Significant conditions for the two-electron reduced density matrix from the constructive solution of N representability

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We recently presented a constructive solution to the N-representability problem of the two-electron reduced density matrix (2-RDM)—a systematic approach to constructing complete conditions to ensure that the 2-RDM represents a realistic N-electron quantum system [D. A. Mazziotti, Phys. Rev. Lett. (to be published)]. In this paper we provide additional details and derive further N-representability conditions on the 2-RDM that follow from the constructive solution. The resulting conditions can be classified into a hierarchy of constraints, known as the $(2,q)$-positivity conditions, where the q indicates their derivation from the non-negativity of q-body operators. In addition to the known T1 and T2 conditions, we derive another class of (2,3)-positivity conditions. We also derive 3 classes of (2,4)-positivity conditions, 6 classes of (2,5)-positivity conditions, and 24 classes of (2,6)-positivity conditions. The constraints obtained can be divided into two general types: (i) *lifting conditions*, that is, conditions which arise from lifting lower $(2,q)$-positivity conditions to higher $(2,q+1)$-positivity conditions, and (ii) *pure conditions*, that is, conditions which cannot be derived from a simple lifting of the lower conditions. All of the lifting conditions and the pure $(2,q)$-positivity conditions for $q > 3$ require tensor decompositions of the coefficients in the model Hamiltonians. Subsets of the derived N-representability conditions can be employed with the previously known conditions to achieve polynomially scaling calculations of ground-state energies and 2-RDMs of many-electron quantum systems even in the presence of strong electron correlation.

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I. INTRODUCTION

Because electrons are indistinguishable with pairwise Coulomb interactions, the energies and properties of many-electron atoms and molecules can be evaluated from a knowledge of the two-electron reduced density matrix (2-RDM) [1–3]. Minimizing the ground-state energy as a functional of the 2-RDM, however, requires nontrivial constraints on the 2-RDM to ensure that it represents an N-electron system (N-representability conditions) [1–24]. While advances in theory and computation enabled the accurate variational calculation of the 2-RDM for a variety of strongly correlated systems in chemistry and physics, from polyaromatic hydrocarbons [25,26] to quantum dots [27], the known N-representability conditions for the 2-RDM, albeit rigorous, remained incomplete. Recently, we presented a constructive solution to the N-representability problem—a systematic approach to constructing complete N-representability conditions on the two-electron reduced density matrix (2-RDM)—as well as examples of new N-representability conditions [28]. In the present paper we present additional details as well as further conditions on the 2-RDM that follow from the constructive solution.

The advantage of reduced variables such as the 2-RDM and the one-electron density is that, unlike the wave function expanded in terms of determinants, their degrees of freedom grow *polynomially* with the size of the quantum system [3] even when the electrons are strongly correlated [29,30]. Direct calculation of the reduced variables, however, requires that they and their functionals be consistent with a realistic N-electron quantum system; in other words, the reduced variables and functionals must be representable by the integration of an N-electron density matrix. Such consistency relations are known as the *N-representability conditions* [1–18,20–24]. These conditions are particularly important to 2-RDM methods, where they enable the direct calculation of the 2-RDM without the wave function, but they are also implicit in the design of realistic approximations to the density functional in density functional theory [31,32].

Minimizing the many-electron energy as a functional of the 2-RDM *without* N-representability conditions produces an energy that is *much lower* than the exact ground-state energy of the quantum system. The energy is too low because both the energy and the computed 2-RDM are not realistic—they are not N representable. In the early 1960s the search for the set of necessary and sufficient N-representability conditions became known as the N-representability problem [4]. Three important constraints, known as the D, Q, and G (or 2-positivity) conditions, were developed by Coleman [4] and Garrod and Percus [5]. The D, Q, and G conditions restrict the probability distributions of two electrons, two holes (where a *hole* is the absence of an electron), and an electron-hole pair to be non-negative. Each condition can be expressed in the form of a matrix constrained to be positive semidefinite. A matrix is *positive semidefinite* if and only if its eigenvalues are non-negative.

In 1978 Erdahl [8] discovered two additional semidefinite constraints on the 2-RDM known as the T1 and T2 (or partial 3-positivity) conditions [15,17,18,33], which are derivable from the non-negativity of the three-electron probability distributions. Finally, Weinhold and Wilson [34], Yoseloff and Kuhn [35], McRae and Davidson [36], and Erdahl [8] derived necessary conditions on the *diagonal* part of the 2-RDM. These diagonal conditions were shown, in the context of the Boole optimization problem [37], to be part of a complete set of

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classical N-representability conditions on the two-electron reduced density function, which is the diagonal part of the 2-RDM in a coordinate representation [38]. Despite the solution of the classical problem, the complete set of quantum N-representability conditions remained unknown except for the D, Q, G, T1, and generalized T2 conditions as well as unitary transformations of the classical N-representability conditions. In 2001 Mazziotti and Erdahl [11] presented a systematic generalization of these constraints known as the *p-positivity conditions* and in 2002 Mazziotti [13,39] introduced the *lifting conditions*; however, except for the conditions given above, the p-positivity conditions and the lifting conditions depend upon not only the 2-RDM but also higher-particle RDMs.

The constructive solution to the N-representability problem provides a systematic approach to building complete N-representability conditions on the 2-RDM [28]. While an example of the derived conditions was given previously, in the present paper we present further N-representability conditions on the 2-RDM that follow from the constructive solution. The conditions are in the form of a set of model Hamiltonians with pairwise interactions whose trace against the 2-RDM must be non-negative. The resulting conditions can be classified into an increasing hierarchy of constraints, known as the $(2,q)$-positivity conditions, where the first number p in the name indicates the highest p-RDM required to evaluate the condition (the 2-RDM in our case) and the second number q indicates the highest q-particle reduced density operators (q-RDOs) canceled by non-negative linear combinations in the derivation of the condition. The (p,p)-positivity conditions are equivalent to the p-positivity conditions introduced earlier in Refs. [10], [11], and [13]. We use the two conventions in nomenclature interchangeably.

In addition to the previously known T1 and T2 conditions [8,15,17,18,33], we derive a class of (2,3)-positivity conditions. We also derive three classes of (2,4)-positivity conditions, 6 classes of (2,5)-positivity conditions, and 24 classes of (2,6)-positivity conditions. The conditions obtained can be divided into two general types: (i) *lifting conditions*, that is, conditions which arise from lifting lower $(2,q)$-positivity conditions to higher $(2,q+1)$-positivity conditions, and (ii) *pure conditions*, that is, conditions which cannot be derived from a simple lifting of the lower conditions. All of the lifting conditions and the pure $(2,q)$-positivity conditions for $q>3$ require that the expansion coefficients in the model Hamiltonians be *tensor decomposed*. Subsets of the N-representability conditions can be employed with previously known conditions for polynomially scaling calculations of ground-state energies and 2-RDMs of many-electron quantum systems in chemistry and physics.

II. THEORY

After the constructive solution of N representability is reviewed in Sec. II A, it is employed in Secs. II C and II D to derive known and additional N-representability conditions, respectively. The additional constraints are organized into sections on (2,3)-, (2,4)-, (2,5)-, and (2,6)-positivity conditions. Two algorithms for implementing the conditions in a variational 2-RDM calculation are briefly discussed in Sec. II B.

