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Scaling of nonlocal operators

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An exact scaling relation developed for nonlocal operators is presented. The matrix elements of a general nonlocal operator are related to a set of reduced matrix elements through scaling coefficients which do not *explicitly* depend on the particular nonlocal operator. The theory reduces to a conventional local scaling formulation in that limit. The guide to developing the nonlocal scaling relation comes from consideration of general symmetry properties of the nonlocal operator in a chosen representation. Operators with high degrees of symmetry will generally lead to scaling relations requiring a small number of scaling coefficients for practical applications. The theory is expected to be useful not only for providing exact nonlocal scaling relations but also as a tool for developing approximate scaling relations which still retain the nonlocal nature of the operator to an appropriate extent.

I. INTRODUCTION

Recently, there have been extensive studies on scaling theories which establish a linear relation between matrix elements of a desired operator and a reduced number of independent (input) matrix elements.[1-17] Most quantum-mechanical expressions for physical observables involve large numbers of matrix elements including cases where sums or averages over the quantum states enter.[18] Thus, the reduction of computational effort implied by scaling can be important in many quantum mechanical calculations where obtaining large numbers of matrix elements is often one of the most time consuming steps. Furthermore, scaling may also be applied to inversion problems where fundamental quantities such as the potential or rate-constant matrices are sought from a set of appropriate experimental observables.[9] In molecular dynamics, scaling relations were first found within the infinite-order sudden approximation[1] and an energy-corrected sudden scaling theory.[2] These techniques have been applied quite successfully to a number of dynamics problems such as the calculation of state-to-state cross sections,[6] the inversion of experimental relaxation data,[9] and the modeling of experiments.[10] A similar scaling idea was also proposed for the calculation of multicenter molecular integrals[15] and for classical observables averaged over phase space.[16]

The scaling theory developed thus far has been mainly restricted to local operators which are multiplicative and diagonal in the chosen representation (usually coordinate space).[1-8] For example, the T-matrix operator in the sudden approximation is local and multiplicative in the internal coordinate space. For such local operators, a scaling relation is found by expanding either the operator or a product of the matrix element wave functions in terms of a complete set of basis functions with an appropriate weighting factor.[2] Then, an entire set of matrix elements can be related to a smaller set of fundamental elements which often correspond to a column (or row) of the original matrix. The scaling coefficients relating various matrix elements to the fundamental elements have been referred to as "spectroscopic,"[1] since they are independent of operator, and therefore they can be calculated once and used for many different operators. The latter property is very important with regard to the practical use of scaling theory, and the scaling theory for nonlocal operators presented in this paper essentially retains this feature.

Many quantum-mechanical operators are inherently nonlocal and therefore are not multiplicative or diagonal in the representation chosen for study.[2,19] Only a few examples of such nonlocal operators are the transition operator (T- or S-matrix operator) in scattering theory and optical spectroscopy,[19] the exchange operator in molecular structure theory,[20,21] Green's functions,[22] and optical potentials.[23] In spite of the richness and importance of nonlocal operators in quantum mechanics, there has been little work on scaling theory which is applicable directly to this class of operators. Instead, a nonlocal operator is often approximated as a local operator (e.g., by using the sudden approximation for the collision transition operators) after which the local scaling technique is applied. Recently, Eno[17] has proposed an exact scaling relation which is capable of treating nonlocal operators. In this technique, a new arbitrary operator is introduced and the matrix of the desired operator is related to the set of matrix elements of the new operator through scaling coefficients which explicitly depend not only on the original operator but also on the new operator introduced in the scaling process. A judicious choice of the extra operator is critical and further study on the convergence behavior is necessary. Because of the complexity of the scaling coefficients, this approach may be useful as a tool for finding approximate scaling relations rather than as an exact scaling relation. The formulation in the present paper, however, avoids any explicit dependence upon the desired operator in the scaling coefficients.

