

## Exact Tensor Hypercontraction: A Universal Technique for the Resolution of Matrix Elements of Local Finite-Range $N$ -Body Potentials in Many-Body Quantum Problems

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Configuration-space matrix elements of  $N$ -body potentials arise naturally and ubiquitously in the Ritz-Galerkin solution of many-body quantum problems. For the common specialization of local, finite-range potentials, we develop the exact tensor hypercontraction method, which provides a quantized renormalization of the coordinate-space form of the  $N$ -body potential, allowing for a highly separable tensor factorization of the configuration-space matrix elements. This representation allows for substantial computational savings in chemical, atomic, and nuclear physics simulations, particularly with respect to difficult “exchangelike” contractions.

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The physics of many-body quantum systems is often captured by local, finite-range  $N$ -body potentials  $\hat{V}(\mathbf{x}_1, \dots, \mathbf{x}_N)$ , where  $\mathbf{x}$  is any convenient parametrization of the physical space, e.g., position space ( $\mathbf{x} \equiv \mathbf{r}$ ) or momentum space ( $\mathbf{x} \equiv \mathbf{k}$ ). Given some real, finite, one-particle Ritz-Galerkin basis set  $\{\psi_i(\mathbf{x})\}$ , the configuration-space representation of  $\hat{V}$  is the integral tensor

$$\begin{aligned} &\langle i \dots n | \hat{V} | i' \dots n' \rangle \\ &= \int d\mathbf{x}_1 \cdots \int d\mathbf{x}_N \psi_i(\mathbf{x}_1) \cdots \psi_n(\mathbf{x}_N) \hat{V}(\mathbf{x}_1, \dots, \mathbf{x}_N) \\ &\quad \times \psi_{i'}(\mathbf{x}_1) \cdots \psi_{n'}(\mathbf{x}_N). \end{aligned} \quad (1)$$

The generation, manipulation, and storage of this tensor is a major hurdle in many-body quantum simulations. In order to overcome the computational difficulties inherent to such high order tensors, it is common to introduce simplifying approximations. For example, the Slater approximation [1] has been applied to reduce the numerical expense of treating exchange terms involving the local, two-body Coulomb potential. Unfortunately, such approximations can fail, as exemplified by the often spectacular self-interaction errors induced by local approximations to exchange interactions [2]. Another canonical example is nuclear density functional theory (DFT), where the need for computational savings is the main driver for the continued usage of energy density functionals (EDFs) derived from the zero-range Skyrme-like pseudopotential [3], in spite of severe problems at both two- and three-body levels [4,5]. At the two-body level, even EDFs derived from the finite-range Gogny pseudopotential [6] (which avoids some of the limitations of Skyrme functionals [7]) contain the same phenomenological density-dependent terms recently shown to cause the collapse of all beyond-mean-field methods [8–11].

Removing density-dependences in the EDF, however, would require introducing explicit finite-range three-body forces, which pose a serious computational challenge with current technology. Thus, it is clear that an improved algorithm for faithful and direct treatment of arbitrary local  $N$ -body potentials (with  $N \geq 2$ ) would be highly desirable.

In this Letter, we show that an exact and separable decomposition exists for any local potential in a finite basis set built from polynomial functions in any desired parametrization of the physical space. This decomposition is motivated by our recently introduced tensor hypercontraction (THC) method for electronic structure [12–14], which provided a phenomenological approximation for the electron repulsion integrals involving the Coulomb potential in nonpolynomial basis sets. The new exact tensor hypercontraction (X-THC) representation reveals two points of great importance for both electronic and nuclear structure problems. First, THC approximation of the Coulomb interaction is exact for basis sets which can be expressed in polynomial form (and thus, the approximation in electronic structure arises only because the basis functions used were of nonpolynomial form). Second, THC approximation is applicable not only to the two-body Coulomb interaction but also to arbitrary local potentials commonly encountered in nuclear structure (such as the Coulomb, Gogny, local forms of realistic three-body potentials, etc.). Since the nuclear problem is already commonly formulated in terms of polynomial basis sets, this implies that many problems in nuclear structure can now be treated exactly with the lossless scaling reduction afforded by the X-THC representation. The first of these points may aid markedly in the search for more efficient THC approximations in electronic structure, while the second may yield unprecedented physical fidelity in

nuclear structure computations (especially within the context of nuclear DFT).

Below, we first demonstrate the key features of the X-THC representation through the representative example of a one-dimensional, two-body problem in Cartesian coordinates using Hermite functions. The  $D$ -dimensional,  $N$ -body generalization of X-THC is then presented. Finally, we present an example implementation of X-THC for the finite-range Gaussian potential in a basis of Hermite functions, demonstrating that X-THC is both lossless and markedly efficient in practice.