A. Constructive solution

The energy of an N-electron quantum system in a stationary state can be computed from the Hamiltonian traced against the state's density matrix,

$$E = \mathrm{Tr}(\hat{H}\,{}^{N}D), \tag{1}$$

where the Hamiltonian operator is expressible in second quantization as

$$\hat{H} = \sum_{ijkl} {}^{2}K^{ij}_{kl}\hat{a}^{\dagger}_{i}\hat{a}^{\dagger}_{j}\hat{a}_{l}\hat{a}_{k}, \tag{2}$$

in which the matrix ${}^{2}K$ is the reduced Hamiltonian operator in a finite one-electron basis set [40] and the indices label the members (orbitals) of the basis set. Because electrons are indistinguishable with pairwise interactions, the energy can also be universally written as a linear functional of only the 2-RDM,

$$E = \mathrm{Tr}(\hat{H}\,{}^{2}D), \tag{3}$$

where the 2-RDM can be formally defined from integration of the N-electron density matrix over all electrons save two:

$${}^{2}D = \frac{N(N-1)}{2}\int {}^{N}D\, d3\cdots dN. \tag{4}$$

The expression of the energy as a functional of the 2-RDM suggests the tantalizing possibility of computing the ground-state energy of any electronic system as a functional of only the 2-RDM [1,2,41]. Early calculations by Coleman [4], Tredgold [42], and others, however, showed that minimization of the energy as a 2-RDM functional produces unphysically low energies without additional constraints on the 2-RDM to ensure that it represents an N-electron density matrix. In 1963 Coleman called these constraints the N-representability conditions [4].

Building upon work by Garrod and Percus [5], Kummer in 1967 showed by the bipolar theorem [43] that there exists a convex set (cone) of two-body operators $\{{}^{2}\hat{O}_{i}\}$ whose trace against a potential 2-RDM will be non-negative,

$$\mathrm{Tr}({}^{2}\hat{O}\,{}^{2}D) \geqslant 0, \tag{5}$$

if and only if the 2-RDM is N representable [6]. Hence, the set of two-body operators $\{{}^{2}\hat{O}_{i}\}$ defines the set P^{2}_{N} of N-representable 2-RDMs. We say that the set $\{{}^{2}\hat{O}_{i}\}$ is the polar of P^{2}_{N} and denote it $P^{2\,*}_{N}$. Characterizing the set P^{2}_{N} of N-representable 2-RDMs, therefore, would be complete if we could characterize its polar set $P^{2\,*}_{N}$. Kummer's original result demonstrates the existence of the set $P^{2\,*}_{N}$, but it does not provide a prescription for constructing it.

Recently, a constructive solution to the N-representability problem has been derived through the complete characterization of the polar set $P^{2\,*}_{N}$ [28]. In Ref. [28] it is proven that the second-quantized representation of the operators $\{{}^{2}\hat{O}_{i}\}$ in $P^{2\,*}_{N}$ can be explicitly constructed as

$${}^{2}\hat{O} = \sum_{i} w_{i}\hat{C}_{i}\hat{C}^{\dagger}_{i}, \tag{6}$$

where $\hat{C}_{i}$ are polynomials in the creation and/or annihilation operators of degree less than or equal to r (the rank of the one-electron basis set) and w_{i} are non-negative integer weights.

The proof relies on the fact that P_N^{2*} is *contained within* the set P_N^{r*} of operators of degree $\leqslant 2r$ whose trace against an N-electron density matrix must be non-negative. Because the extreme elements (rays) of the convex cone P_N^{r*} are readily expressed as [44]

$$\hat{C}_i \hat{C}_i^\dagger, \tag{7}$$

the extreme elements (rays) of P_N^{2*} can be constructed from the *conic combinations* (or non-negative linear combinations) given in Eq. (6). The conic combinations, if divided by $\sum_i w_i$, can be interpreted as *convex combinations*. Conic combinations are contained in P_N^{2*} if and only if they cancel all three- and higher-body operators, that is, polynomials in creation and annihilation operators of degree $\geqslant 6$.

B. Practical implementation

Before developing known and new N-representability conditions in Secs. II C and II D, respectively, in this section we briefly indicate their practical applications by sketching two algorithms for computing the ground-state 2-RDM. Minimizing the ground-state energy as a function of the 2-RDM constrained by these conditions can be formulated as a linear program,

$$\text{minimize} \quad E = \text{Tr}(\hat{H}\, {}^2D) \tag{8}$$

$$\text{such that} \quad \text{Tr}(\hat{O}_j {}^2D) \geqslant 0 \quad \text{for all } j, \tag{9}$$

in which the necessary set of operators (model Hamiltonians) $\hat{O}_j$, defining the boundary of the convex set of 2-RDMs, must be determined iteratively. Given an initial set of model-Hamiltonian constraints that bound the minimum energy, the three key steps in the algorithm are (i) solving the linear program for the optimal 2-RDM, (ii) updating the set of model-Hamiltonian constraints in the linear program, and (iii) repeating steps i and ii until the 2-RDM is non-negative in its trace, with all model Hamiltonians explored in step ii. In the second step, the trace of each model Hamiltonian with the 2-RDM is minimized by optimizing the Hamiltonian's parameters (expansion coefficients), and if the final trace is negative, the model Hamiltonian with its optimized parameters is added to the constraints in Eq. (9). In practice, only a subset of model Hamiltonians from the constructive solution is employed.

Some of the N-representability constraints can be collected together as a single semidefinite constraint on the 2-RDM. The generalization of a linear program to include semidefinite constraints is known as a *semidefinite program*, and the solution of such a program is called *semidefinite programming* [45,46]. Efficient large-scale semidefinite programming algorithms have been developed for the variational calculation of the 2-RDM [14–16,21,23,24,47–49]. While the model Hamiltonians corresponding to previously known N-representability conditions in Sec. II C can be expressed as semidefinite constraints, the model Hamiltonians corresponding to the new conditions in Sec. II D, which use tensor decompositions of the expansion coefficients in the $\hat{C}_i$ operators, cannot be written as traditional semidefinite constraints. In practice, however, we can add these nonstandard constraints to a semidefinite program containing the standard semidefinite constraints by the three-step iterative procedure discussed above for the linear program. A main advantage of this second algorithm is that a large number of model-Hamiltonian constraints can be included by a single semidefinite constraint. A similar algorithm, to which we refer for further details, was proposed in Ref. [50] for imposing the T2 condition by recursively generated linear inequalities.

C. Known conditions

All previously known N-representability conditions are generated by the constructive solution. The most important representability conditions on the 2-RDM, derived by Coleman [4] and Garrod and Percus [5], are the D, Q, and G conditions—also, known as the 2-positivity conditions [11]. These conditions restrict the two-particle RDM ${}^2D$, the two-hole RDM ${}^2Q$, and the particle-hole RDM ${}^2G$ to be positive semidefinite, that is,

$${}^2D \succeq 0, \tag{10}$$

$${}^2Q \succeq 0, \tag{11}$$

$${}^2G \succeq 0, \tag{12}$$

where the elements of the RDMs are given by

$${}^2D^{ij}_{kl} = \langle \Psi | \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_l \hat{a}_k | \Psi \rangle, \tag{13}$$

$${}^2Q^{ij}_{kl} = \langle \Psi | \hat{a}_i \hat{a}_j \hat{a}_l^\dagger \hat{a}_k^\dagger | \Psi \rangle, \tag{14}$$

$${}^2G^{ij}_{kl} = \langle \Psi | \hat{a}_i^\dagger \hat{a}_j \hat{a}_l^\dagger \hat{a}_k | \Psi \rangle, \tag{15}$$

and $M \succeq 0$ indicates that the matrix M is constrained to be positive semidefinite. Physically, these conditions correspond to constraining the probability distributions of two particles and two holes, as well as one particle and one hole, to be non-negative. The 2-positivity conditions are generated from the constructive solution by restricting the following three two-body operators from Eq. (6) to be non-negative for all coefficients b_{ij}:

$${}^2\hat{O}_D = \hat{C}_D \hat{C}_D^\dagger, \tag{16}$$

$${}^2\hat{O}_Q = \hat{C}_Q \hat{C}_Q^\dagger, \tag{17}$$

$${}^2\hat{O}_G = \hat{C}_G \hat{C}_G^\dagger, \tag{18}$$

where $\hat{C}_D$, $\hat{C}_Q$, and $\hat{C}_G$ cover all polynomials in creation and annihilation operators of degree 2:

$$\hat{C}_D = \sum_{ij} b_{ij} \hat{a}_i^\dagger \hat{a}_j^\dagger, \tag{19}$$

$$\hat{C}_Q = \sum_{ij} b_{ij} \hat{a}_i \hat{a}_j, \tag{20}$$

$$\hat{C}_G = \sum_{ij} b_{ij} \hat{a}_i^\dagger \hat{a}_j. \tag{21}$$

Note that conic combinations are not present in these conditions because when the $\hat{C}_i$ operators are of degree 2, the expectation values of the $\hat{O}_i$ operators only involve the 2-RDM [28].