The new approach in this paper for developing an exact scaling relation for a nonlocal operator is based on exploiting any available symmetry properties of the operator in a representation of choice. The notion of the symmetry here is quite general and encompasses any simplifying features of the operator. We thus construct an exact non-

local scaling relation based on utilizing this symmetry to transform the problem into a natural set of variables, which are better able to describe the nonlocal operator. For example, sum and difference variables form a natural choice of variables in many contexts[24] and their use leads to an immediate simplification. In particular, a local operator is a special case of a nonlocal one expressed in these variables. Therefore, we attempt to maximize the use of symmetry of the nonlocal operator to find an exact scaling relation in which the entire set of matrix elements of the nonlocal operator is related to a reduced set of appropriate matrix elements through scaling coefficients which do not explicitly depend on the particular operator. However, the scaling coefficients will generally contain information on the symmetry aspects of the operator. In some cases, it is expected that there may be a significant operational savings achieved by using scaling relations developed in this fashion. It is also expected that these scaling relations may be useful for developing further approximate scaling relations which retain the nonlocal nature of the operator to an appropriate extent.

Section II first briefly summarizes local scaling theory and casts it in a more general form parallel to the nonlocal theory to follow. A presentation is then given of the general concepts behind nonlocal operator scaling. The reduction of the nonlocal scaling relation to local scaling is demonstrated along with an analysis of other special forms of nonlocal operator. In Sec. III, the exact nonlocal scaling relation is applied to the matrix elements of nonlocal operators expressed in terms of harmonic oscillator wave functions. Some concluding remarks are presented in Sec. IV.

II. A SCALING RELATION FOR NONLOCAL OPERATORS

In this section, we present the general concepts needed for the scaling of nonlocal operators. First, we will briefly review and extend the relevant aspects of local scaling theory[5] in order to provide the background to the nonlocal developments. The reduction of the nonlocal scaling relation to special cases will also be discussed.

A. Local operators: Further perspectives

A matrix element of a local operator $A(\mathbf{x})$ is given as

$$A_{ij}=\int_{\Omega_x}\phi_i^*(\mathbf{x})A(\mathbf{x})\phi_j(\mathbf{x})d\mathbf{x}\ , \tag{1}$$

where $\{\phi_i(\mathbf{x})\}$ are the basis functions and Ω_x is the domain of integration for $\mathbf{x}$. The vector $\mathbf{x}$ can be of arbitrary dimension and may be associated with any appropriate space (e.g., coordinate or momentum space). Now, we consider a new variable

$$\mathbf{y}=\mathbf{y}(\mathbf{x}) \tag{2}$$

and an (orthonormal) complete set $\{\psi_i(\mathbf{y})\}$. Here, the transformation between $\mathbf{x}$ and $\mathbf{y}$ must be unique and invertible. The choice of $\mathbf{y}$ should be made to better reflect the structure of the operator $A(\mathbf{x})$. By expanding the operator $A(\mathbf{x})$ in terms of $\{\psi_i(\mathbf{y})\}$ with the appropriate weighting factor $[\psi_0(\mathbf{y})]^{-1}$,

$$A(\mathbf{x})=\sum_k \tilde{A}_{k0}\psi_k(\mathbf{y})/\psi_0(\mathbf{y})\ , \tag{3}$$

we can easily find the following scaling relation:

$$A_{ij}=\sum_k \tilde{I}_{ij,k}\tilde{A}_{k0}\ , \tag{4}$$

where $\tilde{A}_{k0}$ is the matrix element of A in the new basis set $\{\psi_i(\mathbf{y})\}$

$$\tilde{A}_{k0}=\int_{\Omega_y}\psi_k^*(\mathbf{y})A(\mathbf{x})\psi_0(\mathbf{y})d\mathbf{y}\ , \tag{5}$$

and $\tilde{I}_{ij,k}$ is the scaling coefficient given as

$$\tilde{I}_{ij,k}=\int_{\Omega_x}\phi_i^*(\mathbf{x})\frac{\psi_k(\mathbf{x})}{\psi_0(\mathbf{y})}\phi_j(\mathbf{x})d\mathbf{x}\ . \tag{6}$$

