the former can be introduced not only for infinite systems, but also for finite systems. In recent years, the investigation of finite systems has become of high importance due to the widespread technological applications of various finite objects. As examples, we can mention quantum dots, metallic grains, different granular materials, nanoclusters, trapped atoms, and a variety of macromolecules, including biomolecules. For finite systems, as is well known, the order parameters are not defined [7,8]. In that case, the order indices can become principally important, as far as they can be defined for systems of any size. Then the order indices could characterize the amount of order specific for finite systems. It is the aim of the present paper to extend the definition and application of the order indices for finite systems.

In Section 2, we introduce the notion of order indices for arbitrary operators, which is specified for generalized density matrices in Section 3. The application to the usual reduced density matrices of statistical systems is given in Section 4, without invoking thermodynamic limit. In Section 5, we exemplify the consideration for bosonic atoms trapped in a finite box. Calculations for the order index of the first-order density matrix are given in Section 6, where the order index is treated as a function of the number of particles and of atomic interactions. Section 7 concludes.

2. Operator order indices

Order indices can be introduced for operators of any nature [9]. Let $\hat{A}$ be an operator acting on a Hilbert space $\mathcal{H}$. The operator is assumed to possess a norm $\|\hat{A}\|$ and a trace $\mathrm{Tr}\hat{A}$, with the trace taken over the space $\mathcal{H}$. In all other aspects, it can be arbitrary. The *operator order index* is

$$\omega(\hat{A}) \equiv \frac{\log \|\hat{A}\|}{\log |\mathrm{Tr}\hat{A}|}. \tag{1}$$

The logarithm can be taken with respect to any base, since $\log_a z = \log_b z/\log_b a$. This definition connects the norm and trace of the operator through the relation

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$$\|\widehat{A}\| = |\mathrm{Tr}\widehat{A}|^{\omega(\widehat{A})}. \tag{2}$$

An operator $\widehat{A}_1$ is said to be better ordered than $\widehat{A}_2$, if and only if

$$\omega(\widehat{A}_1) > \omega(\widehat{A}_2). \tag{3}$$

Respectively, two operators, $\widehat{A}_1$ and $\widehat{A}_2$ are equally ordered, provided that $\omega(\widehat{A}_1) = \omega(\widehat{A}_2)$.

The operator norm can be defined as a norm associated with the vector norm $|\varphi|$ for a nonzero vector $\varphi \in \mathcal{H}$, so that

$$\|\widehat{A}\| = \sup_{\varphi} \frac{|\widehat{A}\varphi|}{|\varphi|}. \tag{4}$$

Employing the scalar product (φ, φ) for defining the norm yields the Hermitian vector norm $|\varphi| \equiv \sqrt{(\varphi, \varphi)}$. The corresponding *Hermitian operator norm* is

$$\|\widehat{A}\| = \sup_{\varphi} \left[\frac{(\widehat{A}\varphi, \widehat{A}\varphi)}{(\varphi, \varphi)} \right]^{1/2} = \sup_{\varphi} \left[\frac{(\varphi, \widehat{A}^{+}\widehat{A}\varphi)}{(\varphi, \varphi)} \right]^{1/2}. \tag{5}$$

For an orthonormalized basis $\{\varphi_k\}$, labeled with an index k, in $\mathcal{H}$, such that

$$\mathcal{H} = \mathrm{Span}_k\{|\varphi_k\rangle\}, \tag{6}$$

the Hermitian norm (5) becomes

$$\|\widehat{A}\| = \sup_k [(\widehat{A}\varphi_k, \widehat{A}\varphi_k)]^{1/2}. \tag{7}$$

If the operator $\widehat{A}$ is self-adjoint, then its Hermitian norm simplifies to

$$\|\widehat{A}\| = \sup_{\varphi} \frac{|(\varphi, \widehat{A}\varphi)|}{|\varphi|} = \sup_k |(\varphi_k, \widehat{A}\varphi_k)|. \tag{8}$$

The eigenfunctions of a self-adjoint operator, defined by the eigenproblem

$$\widehat{A}\varphi_k = A_k\varphi_k,$$

form an orthogonal basis that can be normalized. The space basis can be chosen as the set of these eigenfunctions of the considered operator. Then the Hermitian norm becomes the *spectral norm*

$$\|\widehat{A}\| = \sup_k |A_k|. \tag{9}$$

When the operator is semi-positive, then $|A_k| = A_k$.