The other previously known N-representability conditions—the T1 and T2 conditions [8,15,17,18,33]—are part of the (2,3) conditions that follow from the constructive solution. These semidefinite conditions on the 2-RDM are obtainable from conic combinations of three-particle metric matrices that cancel their dependence on the 3-RDM [17,18]:

$$T1 = {}^3D + {}^3Q \succeq 0, \tag{22}$$

$$T2 = {}^3E + {}^3F \succeq 0, \tag{23}$$

where in second quantization the matrix elements of these metric matrices are definable as

$${}^3D^{ijk}_{pqs} = \langle\Psi|\hat{a}^\dagger_i\hat{a}^\dagger_j\hat{a}^\dagger_k\hat{a}_s\hat{a}_q\hat{a}_p|\Psi\rangle, \tag{24}$$

$${}^3E^{ijk}_{pqs} = \langle\Psi|\hat{a}^\dagger_i\hat{a}^\dagger_j\hat{a}_k\hat{a}^\dagger_s\hat{a}_q\hat{a}_p|\Psi\rangle, \tag{25}$$

$${}^3F^{ijk}_{pqs} = \langle\Psi|\hat{a}_p\hat{a}_q\hat{a}^\dagger_s\hat{a}_k\hat{a}^\dagger_j\hat{a}^\dagger_i|\Psi\rangle, \tag{26}$$

$${}^3Q^{ijk}_{pqs} = \langle\Psi|\hat{a}_p\hat{a}_q\hat{a}_s\hat{a}^\dagger_k\hat{a}^\dagger_j\hat{a}^\dagger_i|\Psi\rangle. \tag{27}$$

The four metric matrices ${}^3D$, ${}^3E$, ${}^3F$, and ${}^3Q$ correspond to the probability distributions for three particles, two particles and a hole, one particle and two holes, and three holes, respectively [11,13,18]. Restricting the ${}^3D$, ${}^3E$, ${}^3F$, and ${}^3Q$ matrices to be positive semidefinite generates the 3-positivity conditions [11,18] which depend on the 3-RDM. While the T1 and T2 conditions are a subset of the 3-positivity conditions, they depend only on the 2-RDM because the three-particle parts of ${}^3D$ and ${}^3Q$ (and ${}^3E$ and ${}^3F$) cancel upon addition [17,18]. For example, the matrix elements of $T1$ are given by

$$T1^{ijk}_{pqs} = 6\,{}^3I^{ijk}_{pqs} - 18\,{}^1D^i_p \wedge {}^2I^{jk}_{qs} + 9\,{}^2D^{ij}_{pq} \wedge {}^1I^k_s, \tag{28}$$

where ${}^pI$ is the p-particle identity matrix and $\wedge$ denotes the Grassmann wedge product [40,51].

While the T1 condition is unique, three distinct forms of the T2 condition can be generated by rearranging the second-quantized operators in the definition of the ${}^3F$ metric matrix relative to those in the ${}^3E$ metric matrix [18]. Consider the two variants of the ${}^3F$ matrix with the following matrix elements:

$${}^3\bar{F}^{ijk}_{pqs} = \langle\Psi|\hat{a}_p\hat{a}^\dagger_s\hat{a}_q\hat{a}^\dagger_j\hat{a}_k\hat{a}^\dagger_i|\Psi\rangle, \tag{29}$$

$${}^3\tilde{F}^{ijk}_{pqs} = \langle\Psi|\hat{a}^\dagger_s\hat{a}_p\hat{a}_q\hat{a}^\dagger_j\hat{a}^\dagger_i\hat{a}_k|\Psi\rangle. \tag{30}$$

The 3-positivity condition ${}^3F \succeq 0$ implies both ${}^3\bar{F} \succeq 0$ and ${}^3\tilde{F} \succeq 0$ because reordering the creation and annihilation operators does not change the vector space covered by the metric matrix. Changing the ordering of the second-quantized operators in the ${}^3F$ matrix relative to those in the ${}^3E$ matrix, however, does generate two additional T2 conditions:

$$\bar{T}2 = {}^3E + {}^3\bar{F} \succeq 0, \tag{31}$$

$$\tilde{T}2 = {}^3E + {}^3\tilde{F} \succeq 0. \tag{32}$$

It was the $\tilde{T}2$ form of the T2 condition that was originally implemented by Zhao *et al.* [15] and Mazziotti [17,18].

The three T2 conditions are generated in the constructive solution by keeping the following two-body operators from Eq. (6) non-negative:

$${}^2\hat{O}_{T2} = \hat{C}_E\,\hat{C}^\dagger_E + \hat{C}_F\hat{C}^\dagger_F, \tag{33}$$

$${}^2\hat{O}_{\bar{T}2} = \hat{C}_E\hat{C}^\dagger_E + \hat{C}_{\bar{F}}\hat{C}^\dagger_{\bar{F}}, \tag{34}$$

$${}^2\hat{O}_{\tilde{T}2} = \hat{C}_E\hat{C}^\dagger_E + \hat{C}_{\tilde{F}}\hat{C}^\dagger_{\tilde{F}}, \tag{35}$$

where

$$\hat{C}_E = \sum_{ijk} b_{ijk}\hat{a}^\dagger_i\hat{a}^\dagger_j\hat{a}_k, \tag{36}$$

$$\hat{C}_F = \sum_{ijk} b^*_{ijk}\hat{a}_i\hat{a}_j\hat{a}^\dagger_k, \tag{37}$$

$$\hat{C}_{\bar{F}} = \sum_{ijk} b^*_{ijk}\hat{a}_i\hat{a}^\dagger_k\hat{a}_j, \tag{38}$$

$$\hat{C}_{\tilde{F}} = \sum_{ijk} b^*_{ijk}\hat{a}^\dagger_k\hat{a}_i\hat{a}_j. \tag{39}$$

The three T2 conditions can be combined into a single generalized T2 condition as shown in Refs. [18] and [33]. The T1 condition is also produced in the constructive solution by keeping the following two-body operator from Eq. (6) non-negative:

$${}^2\hat{O}_{T1} = \hat{C}_D\,\hat{C}^\dagger_D + \hat{C}_Q\hat{C}^\dagger_Q, \tag{40}$$

where

$$\hat{C}_D = \sum_{ijk} b_{ijk}\hat{a}^\dagger_i\hat{a}^\dagger_j\hat{a}^\dagger_k, \tag{41}$$

$$\hat{C}_Q = \sum_{ijk} b^*_{ijk}\hat{a}_i\hat{a}_j\hat{a}_k. \tag{42}$$

Because the second-quantized operators in $\hat{C}_D$ and $\hat{C}_Q$ are anticommutative, there is only one T1 condition. Unlike the D, Q, and G conditions, both the T1 and the T2 conditions arise from the conic combination of a pair of three-positive operators that cancels their dependence on the 3-RDM.