Here, the function $\psi_0(\mathbf{y})$ is nodeless,[25] usually corresponding to a ground-state function of the set $\{\psi_i(\mathbf{y})\}$. The scaling relation in Eq. (4) can be obtained equivalently by expanding the product of basis functions $\phi_i^*(\mathbf{x})\phi_j(\mathbf{x})$,

$$\phi_i^*(\mathbf{x})\phi_j(\mathbf{x})=\sum_k \tilde{I}_{ij,k}\psi_k^*(\mathbf{y})\psi_0(\mathbf{y})/|J_1| \tag{7}$$

and directly substituting Eq. (7) into Eq. (1) with $J_1=\partial\mathbf{x}/\partial\mathbf{y}$ being the Jacobian for the transformation from $\mathbf{x}$ to $\mathbf{y}$. The local scaling formula in Eq. (4) is an exact relation and no approximation is involved. As evident from Eq. (6), the scaling coefficients are entirely independent of the form of the operator $A(\mathbf{x})$ and therefore they can be calculated once and used as needed for many different operators. However, it is also evident from Eq. (6) that $\{\psi_i(\mathbf{y})\}$ and hence $\{\tilde{I}_{ij,k}\}$ should generally reflect the properties of $A(\mathbf{x})$ and/or the product set $\{\phi_i^*(\mathbf{x})\}\times\{\phi_j(\mathbf{x})\}$. The scaling relation in Eq. (4) has some similarity to the Wigner-Eckart theorem although a fundamental difference is apparent through the presence of the summation. Equation (4) can also be interpreted as the result of generalized Fourier expansions through either Eqs. (3) or (7). The utility of the scaling relation is critically dependent on the convergence of these generalized Fourier expansions as well as the spectroscopic nature of the scaling coefficients. It has been shown that the expansion of Eq. (4) in many cases is finite because of the nature of the scaling coefficients, and thus a significant operational savings is possible. This local scaling relation has been successfully applied to problems in which nonlocal operators (e.g., the transition operator T) are first approximated as local operators by using dynamical simplifications such as the sudden approximation.[5–13]

A significant point with regard to the nonlocal operator discussion below concerns the introduction of the transformation of variables in Eq. (2) and the use of the new basis $\{\psi_i(\mathbf{y})\}$. Traditional local scaling theory has not involved either of these operations. The introduction of the transformation in Eq. (2) should be viewed as being performed to take advantage of the natural variable dependence (i.e., a symmetry in the sense used for nonlocal scaling below) of the operator A. Similarly the use of the set $\{\psi_i(\mathbf{y})\}$ is suggested in order to best span the space of the transformed operator or the wave function product

in Eq. (7). These generalizations of local scaling theory result in the relation of Eq. (4) between the matrix elements of A in the original basis $\{\phi_i(\mathbf{x})\}$ and a column of the matrix in the basis $\{\psi_i(\mathbf{y})\}$. Although this is not the traditional form of local scaling theory, the added complication is minimal. Furthermore, the generalization extends the utility of local scaling theory as well as provides a critical springboard for the nonlocal scaling below.

B. Nonlocal operators

In contrast to Eq. (1), a matrix element of a nonlocal operator $B(\mathbf{x},\mathbf{y})$ takes on the following form,

$$B_{ij}=\int_{\Omega_x}\int_{\Omega_y}\phi_i^*(\mathbf{x})B(\mathbf{x},\mathbf{y})\phi_j(\mathbf{y})d\mathbf{x}\,d\mathbf{y}\ . \tag{8}$$

A nonlocal operator B is not multiplicative or diagonal in a chosen representation, and it may include differential operators. The technique used for scaling local operators is not directly applicable in the present case, although a generalized procedure will now be developed. Guidance in this matter can first be obtained by some qualitative observations. Based on the common local approximation $B(\mathbf{x},\mathbf{y})\approx B(\mathbf{x})\delta(\mathbf{x}-\mathbf{y})$ and more general considerations,[24] one might expect a dominant region of significance for $B(\mathbf{x},\mathbf{y})$ to be in the vicinity of $\mathbf{x}\approx\mathbf{y}$. Other special cases could have different behavior, and the first step in achieving a nonlocal scaling is an examination of $B(\mathbf{x},\mathbf{y})$ for any evident structure as a function of $\mathbf{x}$ and $\mathbf{y}$. Such structure will imply the existence of a natural set of variables which best describes the nature of the operator. Thus, it is possible to choose a set of new variables, $(\mathbf{u},\mathbf{v})$:

$$\mathbf{u}=\mathbf{u}(\mathbf{x},\mathbf{y})\ , \tag{9a}$$

$$\mathbf{v}=\mathbf{v}(\mathbf{x},\mathbf{y})\ . \tag{9b}$$

Here, $\mathbf{u}$ and $\mathbf{v}$ must be linearly independent and the transformation between $(\mathbf{x},\mathbf{y})$ and $(\mathbf{u},\mathbf{v})$ must be unique and invertible. It was noted in the local scaling approach of subsection A that it is also possible to introduce a new variable in similar fashion [see Eq. (2)]. In terms of the new set of variables, the matrix element in Eq. (8) can be rewritten as

$$B_{ij}=\int_{\Omega_u}\int_{\Omega_v}\tilde{\phi}_i^*(\mathbf{u},\mathbf{v})\tilde{B}(\mathbf{u},\mathbf{v})\tilde{\phi}_j(\mathbf{u},\mathbf{v})\,|J|\,d\mathbf{u}\,d\mathbf{v}\ , \tag{10}$$

where $\{\tilde{\phi}_i\}$ and $\tilde{B}$ signify the new functional forms of $\{\phi_i\}$ and B in terms of $(\mathbf{u},\mathbf{v})$, respectively, and $J=\partial(\mathbf{x},\mathbf{y})/\partial(\mathbf{u},\mathbf{v})$ is the Jacobian for the transformation from $(\mathbf{x},\mathbf{y})$ to $(\mathbf{u},\mathbf{v})$. In many problems it is anticipated that a dominance will arise with respect to one or other of the variables $(\mathbf{u},\mathbf{v})$ (e.g., this occurs in the near local operator limit using sum and difference variables), and this behavior can be utilized to simplify the evaluation of the integral in Eq. (10). The basis of the nonlocal scaling technique presented below rests on taking advantage of the existence of a set of natural variables $(\mathbf{u},\mathbf{v})$. The choice of variables would depend not only on the structure of a nonlocal operator but also on the basis set used to calculate the matrix elements. As will be discussed later, the judicious choice of this set is critical for this scaling technique and the possibility of such a choice largely depends on the symmetry of the given nonlocal operator.

In terms of the natural variables $(\mathbf{u},\mathbf{v})$, the operator B (or $\tilde{B}$) is expected to have simpler behavior. Indeed, the choice of $(\mathbf{u},\mathbf{v})$ would largely be guided by seeking such simplifying characteristic behavior. With these comments in mind, we assume the existence of an appropriate complete set of function $\{\eta_i(\mathbf{u})\}$ and $\{\xi_i(\mathbf{v})\}$ which span the domain encompassed by $\mathbf{u}$ and $\mathbf{v}$, respectively.[26] In terms of these functions, $\tilde{B}$ may be expressed as

$$\tilde{B}(\mathbf{u},\mathbf{v})\equiv B(\mathbf{x},\mathbf{y})=\sum_{kl}b_{kl}\eta_k(\mathbf{u})\xi_l^*(\mathbf{v})/[\eta_0(\mathbf{u})\xi_0^*(\mathbf{v})]\ , \tag{11}$$

where $\{b_{kl}\}$ are constant expansion coefficients and $\eta_0(\mathbf{u})$ and $\xi_0(\mathbf{v})$ form nodeless weight functions in the same sense as arose in Eq. (3) for local scaling.[25] The introduction of complex conjugates into Eq. (11) is for convenience and other equivalent choices could as well be made. Since the variables $(\mathbf{u},\mathbf{v})$ and functions $\{\eta_i(\mathbf{u})\}$ and $\{\xi_i(\mathbf{v})\}$ are "natural" for the system, we expect the expansion in Eq. (11) for $\tilde{B}$ not to contain a large number of terms. This is precisely the argument one would put forth for the choice of $\{\psi_i(\mathbf{y})\}$ for the local case in Eq. (4). Assuming the chosen functions are orthonormal, $\langle\eta_i\,|\,\eta_j\rangle=\delta_{ij}$ and $\langle\xi_i\,|\,\xi_j\rangle=\delta_{ij}$, we may readily identify the coefficients,

$$b_{kl}=\int_{\Omega_u}\int_{\Omega_v}\eta_k^*(\mathbf{u})\xi_0^*(\mathbf{v})\tilde{B}(\mathbf{u},\mathbf{v})\eta_0(\mathbf{u})\xi_l(\mathbf{v})d\mathbf{u}\,d\mathbf{v}\ . \tag{12}$$