*X-THC example.*—Consider a one-dimensional ( $D = 1$ ) problem in Cartesian coordinates, involving a finite basis of  $M + 1$  Hermite functions  $\{\psi_i(x)\}$  (labeled from 0 to  $M$ ) with a local two-body ( $N = 2$ ) potential  $\hat{V} \equiv \hat{V}(x_1, x_2)$ . The potential matrix elements are

$$\langle ij|\hat{V}|i'j'\rangle \equiv \iint dx_1 dx_2 \psi_i(x_1) \psi_j(x_2) \times \hat{V}(x_1, x_2) \psi_{i'}(x_1) \psi_{j'}(x_2). \quad (2)$$

The first stage in X-THC is to note that all  $(M + 1)^2$  products  $\psi_i(x_1) \psi_{i'}(x_1)$  are exactly spanned by an orthonormal “auxiliary” basis  $\{\chi_A(x_1)\}$  consisting of  $2M + 1$  Hermite functions with a slightly modified spatial range,  $\chi_A(x_1) \equiv \psi_A(\sqrt{2}x_1)$ ,

$$\psi_i(x_1) \psi_{i'}(x_1) = \sum_A [ii'A] \chi_A(x_1), \quad (3)$$

where

$$[ii'A] \equiv \int_{\mathbb{R}} dx_1 \psi_i(x_1) \psi_{i'}(x_1) \chi_A(x_1). \quad (4)$$

This resolution is well known in the context of nuclear physics [15–17], and is analogous to the popular density fitting (DF) procedure of electronic structure theory [18–20]. In this context, the decomposition is exact thanks to the closure properties of the polynomial-based Hermite functions. The integrals are now given as

$$\langle ij|\hat{V}|i'j'\rangle = \sum_{AB} [ii'A][jj'B] G^{AB}, \quad (5)$$

where

$$G^{AB} \equiv \iint_{\mathbb{R}^2} dx_1 dx_2 \chi_A(x_1) \chi_B(x_2) \hat{V}(x_1, x_2). \quad (6)$$

Thus, the fourth-order integral tensor is expressed as a product of second- and third-order tensors. Even though we have compressed the fourth-order tensor, this representation still precludes scaling reduction in “exchangelike” terms. A canonical example of such a term is the pairing field in Hartree-Fock-Bogoliubov theory,

$$\Delta_{ij} \equiv \sum_{i'j'} \langle ij|\hat{V}|i'j'\rangle \kappa_{i'j'} = \sum_{ABi'j'} [ii'A][jj'B] G^{AB} \kappa_{i'j'}, \quad (7)$$

where  $\kappa$  is the pairing tensor. Despite the factorization, computing this term still scales as  $O(M^4) = O(M^{2ND})$ .

The critical step in THC is to resolve the three-index overlap integral  $[ii'A]$  to “unpin” the indices  $i$  and  $i'$  across some additional linear-scaling index  $P$ . That is, we seek a decomposition of the form  $[ii'A] = \sum_P X_i^P X_{i'}^P Y_A^P$ , where the range of  $P$  is  $O(M)$ . Thanks to the choice of a polynomial basis, the overlap integral is exactly integrated by a  $2M + 1$ -node Gaussian quadrature (in this case, Gauss-Hermite) defined by the nodes and weights  $\{(x_P, w_P)\}$  [21]. Therefore, the quadrature grid index provides a natural decomposition of the overlap integral

$$[ii'A] = \sum_P w_P \psi_i(x_P) \psi_{i'}(x_P) \chi_A(x_P) = \sum_P X_i^P X_{i'}^P Y_A^P, \quad (8)$$

where  $X_i^P \equiv \psi_i(x_P)$  and  $Y_A^P \equiv w_P \chi_A(x_P)$ . This is reminiscent of the discrete variable representation (DVR) [22–25] or pseudospectral [26] techniques of chemical physics. Thus, defining the intermediate  $Z^{PQ} = \sum_{AB} Y_A^P G^{AB} Y_B^Q$ , the full integral (2) is expressed as

$$\langle ij|\hat{V}|i'j'\rangle = \sum_{PQ} X_i^P X_j^Q Z^{PQ} X_{i'}^P X_{j'}^Q. \quad (9)$$