D. Additional conditions

The constructive solution also produces new N-representability conditions on the 2-RDM [28]. In this section we discuss the further conditions on the 2-RDM that emerge from conic combinations of three-, four-, five-, and six-particle operators in Eq. (6), which we denote the (2,3)-, (2,4)-, (2,5)-, and (2,6)-positivity conditions, respectively. All of the new N-representability conditions require a nonlinear factorization of the expansion coefficients to cancel the higher particle operators.

1. (2,3)-positivity conditions

In addition to the T1 and T2 conditions, there exists a second class of (2,3)-positivity conditions that can be generated from lifting the 2-positivity conditions to the three-particle space and then canceling the three-particle operators. Consider the pair of three-body operators

$$\hat{O}(i,j,k) = \hat{C}(i,j,k)\hat{C}(i,j,k)^\dagger, \tag{43}$$

$$\hat{O}(i,j,\bar{k}) = \hat{C}(i,j,\bar{k})\hat{C}(i,j,\bar{k})^\dagger, \tag{44}$$

where

$$\hat{C}(i,j,k) = \sum_{ijk} b_{ij} d_k \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k^\dagger, \tag{45}$$

$$\hat{C}(i,j,\bar{k}) = \sum_{ijk} b_{ij} d_k^* \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k. \tag{46}$$

The notation for the operators $\hat{O}(i,j,k)$ and $\hat{C}(i,j,k)$ includes their internal summation indices to indicate succinctly (i) the ordering of the second-quantized operators with indices i, j, and k and (ii) the type of second-quantized operator, with k denoting $\hat{a}_k^\dagger$ and $\bar{k}$ denoting $\hat{a}_k$. Note that the notation does not indicate the ordering of the indices on the tensor coefficients, which is alphabetical in both $\hat{C}(i,j,k)$ in Eq. (46) and $\hat{C}(k,i,j)$ in Eq. (52). Although the summation indices within $\hat{C}$ and its adjoint are distinct, we only show primes on the indices of the adjoint when the indices of the two operators appear in the same sum. Finally, for the N-representability conditions to be valid for real symmetric and general Hermitian RDMs, one-index tensors d_k and $d_{\bar{k}}$ denote d_k and d_k^*, respectively. For multi-index tensors we employ the convention that the first subscript determines conjugacy, that is, $b_{ij..m} = b_{ij..m}$ and $b_{\bar{i}j..m} = b_{ij..m}^*$.

The first operator $\hat{O}(i,j,k)$ arises from lifting the D condition through the insertion of a *particle* projection operator,

$$\sum_{k,k'} d_k d_{k'}^* \hat{a}_k^\dagger \hat{a}_{k'}, \tag{47}$$

while the second operator $\hat{O}(i,j,\bar{k})$ arises from lifting the D condition through the insertion of a *hole* projection operator,

$$\sum_{k,k'} d_k^* d_{k'} \hat{a}_k \hat{a}_{k'}^\dagger. \tag{48}$$

The non-negativity of $\hat{O}(i,j,k)$ and $\hat{O}(i,j,\bar{k})$ generates a pair of *lifting conditions* discussed in Refs. [13] and [39]. While these two conditions depend not just on the 2-RDM but on parts of the 3-RDM, the sum of these two three-body operators produces a two-body operator:

$${}^2\hat{O}_{L1} = \hat{O}(i,j,k) + \hat{O}(i,j,\bar{k}). \tag{49}$$

Because the two-body operator ${}^2\hat{O}_{L1}$ simplifies to the two-body operator ${}^2\hat{O}_D$ in Eq. (16), its non-negativity regenerates the D condition. With a generalization of this lifting process, however, we can generate (2,3)-positivity conditions that are distinct from the known conditions.

We can generalize the lifting process by inserting the creation operator and the annihilation operator responsible for lifting at nonadjacent positions. For example, consider the pair of three-body operators

$$\hat{O}(k,i,j) = \hat{C}(k,i,j)\hat{C}(k,i,j)^\dagger, \tag{50}$$

$$\hat{O}(\bar{k},i,j) = \hat{C}(\bar{k},i,j)\hat{C}(\bar{k},i,j)^\dagger, \tag{51}$$

where

$$\hat{C}(k,i,j) = \sum_{ijk} b_{ij} d_k \hat{a}_k^\dagger \hat{a}_i^\dagger \hat{a}_j^\dagger, \tag{52}$$

$$\hat{C}(\bar{k},i,j) = \sum_{ijk} b_{ij} d_k^* \hat{a}_k \hat{a}_i^\dagger \hat{a}_j^\dagger. \tag{53}$$

In $\hat{O}(k,i,j)$ the creation operator $\hat{a}_k^\dagger$ in $\hat{C}$ and the annihilation operator $\hat{a}_{k'}$ in the adjoint of $\hat{C}$, which perform the lifting of the D condition, are separated from each other by four second-quantized operators; similarly, in $\hat{O}(\bar{k},i,j)$ the creation and annihilation operators, $\hat{a}_k$ and $\hat{a}_{k'}^\dagger$, respectively, are separated from each other by four second-quantized operators. Because the components of the projectors are separated, the non-negativity of $\hat{O}(k,i,j)$ and $\hat{O}(\bar{k},i,j)$ generates a pair of generalized lifting conditions that extend those discussed in Refs. [13] and [39].

While individually $\hat{O}(k,i,j)$ and $\hat{O}(\bar{k},i,j)$ depend on three-particle operators, their sum generates a two-body operator,

$${}^2\hat{O}_{L2} = \hat{O}(k,i,j) + \hat{O}(\bar{k},i,j). \tag{54}$$

Unlike ${}^2\hat{O}_{L1}$, the non-negativity of the lifted operator ${}^2\hat{O}_{L2}$ is not necessarily implied by the D, Q, G, T1, and T2 conditions. Importantly, ${}^2\hat{O}_{L2}$ does not simply rearrange to ${}^2\hat{O}_{L1}$ because the creation and annihilation operators are noncommutative. Based on the possible orderings of the fundamental second-quantized operators, there are nine distinct ways to lift the D condition while canceling the resulting three-particle operators and, hence, nine distinct lifting conditions from the D condition. Similarly, there are nine distinct (2,3)-positivity conditions from lifting the Q condition and nine from lifting the G condition. Three of these 27 lifting conditions reduce to the D, Q, and G conditions, respectively, while the other conditions are distinct because the second-quantized operators in quantum mechanics form a noncommutative algebra.

Table I summarizes the (2,3)-positivity conditions by giving a representative condition from each of the two classes: (i) the lifting conditions and (ii) the pure conditions. While the lifting conditions arise from lifting the 2-positivity conditions, the pure conditions cannot be obtained by lifting any of the lower conditions. Table I gives non-negativity of ${}^2\hat{O}_{L2}$ and the T1 condition as representative conditions of the lifting and pure (2,3)-positivity conditions, respectively. All of the other (2,3) conditions can be obtained from these representative conditions through two processes: (i) *switching* of the second-quantized operators in the $\hat{C}(i,j,k)$ between

TABLE I. The (2,3)-positivity conditions can be derived from conic (linear non-negative) combinations of the (3,3)-positivity conditions that cancel the three-particle operators.

Class	Type	Representative condition	$\hat{C}$ definition
1	Lifted (2,2)	$\mathrm{Tr}[(\hat{O}(k,i,j) + \hat{O}(\bar{k},i,j))^2D] \geqslant 0$	Eq. (52)
2	Pure (2,3)	$\mathrm{Tr}[(\hat{O}(i,j,k) + \hat{O}(\bar{i},\bar{j},\bar{k}))^2D] \geqslant 0$	Eq. (41)

creators and annihilators and (ii) *reordering* of the second-quantized operators in the $\hat{C}(i,j,k)$.