Substitution of Eq. (11) into Eq. (10) will finally yield the desired scaling relation,

$$B_{ij}=\sum_{kl}I_{ij,kl}b_{kl}\ , \tag{13}$$

where

$$I_{ij,kl}=\int_{\Omega_u}\int_{\Omega_v}\tilde{\phi}_i^*(\mathbf{u},\mathbf{v})\frac{\eta_k(\mathbf{u})\xi_l^*(\mathbf{v})}{\eta_0(\mathbf{u})\xi_0^*(\mathbf{v})}\tilde{\phi}_j(\mathbf{u},\mathbf{v})\,|J|\,d\mathbf{u}\,d\mathbf{v}\ . \tag{14}$$

In parallel with local operator scaling, it is significant to point out that the scaling relation in Eq. (13) may equally be derived from expanding the product function $\phi_i^*(\mathbf{x})\phi_j(\mathbf{y})$ in Eq. (10) in terms of the same set of new functions introduced above:

$$\phi_i^*(\mathbf{x})\phi_j(\mathbf{y})=\sum_{kl}I_{ij,kl}\eta_k^*(\mathbf{u})\eta_0(\mathbf{u})\xi_0^*(\mathbf{v})\xi_l(\mathbf{v})/|J|\ . \tag{15}$$

Direct substitution of this expansion into Eq. (8) will again lead to the scaling relation in Eq. (13). The scaling coefficients in Eq. (14) and the reduced matrix elements in Eq. (12) may be calculated analytically if possible, or numerically. The above nonlocal scaling relation is exact and there is no approximation involved. It shows that a matrix element B_{ij} can be expressed in terms of the scaling coefficients $\{I_{ij,kl}\}$ and reduced matrix elements $\{b_{kl}\}$. Notice that the scaling coefficients do not *explicitly* depend on the operator B. In cases of related sets of operators, for which the same set of natural variables $(\mathbf{u},\mathbf{v})$ and basis sets $\{\eta_i(\mathbf{u})\}$ and $\{\xi_i(\mathbf{v})\}$ can be used, it should be possible to treat $\{I_{ij,kl}\}$ as spectroscopic in the same sense as for local scaling.

The utility of the above nonlocal scaling relation would depend on the ease of calculating the scaling coefficients and the reduced matrix elements. It would also depend on the speed of convergence of the expansion in Eq. (13). As mentioned before, one of the major goals of the scaling approach is the achievement of a significant operational savings for the calculation of matrix elements. Evidently, there would be no operational savings if we need as many reduced matrix elements $\{b_{kl}\}$ as the original matrix elements $\{B_{ij}\}$. The essence of finding the symmetry of $B(\mathbf{x},\mathbf{y})$ leading to Eq. (13) indicates that there will generally be fewer reduced elements than in the original set. This point is especially clear if $\widetilde{B}$ is exactly expressed, or reasonably well approximated, in terms of a finite set of product functions,

$$\widetilde{B}(\mathbf{u},\mathbf{v})=\sum_{m=1}^{M}\alpha_m(\mathbf{u})\beta_m(\mathbf{v})\ . \tag{16}$$

Then, a reduced matrix element b_{kl} can be written as

$$b_{kl}=\sum_{m=1}^{M}(\alpha_m)_{k0}(\beta_m)_{0l}\ , \tag{17}$$

where

$$(\alpha_m)_{k0}=\int_{\Omega_u}\eta_k^*(\mathbf{u})\alpha_m(\mathbf{u})\eta_0(\mathbf{u})d\mathbf{u}\ , \tag{18a}$$

$$(\beta_m)_{0l}=\int_{\Omega_v}\xi_0^*(\mathbf{v})\beta_m(\mathbf{v})\xi_l(\mathbf{v})d\mathbf{v}\ . \tag{18b}$$