This X-THC representation of the integral tensor is the key for the exact  $O(M^3) = O(M^{ND+1})$  treatment of the pairing term, via several intermediate summations, indicated here by brackets for clarity,

$$\begin{aligned} \Delta_{ij} &= \sum_{PQ i'j'} X_i^P X_j^Q Z^{PQ} X_{i'}^P X_{j'}^Q \kappa_{i'j'} \\ &= \sum_P X_i^P \left[ \sum_Q X_j^Q \left[ Z^{PQ} \left[ \sum_{i'} X_{i'}^P \left[ \sum_{j'} X_{j'}^Q \kappa_{i'j'} \right] \right] \right] \right]. \end{aligned} \quad (10)$$

*Interpretation.*—At first glance, the  $Z$  operator is a mere mathematical intermediate, but there exists a much richer interpretation: it is a quantized renormalization of the coordinate-space representation of the potential operator  $\hat{V}$ . To see this, we first consider the continuous, renormalized potential operator  $\bar{V}$ , defined as

$$\bar{V}(x_1, x_2) \equiv \sum_{AB} \chi_A(x_1) \chi_B(x_2) G^{AB}. \quad (11)$$

This operator is not equivalent to the original in physical space, i.e.,  $\hat{V}(x_1, x_2) \neq \bar{V}(x_1, x_2)$ , yet the matrix elements of both operators are identical, i.e.,  $\langle ij|\hat{V}|i'j'\rangle = \langle ij|\bar{V}|i'j'\rangle$ . The renormalized operator is simply the raw operator  $\hat{V}$  with all components outside of the finite product space  $\{\psi_i(x_1) \psi_{i'}(x_1)\} \Leftrightarrow \{\chi_A(x_1)\}$  projected out in each coordinate. This projection is serendipitous: the coordinate-space integrand involving  $\bar{V}$  and the products of basis functions are exactly resolved by the Gaussian quadrature for the auxiliary basis, while the corresponding integrand for  $\hat{V}$  is not exact under any finite quadrature due to the presence of

“alias” components outside of  $\{\psi_i(x_1)\psi_{i'}(x_1)\}$ . Applying the Gaussian quadrature, we can quantize the renormalized operator  $\tilde{V}$  to produce the discrete operator  $\hat{V}$ , adding quadrature weights to account for the spatial contribution of each point,

$$\tilde{V}(x_1, x_2) \equiv w_P w_Q \delta(x_1 - x_P) \delta(x_2 - x_Q) \tilde{V}(x_1, x_2). \quad (12)$$

As with  $\tilde{V}$ , the matrix elements of  $\hat{V}$  are identical to those of  $\tilde{V}$ . Integrating  $\tilde{V}$  instead of  $\hat{V}$  naturally exposes the X-THC factorization,

$$\begin{aligned} \langle ij | \hat{V} | i' j' \rangle &= \langle ij | \tilde{V} | i' j' \rangle \\ &= \iint dx_1 dx_2 \psi_i(x_1) \psi_j(x_2) \tilde{V}(x_1, x_2) \psi_{i'}(x_1) \psi_{j'}(x_2) \\ &= \sum_{PQ} X_i^P X_j^Q Z^{PQ} X_{i'}^P X_{j'}^Q. \end{aligned} \quad (13)$$

Here, the elements  $Z^{PQ}$  are simply the quantized values of the renormalized potential, with the weights rolled in, i.e.,  $Z^{PQ} = w_P w_Q \tilde{V}(x_P, x_Q)$ . An example involving a Gaussian potential in Hermite functions is shown in Fig. 1. The renormalized potential (right) clearly shows the effects of projection from the raw potential (left). The locations of the quantization to  $Z^{PQ}$  (the positions at which  $\tilde{V}$  can be discretized in a lossless manner) are indicated with small white x's on the right.

This understanding of the  $Z$  operator reveals that while X-THC is built from DF and DVR techniques, the resultant supersedes both of the originals. In the context of local potentials and polynomial basis sets, DF is always exact, but does not provide separability of the  $i$  and  $i'$  indices, precluding scaling reductions. DVR techniques do provide separability, but are only exact when an infinite quadrature is used, for an arbitrary choice of local potential. By contrast, X-THC's particular merger of DF and DVR yields a perfect dealiasing renormalization within a finite quadrature, providing a decomposition that is both exact and separable for an arbitrary choice of local potential.