Switching the second-quantized operators with index j in the L2 condition of Eq. (54), for example, generates a lifted G condition:

$$^{2}\hat{O}_{L3} = \hat{O}(k,i,\bar{j}) + \hat{O}(\bar{k},i,\bar{j}). \quad (55)$$

Note that switching the second-quantized operators with index k in Eq. (54) simply regenerates the same condition while switching the second-quantized operators associated with indices i and j generates lifted G and Q conditions from the lifted D condition. Reordering of the second-quantized operators in the L2 condition of Eq. (54), by contrast, produces the other nine lifted D conditions; for example, reordering L2 yields the L1 condition in Eq. (49). Similarly, for the pure (2,3)-positivity conditions, switching of the second-quantized operators with index k in T1 produces the T2 condition in Eq. (23). The other two distinct T2 conditions, $\bar{T}2$ and $\tilde{T}2$, in Eqs. (31) and (32) are generated not by switching but by reordering the second-quantized operators in the T2 condition of Eq. (23).

2. (2,4)-positivity conditions

The (2,4)-positivity conditions, arising from considering all $\hat{C}_i$ operators of degree $\leqslant 4$ in Eq. (6), consist of two classes of lifting conditions and one class of pure conditions, which are summarized in Table II. The two classes of lifting conditions are generated from lifting the two classes of (2,3)-positivity conditions. As in the previous section, the generalized lifting is performed by (i) inserting a creation operator into each $\hat{C}_i$ operator contributing to the condition, (ii) converting the inserted creation operator into an annihilation operator in the operator produced from step i, and (iii) adding the two lifted operators from steps i and ii together to produce a two-particle operator. The non-negativity of the resulting two-particle operator generates a lifting (2,4)-positivity condition. Representative lifting conditions for both classes are reported in Table II. The $\hat{C}$ operators in the first and second classes of lifted (2,3)-positivity conditions and the pure (2,4)-positivity condition are given by

$$\hat{C}(l,k,i,j) = \sum_{ijkl} b_{ij} d_k e_l \hat{a}_l^\dagger \hat{a}_k^\dagger \hat{a}_i^\dagger \hat{a}_j^\dagger, \quad (56)$$

$$\hat{C}(l,i,j,k) = \sum_{ijkl} b_{ijk} d_l \hat{a}_l^\dagger \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k^\dagger, \quad (57)$$

$$\hat{C}(i,j,k,l) = \sum_{ijkl} b_i d_j e_k f_l \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k^\dagger \hat{a}_l^\dagger, \quad (58)$$

where b_i, d_i, e_i, f_i, b_{ij}, b_{ijk}, and $\hat{a}_i^\dagger$ become b_i^*, d_i^*, e_i^*, f_i^*, b_{ij}^*, b_{ijk}^*, and $\hat{a}_i$, respectively, when $i = \bar{i}$. The rank of the largest tensor changes from 3 in Eq. (56) to 1 in Eq. (58) to effect the cancellation of the 3- and 4-RDOs in the combinations of operators in Table II. Fusing the tensors b_i and d_j into a single rank 2 tensor b_{ij} in Eq. (58), for example, would cause the operator combinations in Table II to depend on the 3- and 4-RDOs. Additional (2,4)-positivity conditions can be generated from the representative conditions through a combination of switching and reordering of the creation and annihilation operators.

The pure (2,4)-positivity conditions, presented in Ref. [28], depend upon only the 2-RDM through conic combinations that cancel the 3- and 4-RDMs. As in the (2,3) conditions, the cancellations depend upon the conic combination of pairs of operators that differ from each other by an odd number of switchings—exchanges of creators and annihilators. Generating an extreme condition on the 2-RDM requires that we consider the minimum number of conic combinations that effect the cancellation of the higher RDMs. Each pure (2,4)-positivity condition involves the conic combination of eight four-particle operators by Eq. (6). These eight four-particle operators can be grouped into the four pairs that depend upon only three-particle operators:

$$\hat{O}(\bar{i},j,k,l) + \hat{O}(\bar{i},\bar{j},\bar{k},\bar{l}), \quad (59)$$

$$\hat{O}(i,\bar{j},k,l) + \hat{O}(i,j,k,l), \quad (60)$$

$$\hat{O}(i,j,\bar{k},l) + \hat{O}(i,j,k,l), \quad (61)$$

$$\hat{O}(i,j,k,\bar{l}) + \hat{O}(i,j,k,l). \quad (62)$$

The operators in the first pair differ from each other by the switching of three creation and annihilation operators, while the operators in the other three pairs differ from each other by the switching of one creation operator and one annihilation operator. Rearranging the second-quantized operators in the four pairings into normal order with creators to the left of the annihilators generates expressions involving the sum of nine, five, three, and one 3-RDOs, respectively. Upon summation, the nine 3-RDOs from the one pairing with three switchings cancel with the five, three, and one 3-RDOs from the three pairings with one switching, and hence the final operator depends upon only the 2-RDO.

Other pure (2,4)-positivity conditions can be generated from the representative condition through switching and reordering of the second-quantized operators. To maintain the cancellation of the 3- and 4-RDOs, we must perform the same switching of creation and annihilation operators in each operator $\hat{C}(i,j,k,l)$ contributing to the condition. Because each fundamental second-quantized operator can be either a creation or an annihilation operator, there are 2^4, or 16, conditions from switching. Eight of these conditions can be

TABLE II. The (2,4)-positivity conditions can be derived from conic (linear non-negative) combinations of the (4,4)-positivity conditions that cancel the three- and four-particle operators.

Class	Type	Representative condition	$\hat{C}$ definition
1	Lifted (2,2)	$\mathrm{Tr}[(\hat{O}(l,k,i,j) + \hat{O}(l,\bar{k},i,j) + \hat{O}(\bar{l},k,i,j) + \hat{O}(\bar{l},\bar{k},i,j))\,^2D] \geqslant 0$	Eq. (56)
2	Lifted (2,3)	$\mathrm{Tr}[(\hat{O}(l,i,j,k) + \hat{O}(l,\bar{i},\bar{j},\bar{k}) + \hat{O}(\bar{l},\bar{i},\bar{j},\bar{k}) + \hat{O}(\bar{l},i,j,k))\,^2D] \geqslant 0$	Eq. (57)
3	Pure (2,4)	$\mathrm{Tr}[(3\hat{O}(i,j,k,l) + \hat{O}(i,j,k,\bar{l}) + \hat{O}(i,j,\bar{k},l) + \hat{O}(i,\bar{j},k,l) + \hat{O}(\bar{i},j,k,l) + \hat{O}(\bar{i},\bar{j},\bar{k},\bar{l}))\,^2D] \geqslant 0$	Eq. (58)

TABLE III. The representative pure (2,4)-positivity condition $g_1 \geqslant 0$ as well as three other conditions generated from its reordering, $g_2 \geqslant 0$, $g_3 \geqslant 0$, and $g_4 \geqslant 0$. Unlike the situation in the classical limit, in the quantum case additional conditions can be generated from each of the 16 conditions obtained from switching by reordering the creation and annihilation operators while preserving the cancellation of the three- and four-particle operators.