These two reduced matrices have exactly the same forms as the reduced matrices entering into the local scaling theory of Eq. (4). We can calculate $(\alpha_m)_{k0}$ and $(\beta_m)_{0l}$ separately and combine them together as necessary to construct a reduced matrix b_{kl}. This separability of the reduced matrix elements can lead to a significant operational savings for the nonlocal scaling approach. For example, suppose we desire to calculate the $N\times N$ matrix $\{B_{ij}\}$ and we need a $K\times K'$ matrix of reduced elements $\{b_{kl}\}$. If Eq. (17) holds, only KM and $K'M$ matrix elements of α_m and β_m, respectively, would be necessary. When M is small enough and K and K' is not too large compared to N, the operational savings by using this scaling technique can be significant. It should now be clear that, if a nonlocal operator has some degree of symmetry, Eq. (13) can be useful as an exact scaling relation with a potential for significant operational savings.

The exact scaling relation Eq. (13) can also be used as a tool for finding approximate nonlocal scaling relations taking into account the nonlocal nature of the operator to an appropriate extent. For example, we may approximate $\widetilde{B}(\mathbf{u},\mathbf{v})$ if it is a slowly varying function of one of the variables. This possibility is evident in the form of Eq. (17). In addition, it may also be possible to approximate the scaling coefficients $\{I_{ij,kl}\}$ in some problems.

At this point, some discussion on special cases is appropriate. The choice of variables $(\mathbf{u},\mathbf{v})$ was arbitrary above, but a commonly expected case[24] consists of sum and difference variables

$$\mathbf{u}=(\mathbf{x}+\mathbf{y})/2\ , \tag{19a}$$

$$\mathbf{v}=(\mathbf{x}-\mathbf{y})/2\ . \tag{19b}$$

Furthermore, many cases may be dominated by a strong dependence on $\mathbf{v}$ and a weak dependence on $\mathbf{u}$. A Green's function $G(\mathbf{x}-\mathbf{y})$ is clearly an extreme example with dependence only on $\mathbf{v}$. Under these latter conditions, the analysis based on Eq. (17) is quite simple with $M=1$. The choice of variables in Eq. (19) is also natural in momentum (or quantum number) space from semiclassical arguments again leading to a suggested weak dependence on $\mathbf{u}$ over that of $\mathbf{v}$.

The nonlocal scaling relation in Eq. (13) reduces to local scaling when the nonlocal operator $B(\mathbf{x},\mathbf{y})$ can be written as

$$B(\mathbf{x},\mathbf{y})=A(\mathbf{x})\delta(\mathbf{x}-\mathbf{y})\ , \tag{20}$$

where $A(\mathbf{x})$ is a local operator, and clearly in this limit $B_{ij}=A_{ij}$. This limit corresponds to the sudden approximation for the transition operator in dynamics problems.[1,2] A nonlocal operator of this form can be also viewed as a simple separable case in Eq. (17) with $\alpha(\mathbf{u})=A((\mathbf{x}+\mathbf{y})/2)$, $\beta(\mathbf{v})=\delta(\mathbf{x}-\mathbf{y})$, and $M=1$. Thus, it is understandable from the above discussion on matrix dimensionality issues for the nonlocal scaling relations how the local scaling limit can achieve such significant operational savings. In this case, we choose $(\mathbf{u},\mathbf{v})$ in Eq. (19) and $\{\phi_i\}=\{\eta_i\}=\{\xi_i\}$. Then, a reduced matrix element is expressed as

$$b_{kl}=\phi_0^*(0)\phi_l(0)A_{k0}\ . \tag{21}$$

The local scaling relation in Eq. (4) with $\{\phi_i\}=\{\psi_i\}$ and $\mathbf{y}=\mathbf{x}$ is readily obtained by substituting Eq. (21) into Eq. (13) and the use of the closure relation as well as the fact that $\widetilde{\phi}_i(\mathbf{u},\mathbf{0})=\phi_i(\mathbf{x})$.