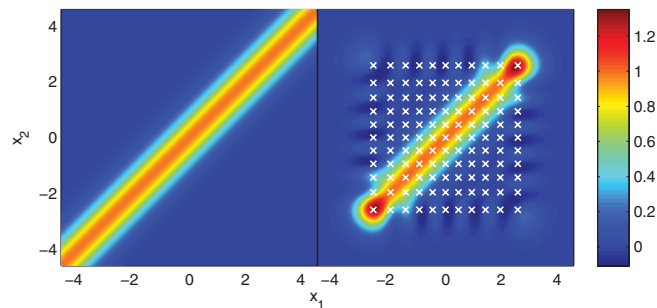


FIG. 1 (color). Example of the X-THC process for a one-dimensional, two-body Gaussian potential  $\hat{V}(x_1, x_2) = \exp(-x_1^2 - x_2^2)$  in Hermite functions  $\{\psi_i(x)\}$  up to  $M = 5$ . Left: raw  $\hat{V}(x_1, x_2)$ . Right: renormalized  $\tilde{V}(x_1, x_2)$ . White x's indicate the collocation locations of the Gauss-Hermite quadrature to the quantized operator  $\tilde{V}(x_1, x_2)$ .

*Generalized X-THC.*—The generalization of the one-dimensional, two-body, Hermite function example above to  $N$ -body potentials in  $D$  dimensions and other choices of polynomial direct-product bases is straightforward. For X-THC to hold, the one-particle basis must be of the  $D$ -dimensional direct-product polynomial type, i.e.,  $\psi_i(\mathbf{r}) \equiv \prod_{\mu=1}^D P_{i_\mu}(r_\mu) v_\mu(r_\mu)$ . In each dimension  $\mu$ ,  $P_{i_\mu}$  is a polynomial of up to degree  $i_\mu$ , and  $v_\mu$  is an arbitrary weight function (analogous to the Gaussian term in the Hermite functions above). Such basis sets are widely used in atomic and nuclear many-body physics in various coordinate systems. Use of a direct-product polynomial basis automatically guarantees closure: for the  $M_\mu + 1$  functions in the  $\mu$ th dimension, the span  $\langle \psi_{i_\mu}(r_\mu) \psi_{i'_\mu}(r_\mu) \rangle$  lies wholly inside a  $(2M_\mu + 1)$ -function auxiliary basis, defined by a set of polynomials orthogonal with respect to the weight  $|v_\mu(r_\mu)|^4$ . Additionally, all quadratic products of auxiliary functions are exactly integrated by a  $(2M_\mu + 1)$ -node Gaussian quadrature  $\{\langle r_{P_\mu}, w_{P_\mu} \rangle\}$  which can always be found, e.g., by the Golub-Welsch algorithm [27].

These properties allow for the X-THC factorization

$$\langle i \dots n | \hat{V} | i' \dots n' \rangle = \sum_{P \dots W} X_i^P \dots X_n^W Z^{P \dots W} X_{i'}^P \dots X_{n'}^W, \quad (14)$$

with each  $X_i^P$  being the direct product of the  $D$  underlying  $X_{i_\mu}^{P_\mu}$ .  $Z^{P \dots W}$  is the generalization of  $Z^{PQ}$  to the case with  $N$ -body auxiliary integrals  $G^{A \dots N}$ .

Within the X-THC representation, the representative generalization of the pairing term,  $\Delta_{i \dots n} \equiv \langle i \dots n | \hat{V} | i' \dots n' \rangle \kappa_{i' \dots n'}$ , now scales as  $O(M_\mu^{ND+1})$ , rather than  $O(M_\mu^{2ND})$ , with no approximation or restriction on the form of the local, finite-range potential  $\hat{V}$ .

It is worth noting that common techniques to reduce the cost of treating exchange-like terms involve approximating the potential to be direct-product separable over  $N_w$  terms, e.g., by approximating the Coulomb operator as a sum of separable Gaussians [28,29]. This reduces the conventional or DF cost of forming the generalized pairing tensor to  $O(M_\mu^{ND+N})$ . X-THC can be applied to this approximate separable potential, producing an  $O(M_\mu^{ND+1})$  implementation. However, the separable form gives no particular scaling advantage in the X-THC formalism, and can only reduce the prefactor and memory requirements. A more severe approximation is the invocation of a zero-range potential. This is typically formulated as a DVR-type quadrature in coordinate space, which can be exact depending on the form of the zero-range operator [30]. The asymptotic scaling of a pairing term involving a zero-range potential is  $O(M_\mu^{ND+1})$ , due to the first or last transformation into or out of the grid index. Remarkably, this is the same asymptotic scaling as X-THC. The zero-range potential will generally have a lower prefactor than X-THC (as there is only one grid coordinate in the zero-range potential), but the asymptotic scalings are identical, and thus, the tractability limits

TABLE I. Computational scalings for the pairing term of an arbitrary local potential in several approaches.  $M_\mu$  is the order of the polynomial basis in the  $\mu$ th degree of freedom, and the potential is  $N$  body in  $D$  dimensions. For simplicity, we consider the isotropic case where  $M_\mu$  is the same in all dimensions in this comparison.  $N_w$  is the number of terms retained in a separable approximation to the potential.