Condition	$\hat{C}$ definition
$g_1(^2D) = \mathrm{Tr}[(3\hat{O}(i,j,k,l) + \hat{O}(i,j,k,\bar{l}) + \hat{O}(i,j,\bar{k},l) + \hat{O}(i,\bar{j},k,l) + \hat{O}(\bar{i},j,k,l) + \hat{O}(\bar{i},\bar{j},\bar{k},\bar{l}))^2 D] \geqslant 0$	Eq. (58)
$g_2(^2D) = \mathrm{Tr}[(3\hat{O}(i,j,k,l) + \hat{O}(i,j,k,\bar{l}) + \hat{O}(i,\bar{k},j,l) + \hat{O}(k,\bar{j},i,l) + \hat{O}(j,\bar{i},k,l) + \hat{O}(\bar{i},\bar{j},\bar{k},\bar{l}))^2 D] \geqslant 0$	Eq. (58)
$g_3(^2D) = \mathrm{Tr}[(3\hat{O}(i,j,k,l) + \hat{O}(i,j,\bar{l},k) + \hat{O}(i,l,\bar{k},j) + \hat{O}(k,\bar{j},i,l) + \hat{O}(j,\bar{i},k,l) + \hat{O}(\bar{i},\bar{j},\bar{k},\bar{l}))^2 D] \geqslant 0$	Eq. (58)
$g_4(^2D) = \mathrm{Tr}[(3\hat{O}(i,j,k,l) + \hat{O}(i,j,k,\bar{l}) + \hat{O}(i,\bar{k},j,l) + \hat{O}(k,\bar{j},i,l) + \hat{O}(j,\bar{i},k,l) + \hat{O}(\bar{i},\bar{j},\bar{k},\bar{l}))^2 D] \geqslant 0$	Eq. (58)

generated from the other eight conditions by switching all creation and annihilation operators by particle-hole symmetry. In the limit that the expansion coefficients b_i, d_j, e_k, and f_l become orthogonal unit vectors, these 16 conditions reduce to the 16 conditions in the (2,4) class of the classical (or diagonal) N-representability problem [8,36,37]. The quantum mechanical formulation of these conditions, however, is much more general because the expansion coefficients need not be orthogonal. When the expansion coefficients are nonorthogonal, the creation and annihilation operators become noncommutative operators, and hence, the conditions depend upon their ordering.

In the quantum case additional conditions can be generated from each of the 16 conditions by reordering the creation and annihilation operators while preserving the cancellation of the 3- and 4-RDOs. These additional conditions are related to the original 16 conditions as the generalized T2 conditions are related to the T2 condition in the (2,3)-positivity conditions. Table III reports the representative pure (2,4)-positivity condition as well as three other conditions generated from its reordering. Each of these four conditions differs from the others by a few terms involving the 2-RDM. For example, the first and second conditions differ by only one term,

$$g_2 = g_1 + 4\mathrm{Re}\left(\alpha\beta \sum_{ik;i'l'} b_i e_k\, {}^2D^{ik}_{i'l'}\, b^*_{i'} f^*_{l'}\right) \geqslant 0, \tag{63}$$

where

$$\alpha = \sum_j d_j e^*_j, \tag{64}$$

$$\beta = \sum_j f_j d^*_j, \tag{65}$$

and Re selects the real part of the expression. When this term is negative, inequality g_2 is stronger than g_1, but when this term is positive, inequality g_1 is stronger than g_2. In the classical case, where the expansion coefficients are orthogonal, these two conditions are equivalent because both α and β are 0, and hence, this additional term vanishes.

3. (2,5)-positivity conditions

The (2,5)-positivity conditions are generated by considering all $\hat{C}_i$ operators of degree $\leqslant$5 in Eq. (6). These conditions consist of three classes of lifting conditions and three classes of pure conditions, which are listed in Table IV. The lifting conditions arise from lifting the three classes of (2,4)-positivity conditions. The $\hat{C}$ operators of the first, second, and third classes of lifting conditions are given by

$$\hat{C}(m,l,k,i,j) = \sum_{ijklm} b_{ij} d_k e_l f_m \hat{a}^\dagger_m \hat{a}^\dagger_l \hat{a}^\dagger_k \hat{a}^\dagger_i \hat{a}^\dagger_j, \tag{66}$$

$$\hat{C}(m,l,i,j,k) = \sum_{ijklm} b_{ijk} d_l e_m \hat{a}^\dagger_m \hat{a}^\dagger_l \hat{a}^\dagger_i \hat{a}^\dagger_j \hat{a}^\dagger_k, \tag{67}$$

$$\hat{C}(m,i,j,k,l) = \sum_{ijklm} b_i d_j e_k f_l g_m \hat{a}^\dagger_m \hat{a}^\dagger_i \hat{a}^\dagger_j \hat{a}^\dagger_k \hat{a}^\dagger_l, \tag{68}$$

respectively, and the $\hat{C}$ operators of the three classes of pure conditions are given by

$$\hat{C}(i,j,k,l,m) = \sum_{ijklm} b_i d_j e_k f_l g_m \hat{a}^\dagger_i \hat{a}^\dagger_j \hat{a}^\dagger_k \hat{a}^\dagger_l \hat{a}^\dagger_m, \tag{69}$$

where b_i, d_i, e_i, f_i, g_i, b_{ij}, b_{ijk}, and $\hat{a}^\dagger_i$ become b^*_i, d^*_i, e^*_i, f^*_i, g^*_i, b^*_{ij}, b^*_{ijk}, and $\hat{a}_i$, respectively, when $i = \bar{i}$. Note that the operators in Eqs. (68) and (69) are not equivalent after switching. Switching of creators to annihilators in the $\hat{C}$ operators in the representative conditions in Table IV produces 16, 32, and 32 conditions in the pure classes 4, 5, and 6, respectively. Class 4 has fewer conditions because its conditions, unlike those in classes 5 and 6, possess particle-hole symmetry. Particle-hole symmetry is present in all of the pure (2,3)-positivity conditions and none of the pure (2,4) conditions. Additional conditions can be generated from the representative conditions through reordering of the creation and annihilation operators. Like the (2,3)- and (2,4)-positivity conditions, the (2,5) conditions generate all of the classical (diagonal) N-representability conditions when the expansion coefficients b_i, d_j, e_k, f_l, and g_m are chosen to be orthogonal unit vectors.

4. (2,6)-positivity conditions

As with the (2,q)-positivity conditions for $q \leqslant 5$, the (2,6)-positivity conditions are generated from Eq. (6) by considering all $\hat{C}_i$ operators of degree $\leqslant$6. Six classes of lifting (2,6)-positivity conditions arise from lifting the six classes of (2,5)-positivity conditions. While not shown explicitly, the representative conditions can be readily constructed from the conditions in Table IV. There are also 18 classes of pure (2,6)-positivity conditions. The $\hat{C}$ operators of these 18 conditions are given by

$$\hat{C}(ijklmn) = \sum_{ijklmn} b_i d_j e_k f_l g_m h_n \hat{a}^\dagger_i \hat{a}^\dagger_j \hat{a}^\dagger_k \hat{a}^\dagger_l \hat{a}^\dagger_m \hat{a}^\dagger_n, \tag{70}$$

where b_i, d_i, e_i, f_i, g_i, h_i, and $\hat{a}^\dagger_i$ become b^*_i, d^*_i, e^*_i, f^*_i, g^*_i, h^*_i, and a_i, respectively, when $i = \bar{i}$. Table V lists a representative

TABLE IV. The (2,5)-positivity conditions can be derived from conic (linear non-negative) combinations of the (5,5)-positivity conditions that cancel the three-, four-, and five-particle operators.