Another interesting special case of nonlocal operator scaling occurs when the nonlocal operator takes on the following form,

$$B^{mn}(\mathbf{x},\mathbf{y})=\phi_m(\mathbf{x})D(\mathbf{x},\mathbf{y})\phi_n^*(\mathbf{y})\ , \tag{22}$$

where $\phi_m(\mathbf{x})$ and $\phi_n^*(\mathbf{y})$ are members of the same basis set used in Eq. (8) and $D(\mathbf{x},\mathbf{y})$ can be an arbitrary operator. In this case, because of the presence of $\phi_m(\mathbf{x})$ and $\phi_n^*(\mathbf{y})$ in the operator, its scaling relation involves double application of the local scaling relation in Eq. (4) for $\mathbf{x}$ and $\mathbf{y}$ separately.[15] It is noted that $D(\mathbf{x},\mathbf{y})$ is independent of m and n. All two-electron integrals in molecular structure calculations belong to this category with $D(\mathbf{x},\mathbf{y})=1/|\mathbf{x}-\mathbf{y}|$[15]. Other special cases may also arise in various areas of quantum mechanics, with each having its own particular features.

III. AN EXAMPLE WITH HARMONIC OSCILLATOR FUNCTIONS

As an example of the exact nonlocal scaling relation in Eq. (13), we consider a case in which $\{\phi_i\}=\{\eta_i\}=\{\xi_i\}$ are harmonic oscillator basis functions in one dimension. We choose the sum and difference variables in Eq. (19) because the harmonic oscillator basis sets can be easily manipulated with this variable transformation. At this point the form of the operator $B(\mathbf{x},\mathbf{y})\equiv\widetilde{B}(\mathbf{u},\mathbf{v})$ will be taken as *arbitrary*. In order to implement the scaling relation in Eq. (13), we first need to calculate the scaling coef-

TABLE I. Computational operation counts for nonlocal scaling using Eq. (23).

Operator $\tilde{B}(\mathbf{u},\mathbf{v})$	Reduced matrix type	Operation count	Ratio[a]
General[b]	b_{kl}	$2N^2$	2
$\sum_{m=1}^{M}\alpha_m(\mathbf{u})\beta_m(\mathbf{v})$	$(\alpha_m)_{k0}$ and $(\beta_m)_{0l}$	$4NM$	$4M/N$
$\alpha(\mathbf{u})\beta(\mathbf{v})$	α_{k0} and β_{0l}	$4N$	$4/N$
$\alpha(\mathbf{u})$ or $\beta(\mathbf{v})$	α_{k0} or β_{0l}	$2N$	$2/N$

[a]Ratio of the operation counts in scaling approach to the number of original elements, N^2.
[b]An operator having no evident symmetry.

ficients $\{I_{ij,kl}\}$ in Eq. (14). By using the generating function for Hermite polynomials,[27] we can readily obtain the analytic expression for the scaling coefficient $\{I_{jk,kl}\}$:

$$I_{ij,kl}=\left[\frac{\pi k!l!}{i!j!2^{i+j+k+l}}\right]^{1/2}\sum_r(-1)^{i+k}a^i_{k+r}a^j_{l-r}J_{klr} \tag{23a}$$

for $i+j\geq k+l$ and $i+j+k+l$=even, and otherwise

$$I_{ij,kl}=0\ . \tag{23b}$$

In Eq. (23a), the symbol J_{klr} is

$$J_{klr}=\sum_q(-1)^q\begin{bmatrix}k+r\\ q\end{bmatrix}\begin{bmatrix}l-r\\ k-q\end{bmatrix} \tag{24}$$

and a^i_k is given by the following recursion relation,

$$a^i_k=2a^{i-1}_{k-1}+(i+1)a^{i-1}_{k+1} \tag{25}$$

with $a^0_0=1$ and $a^i_p=a^j_{i+p}=0$ for $p>0$. In the above equations, the summations are over all possible values of the indices. In practice, tables of $\{J_{klr}\}$ and $\{a^i_k\}$ can be prepared first and stored to be used for construction of the scaling coefficients $\{I_{ij,kl}\}$. Implementation of Eq. (23a) is then very efficient. Since B was arbitrary here, it is clearly evident that the scaling coefficients have no explicit dependence on the operator.