For a semi-positive operator,

$$\|\widehat{A}\| \leqslant \mathrm{Tr}\widehat{A} \qquad (\widehat{A} \geqslant 0).$$

Therefore, for such an operator,

$$\omega(\widehat{A}) \leqslant 1 \qquad (\widehat{A} \geqslant 0). \tag{10}$$

In that way, the order index (1) makes it possible to characterize the level of order in operators and to compare the operators as being more or less ordered. Instead of the Hermitian norm, one could employ some other types of operator norms, for instance, the trace norm [9]. But the use of the Hermitian norm is more convenient for physical and chemical applications.

3. Generalized density matrices

Self-adjoint operators play a special role in applications, defining the operators of observable quantities. One can resort to the coordinate representation, defining the physical coordinates through x, implying the set of all variables characterizing a particle. These can include Cartesian coordinates, spin, isospin, component-enumerating labels, and like that. The arithmetic space of all admissible values of the physical coordinates is denoted as $\mathcal{X} \equiv \{x\}$.

Let $\hat{A}(x)$ be an operator of a local observable from the algebra of local observables $\mathcal{A} \equiv \{\widehat{A}(x)\}$ given on the Fock space $\mathcal{F}$. And let $\mathcal{A}_\psi \equiv \{\hat{\psi}(x), \hat{\psi}^{\dagger}(x)\}$ be the algebra of field operators on $\mathcal{F}$, describing the system. The direct sum of these algebras is an *extended local algebra*

$$\mathcal{A}_{ext} \equiv \mathcal{A} \bigoplus \mathcal{A}_\psi. \tag{11}$$

The set $x^n \equiv \{x_1, x_2, \ldots, x_n\}$ of the coordinates of n particles pertains to the arithmetic space

$$\mathcal{X}^n \equiv \mathcal{X} \times \mathcal{X} \times \cdots \times \mathcal{X}$$

that is an n-fold tensor product. The differential measure on the above space $\mathcal{X}^n$ is defined as

$$dx^n \equiv dx_1 dx_2 \cdots dx_n.$$

A function $\varphi(x^n)$ can be treated as a vector

$$\varphi_n \equiv [\varphi(x^n)] \in \mathcal{H}_n \tag{12}$$

in a Hilbert space $\mathcal{H}_n$, where the scalar product is given by

$$\varphi_n^{+}\varphi_n \equiv \int \varphi^{*}(x^n)\varphi(x^n)dx^n. \tag{13}$$

We consider a quantum system, whose state is given by a statistical operator $\hat{\rho}$ being a semi-positive self-adjoint operator normalized as

$$\mathrm{Tr}_{\mathcal{F}}\hat{\rho} = 1 \qquad (\hat{\rho}^{+} = \hat{\rho} \geqslant 0). \tag{14}$$

Taking any representative $A(x)$ of the extended algebra (11), we can define a matrix

$$\widehat{D}_A^n \equiv [D_A(x^n, y^n)], \tag{15}$$

which is a matrix with respect to the variables x, with the components

$$\widehat{D}_A(x^n, y^n) \equiv \mathrm{Tr}_{\mathcal{F}} A(x_1)\ldots A(x_n)\hat{\rho}A^{+}(y_n)\ldots A^{+}(y_1). \tag{16}$$

The action of matrix (15) on vector (12) is defined as the vector with the components

$$\widehat{D}_A^n\varphi_n = \left[\int D_A(x^n, y^n)\varphi(y^n)dy^n \right]. \tag{17}$$

As is seen from construction, matrix (15) is self-adjoint and semi-positive, because of which it can be termed the generalized density matrix.

The norm of matrix (15) is defined as

$$\left\| \widehat{D}_A^n \right\| = \sup_{\varphi_n} \frac{\varphi_n^{+}\widehat{D}_A^n\varphi_n}{\varphi_n^{+}\varphi_n}. \tag{18}$$

And the trace of this matrix is

$$\mathrm{Tr}\widehat{D}_A^n \equiv \int D_A(x^n, x^n)dx^n. \tag{19}$$

The order index of the generalized density matrix (15) is given by the expression

$$\omega\left(\widehat{D}_A^n\right) \equiv \frac{\log \left\| \widehat{D}_A^n \right\|}{\log \left| \mathrm{Tr}\widehat{D}_A^n \right|}, \tag{20}$$

with the norm and trace defined as above.