Class	Type	Representative condition	$\hat{C}$ definition
1	Lifted (2,2)	$\mathrm{Tr}[(\hat{O}(m,l,k,i,j)+\hat{O}(m,\bar{l},k,i,j)+\hat{O}(\bar{m},l,k,i,j)+\hat{O}(\bar{m},\bar{l},k,i,j)$ $+\hat{O}(m,l,\bar{k},i,j)+\hat{O}(m,\bar{l},\bar{k},i,j)+\hat{O}(\bar{m},l,\bar{k},i,j)+\hat{O}(\bar{m},\bar{l},\bar{k},i,j))^2D]\geqslant 0$	Eq. (66)
2	Lifted (2,3)	$\mathrm{Tr}[(\hat{O}(m,l,i,j,k)+\hat{O}(m,l,\bar{i},\bar{j},\bar{k})+\hat{O}(\bar{m},l,\bar{i},\bar{j},\bar{k})+\hat{O}(\bar{m},l,i,j,k)$ $+\hat{O}(m,\bar{l},i,j,k)+\hat{O}(m,\bar{l},\bar{i},\bar{j},\bar{k})+\hat{O}(\bar{m},\bar{l},\bar{i},\bar{j},\bar{k})+\hat{O}(\bar{m},\bar{l},i,j,k))^2D]\geqslant 0$	Eq. (67)
3	Lifted (2,4)	$\mathrm{Tr}[(3\hat{O}(m,i,j,k,l)+\hat{O}(m,i,j,k,\bar{l})+\hat{O}(m,i,j,\bar{k},l)$ $+\hat{O}(m,i,\bar{j},k,l)+\hat{O}(m,\bar{i},j,k,l)+\hat{O}(m,\bar{i},\bar{j},\bar{k},\bar{l})$ $+3\hat{O}(\bar{m},i,j,k,l)+\hat{O}(\bar{m},i,j,k,\bar{l})+\hat{O}(\bar{m},i,j,\bar{k},l)$ $+\hat{O}(\bar{m},i,\bar{j},k,l)+\hat{O}(\bar{m},\bar{i},j,k,l)+\hat{O}(\bar{m},\bar{i},\bar{j},\bar{k},\bar{l}))^2D]\geqslant 0$	Eq. (68)
4	Pure (2,5)	$\mathrm{Tr}[(3\hat{O}(i,j,k,l,m)+\hat{O}(i,j,k,l,\bar{m})+\hat{O}(i,j,k,\bar{l},m)$ $+\hat{O}(i,j,\bar{k},l,m)+\hat{O}(i,\bar{j},k,l,m)+\hat{O}(\bar{i},j,k,l,m)$ $+3\hat{O}(\bar{i},\bar{j},\bar{k},\bar{l},\bar{m})+\hat{O}(\bar{i},\bar{j},\bar{k},\bar{l},m)+\hat{O}(\bar{i},\bar{j},\bar{k},l,\bar{m})$ $+\hat{O}(\bar{i},\bar{j},k,\bar{l},\bar{m})+\hat{O}(\bar{i},j,\bar{k},\bar{l},\bar{m})+\hat{O}(i,\bar{j},\bar{k},\bar{l},\bar{m}))^2D]\geqslant 0$	Eq. (69)
5	Pure (2,5)	$\mathrm{Tr}[(6\hat{O}(i,j,k,l,m)+3\hat{O}(i,j,k,l,\bar{m})+3\hat{O}(i,j,k,\bar{l},m)$ $+3\hat{O}(i,j,\bar{k},l,m)+3\hat{O}(i,\bar{j},k,l,m)+3\hat{O}(\bar{i},j,k,l,m)$ $+\hat{O}(i,j,k,\bar{l},\bar{m})+\hat{O}(i,j,\bar{k},l,\bar{m})+\hat{O}(i,j,\bar{k},\bar{l},m)$ $+\hat{O}(i,\bar{j},k,l,\bar{m})+\hat{O}(i,\bar{j},k,\bar{l},m)+\hat{O}(i,\bar{j},\bar{k},l,m)$ $+\hat{O}(\bar{i},j,k,l,\bar{m})+\hat{O}(\bar{i},j,k,\bar{l},m)+\hat{O}(\bar{i},j,\bar{k},l,m)$ $+\hat{O}(\bar{i},\bar{j},k,l,m)+\hat{O}(\bar{i},\bar{j},\bar{k},\bar{l},\bar{m}))^2D]\geqslant 0$	Eq. (69)
6	Pure (2,5)	$\mathrm{Tr}[(6\hat{O}(i,j,k,l,m)+3\hat{O}(i,j,k,l,\bar{m})+3\hat{O}(i,j,k,\bar{l},m)$ $+3\hat{O}(i,j,\bar{k},l,m)+3\hat{O}(i,\bar{j},k,l,m)+\hat{O}(\bar{i},j,k,l,m)$ $+\hat{O}(i,j,k,\bar{l},\bar{m})+\hat{O}(i,j,\bar{k},l,\bar{m})+\hat{O}(i,j,\bar{k},\bar{l},m)$ $+\hat{O}(i,\bar{j},k,l,\bar{m})+\hat{O}(i,\bar{j},k,\bar{l},m)+\hat{O}(i,\bar{j},\bar{k},l,m)$ $+\hat{O}(i,j,k,l,\bar{m})+\hat{O}(i,j,k,\bar{l},m)+\hat{O}(i,j,\bar{k},l,m)$ $+\hat{O}(i,\bar{j},k,l,m)+3\hat{O}(\bar{i},\bar{j},\bar{k},\bar{l},\bar{m}))^2D]\geqslant 0$	Eq. (69)

operator for each of the 18 classes. Each representative operator arises from the conic combination of potentially 2^6 (or 64) six-particle operators, which are distinguished from each other by the switching between creation and annihilation operators. These 64 operators are grouped into 32 particle-hole pairs listed in the rows in Table V. For each of the 18 representative conditions, the non-negative integer weights α and β of the operators in each pair are reported. The conic combination of all 32 pairs with the weights in the xth column generates a representative operator for class x. The operator for each class depends only on the 2-RDO, with the dependence on the three-, four-, five-, and six-RDOs canceling through the conic combination. The trace of each representative operator against the 2-RDM generates a representative condition on the 2-RDM. Additional (2,6)-positivity conditions can be generated from the representative conditions through a combination of switching and reordering of the creation and annihilation operators. From the particle-hole pairing it is easy to observe that only one class of the (2,6) conditions—class 4—has particle-hole symmetry, that is, $\alpha=\beta$ in all pairs.

The (2,6)-positivity conditions yield all classes of the classical (diagonal) N-representability conditions when the expansion coefficients b_i, d_j, e_k, f_l, g_m, and h_n are chosen to be orthogonal unit vectors. Classically, all classes of (2,q) conditions for $q\leqslant 5$ are in the form of hypermetric inequalities [36,37]. When $q=6$, however, new classes of classical N-representability conditions emerge [8,36,37,52]. In the classical limit, the first 6 classes of pure (2,6)-positivity conditions in Table V reduce to hypermetric inequalities, while the remaining 12 can be grouped into cycle, parachute, and Grishukhin inequalities [52].

III. DISCUSSION AND CONCLUSIONS

Both new and known N-representability conditions on the 2-RDM have been derived from the constructive solution to the N-representability problem [28]. In addition to all of the previously known conditions, we generate new (2,3)-, (2,4)-, (2,5), and (2,6)-conditions where the first number p in each pair indicates the highest p-RDM required to evaluate the condition (the 2-RDM in our case) and the second number q indicates the highest RDMs canceled by conic (linear non-negative) combinations in the derivation of the condition. There are two classes of (2,3) conditions: (i) lifting conditions. which are derivable from lifting the D, Q, and G (2-positivity) conditions to the three-particle space, and (ii) pure conditions, which are not derivable from lifting and, hence, are without precedent in the 2-positivity conditions. The (2,4) conditions have 2 classes of lifting conditions and 1 class of pure conditions, the (2,5) conditions have 3 classes of lifting conditions and 3 classes of pure conditions, and the (2,6) conditions have 6 classes of lifting conditions and 18 classes of pure conditions. A similar procedure of using conic combinations to cancel operators higher than two-body can be followed to derive the (2,q) conditions for $q>6$.