In Table I, we summarize the computational operation counts in the scaling approach for calculating a $N\times N$ matrix of various types of nonlocal operators with harmonic oscillator basis functions. Since the scaling coefficients in Eq. (23) are spectroscopic, the operation counts include only the effort (i.e., the number of independent matrix elements) for calculating the reduced matrix $\{b_{kl}\}$. The scaling expansion in Eq. (13) is finite because of Eq. (23b) and we only need to calculate the reduced matrix elements $\{b_{kl}\}$ for $k+l\leq 2N$. As evident from Table I, there is no operational savings achieved by the scaling approach for a nonlocal operator with no distinct symmetry. On the other hand, if the operator can be expressed as a function of only $\mathbf{u}$ or $\mathbf{v}$, there is clearly a dramatic operational savings in the scaling approach. In fact, this limit includes the local operator case for which the advantage of the scaling approach has been demonstrated through various practical application. Table I also shows that there are other cases where we can achieve significant operational savings through the nonlocal scaling approach, while the nonlocal nature of the operator is still retained to an appropriate extent. The magnitude of the operational savings depends largely on the degree of symmetry in the nonlocal operator.

IV. CONCLUDING REMARKS

We have presented the general concepts needed to establish exact nonlocal scaling relations. The procedure rests on the ability to identify any meaningful systematic behavior of the nonlocal operator in a chosen representation. If no symmetries in this sense can be found, then there is nothing to be gained by scaling. On the other hand, most physical problems are expected to have varying degrees of symmetry and thus result in a concomitant savings through scaling. In this sense, local behavior represents an extremely high order of symmetry. By using a set of natural variables which best characterizes the nature of the nonlocal operator, it is possible to relate an entire set of nonlocal matrix elements to a reduced set of matrix elements through scaling coefficients. The scaling coefficients suggested in this paper maintain their spectroscopic nature, although they depend implicitly on the structure of the operator as well as the nature of basis set through the choice of a set of natural variables. However, we also point out that these same comments apply to the general form of the local scaling relation in Eq. (4).

Three broad general applications can be envisioned for the scaling theory presented in this paper. First, if the operator B is explicitly known beforehand, then the necessary symmetry analysis discussed above may be carried forth. Each operator will have to be evaluated on its own merit with respect to the degree that it can be scaled. In this regard, approximations of the operator, scaling coefficients, or reduced matrix elements should also be considered when appropriate. The second class of scaling applications arises for solving the Schrödinger equation. As a specific application, we could consider the integral equation formulation where matrix elements of the transition operator T represent the solution. Since the exact form of T is not known beforehand, an ansatz needs to be made. A general scaling theory ansatz for T_{ij}, as in Eq. (11), involves no approximation, but this approach is likely not to lead to a simplification of the computational effort. A more fruitful approach would consist of making an ansatz on the symmetry structure for T and then proceed by using this in the Lippmann-Schwinger equation to calculate

the hopefully smaller number of reduced T-matrix elements.[24] For example, the well established reference form of a local T operator with a (weak) nonlocal correction in Eq. (17) could be proposed for analysis.

Finally, the third broad application would be to problems in the inversion of appropriate experimental data back to more fundamental underlying information. If sufficient data were available, one might try to scale the local or nonlocal (including optical potentials) potential operator in order to reduce the number of unknowns to a minimal level. More typically, such extensive data will not be available, but inversion of a more modest extent may still be possible. This notion has been central to recent efforts at inverting various types of relaxation data back to more fundamental collisional rate constants.[9] Thus far, the energy-corrected sudden scaling theory has been the principal tool employed for this purpose. The energy-correcting aspect of the scaling is an attempt to go beyond the local nature of the sudden approximation transition operator. There is clearly room for more systematic development of hierarchical approximate dynamical scaling relations, and the formulations presented here could provide such an approach. In particular, again a (simplified) nonlocal scaling ansatz would be made with the reduced matrix elements now established by fitting the experimental data. There are surely other applications beyond those listed here, and only further work will elucidate this matter.

In summary, we have shown that a significant operational savings can be achieved depending on the symmetry of the nonlocal operator as well as the nature of the basis set. Thus, the approach can be useful for providing an exact scaling relation for those nonlocal operators with high degrees of symmetry. In addition, the rigorous nonlocal scaling theory can also be useful as a tool for developing approximate scaling relations by studying the nature of the nonlocal operators in their natural variable space.

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