Approach	General local	Separable local	Zero range
Conventional	$O(M_\mu^{2ND})$	$O(N_w M_\mu^{ND+N})$	$O(M_\mu^{ND+1})$
X-THC	$O(M_\mu^{ND+1})$	$O(N_w M_\mu^{ND+1})$	$O(M_\mu^{ND+1})$

should be comparable. A summary of the scaling reductions afforded with various factorization approaches and local potentials is shown in Table I.

*Practical demonstration.*—To illustrate the numerical equivalence and practical utility of the X-THC approach, a hybrid MATLAB-C++ code was developed to produce generalized pairing fields for  $D$ -dimensional,  $N$ -body forces in Hermite functions. A complete description of the code is presented in the Supplemental Material [31].

We have verified that the X-THC generalized pairing fields are exact within machine precision (as expected mathematically). Figure 2 shows the computational gains which can be achieved from the X-THC factorization using a representative example of  $N = 2$  and  $D = 1, 2, 3$ . For a general local potential, X-THC is several orders of magnitude faster than conventional approaches for the largest  $M_\mu$  studied here. When the potential is written in separable form, the X-THC scaling advantage is less dramatic, but

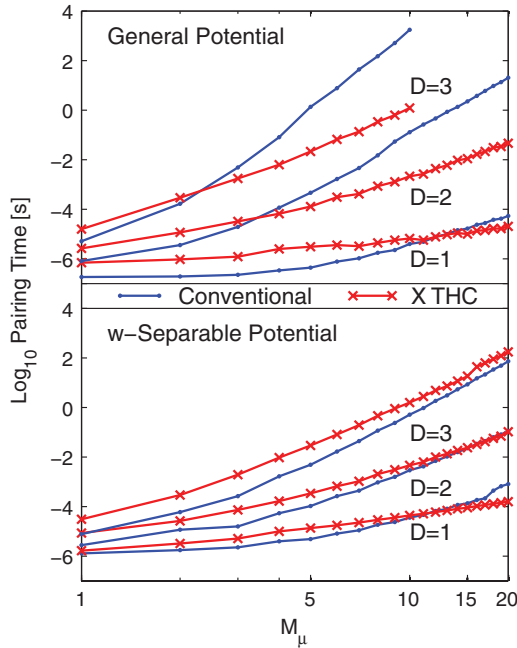


FIG. 2 (color). Wall times for pairing tensor formation as a function of  $M_\mu$  for  $N = 2$  (log-log scale).  $N_w = 8$  for the separable potential.

X-THC becomes less costly for the largest  $M_\mu$  used in Figure 2. The X-THC approach allows one to retain the general local potential and calculate the exact pairing tensor in similar (or even less) computational effort as with an approximate separable potential.

*Summary and outlook.*—In this Letter, we have demonstrated that an exactly quantized renormalization of any local, finite-range  $N$ -body potential exists in any situation where the primary basis set may be composed of polynomial-based functions. This X-THC representation provides for substantial computational scaling reduction of contractions involving the local potential integral tensor, for instance by reducing the formation of a representative generalization of the pairing tensor from  $O(M_\mu^{2ND})$  to  $O(M_\mu^{ND+1})$ .

In electronic structure, the concept of X-THC helps to codify and rationalize our existing least-squares tensor hypercontraction (LS-THC) approximation for nonpolynomial basis sets [13]. The least squares procedure introduced in that work actually performs an implicit renormalization of the potential. Since the basis sets used in our previous applications of LS-THC were not direct products of polynomials (but rather atom-centered Gaussian functions), the decomposition was necessarily an approximation. As the X-THC limit is approached, the fidelity of the approximation will depend on both the basis set resemblance to a set of polynomial-based functions and the efficiency of the quadrature. The physical picture provided by X-THC's explicit renormalization process will almost certainly aid in the search for enhanced approximate THC recipes for nonpolynomial basis sets.

In nuclear structure, the potential applications for X-THC are immediate and substantial. A crucial finding of this Letter is that the formal scaling of operations involving arbitrary local potential operators is identical to that of zero-range operators, without any loss in accuracy. This implies that the finite-range two-body Gogny potentials of nuclear DFT can immediately be applied with the same computational complexity as the more approximate zero-range Skyrme potentials. Tractability gains should be even more marked for three-body potentials, paving the way for Hamiltonian-based nuclear energy densities derived from effective, local, finite-range, density-independent, two- and three-nucleon pseudopotentials, which, by construction, would be free of the current artifacts of nuclear DFT.

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