The classical (diagonal) N-representability conditions [8, 34–37] are constraints on the two-electron reduced density function, the diagonal part of the 2-RDM, to ensure that

TABLE V. The (2,6)-positivity conditions can be derived from conic combinations of the (6,6)-positivity conditions that cancel the three-, four-, five-, and six-particle operators. There are six classes of lifting conditions (not shown) and 18 classes of pure conditions (shown). The table lists a representative operator for each of the 18 classes. The conic combination of all 32 pairs with the weights in the xth column generates a representative operator for class x. The trace of each representative operator against the 2-RDM generates a representative condition on the 2-RDM.

	Weight (α/β)																	
Operator	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
$\alpha\hat{O}(ijklmn)+\beta\hat{O}(\bar{i}\bar{j}\bar{k}\bar{l}\bar{m}\bar{n})$	20/2	12/6	20/6	12/12	20/12	20/12	9/6	5/3	9/5	9/3	5/2	14/9	14/6	14/3	6/3	6/5	1/6	3/3
$\alpha\hat{O}(ijklm\bar{n})+\beta\hat{O}(\bar{i}\bar{j}\bar{k}\bar{l}\bar{m}n)$	12/0	6/2	12/2	6/6	12/6	12/6	5/3	2/1	3/1	5/1	3/1	9/5	9/3	9/1	5/2	5/3	0/3	2/1
$\alpha\hat{O}(ijkl\bar{m}n)+\beta\hat{O}(\bar{i}\bar{j}\bar{k}\bar{l}m\bar{n})$	12/0	6/2	12/2	6/6	12/6	12/6	6/3	3/1	6/3	6/1	3/1	9/5	9/3	9/1	3/1	3/3	0/3	1/1
$\alpha\hat{O}(ijkl\bar{m}\bar{n})+\beta\hat{O}(\bar{i}\bar{j}\bar{k}\bar{l}mn)$	6/0	2/0	6/0	2/2	6/2	6/2	3/1	1/0	1/0	3/0	1/0	5/2	5/1	5/0	3/1	2/1	0/1	1/0
$\alpha\hat{O}(ijk\bar{l}mn)+\beta\hat{O}(\bar{i}\bar{j}\bar{k}l\bar{m}\bar{n})$	12/0	6/2	12/2	6/6	12/6	12/6	5/3	2/1	5/2	5/1	3/1	9/5	9/3	9/1	3/1	3/2	0/3	3/2
$\alpha\hat{O}(ijk\bar{l}m\bar{n})+\beta\hat{O}(\bar{i}\bar{j}\bar{k}l\bar{m}n)$	6/0	2/0	6/0	2/2	6/2	6/2	2/1	0/0	1/0	2/0	1/0	5/2	5/1	5/0	2/0	3/1	0/1	3/1
$\alpha\hat{O}(ijk\bar{l}\bar{m}n)+\beta\hat{O}(\bar{i}\bar{j}\bar{k}lm\bar{n})$	6/0	2/0	6/0	2/2	6/2	6/2	3/1	1/0	3/1	3/0	2/1	5/2	5/1	5/0	1/0	1/1	0/1	2/1
$\alpha\hat{O}(ijk\bar{l}\bar{m}\bar{n})+\beta\hat{O}(\bar{i}\bar{j}\bar{k}lmn)$	2/2	0/0	2/0	0/0	2/0	2/0	1/0	0/0	0/0	1/0	0/0	2/0	2/0	2/0	1/0	1/0	1/0	3/1
$\alpha\hat{O}(ij\bar{k}lmn)+\beta\hat{O}(\bar{i}\bar{j}k\bar{l}\bar{m}\bar{n})$	12/0	6/2	12/2	6/6	12/6	12/6	3/2	3/2	6/3	6/2	3/1	6/3	9/3	6/0	3/1	3/2	1/5	2/3
$\alpha\hat{O}(ij\bar{k}lm\bar{n})+\beta\hat{O}(\bar{i}\bar{j}k\bar{l}\bar{m}n)$	6/0	2/0	6/0	2/2	6/2	6/2	1/1	1/1	2/1	3/1	2/1	3/1	5/1	3/0	3/1	3/1	0/2	1/1
$\alpha\hat{O}(ij\bar{k}l\bar{m}n)+\beta\hat{O}(\bar{i}\bar{j}k\bar{l}m\bar{n})$	6/0	2/0	6/0	2/2	6/2	6/2	1/0	1/0	3/1	3/0	1/0	3/1	5/1	3/0	1/0	1/1	0/2	0/1
$\alpha\hat{O}(ij\bar{k}l\bar{m}\bar{n})+\beta\hat{O}(\bar{i}\bar{j}k\bar{l}mn)$	2/2	0/0	2/0	0/0	2/0	2/0	0/0	0/0	0/0	1/0	0/0	1/0	2/0	1/1	2/1	1/0	0/0	0/0
$\alpha\hat{O}(ij\bar{k}\bar{l}mn)+\beta\hat{O}(\bar{i}\bar{j}kl\bar{m}\bar{n})$	6/0	2/0	6/0	2/2	6/2	6/2	1/1	1/1	3/1	3/1	2/1	3/1	5/1	3/0	1/0	1/0	1/3	1/1
$\alpha\hat{O}(ij\bar{k}\bar{l}m\bar{n})+\beta\hat{O}(\bar{i}\bar{j}kl\bar{m}n)$	2/2	0/0	2/0	0/0	2/0	2/0	0/1	0/1	1/1	1/1	1/1	1/0	2/0	1/1	1/0	2/0	1/1	1/0
$\alpha\hat{O}(ij\bar{k}\bar{l}\bar{m}n)+\beta\hat{O}(\bar{i}\bar{j}klm\bar{n})$	2/2	0/0	2/0	0/0	2/0	2/0	0/0	0/0	1/0	1/0	1/1	1/0	2/0	1/1	0/0	0/0	1/1	0/0
$\alpha\hat{O}(i\bar{j}klmn)+\beta\hat{O}(\bar{i}j\bar{k}\bar{l}\bar{m}\bar{n})$	12/0	6/2	12/2	6/6	6/2	12/6	3/1	3/1	5/2	5/1	2/0	3/1	3/0	9/1	1/0	1/1	1/5	1/1
$\alpha\hat{O}(i\bar{j}klm\bar{n})+\beta\hat{O}(\bar{i}j\bar{k}\bar{l}\bar{m}n)$	6/0	2/0	6/0	2/2	2/0	6/2	1/0	1/0	1/0	2/0	1/0	1/0	1/0	5/0	1/0	1/0	1/3	1/0
$\alpha\hat{O}(i\bar{j}kl\bar{m}n)+\beta\hat{O}(\bar{i}j\bar{k}\bar{l}m\bar{n})$	6/0	2/0	6/0	2/2	2/0	6/2	2/0	2/0	3/1	3/0	1/0	1/0	1/0	5/0	0/0	0/1	1/3	0/0
$\alpha\hat{O}(i\bar{j}kl\bar{m}\bar{n})+\beta\hat{O}(\bar{i}j\bar{k}\bar{l}mn)$	2/2	0/0	2/0	0/0	0/0	2/0	1/0	1/0	0/0	1/0	0/0	0/0	0/1	2/0	1/1	0/0	2/2	1/0
$\alpha\hat{O}(i\bar{j}k\bar{l}mn)+\beta\hat{O}(\bar{i}j\bar{k}l\bar{m}\bar{n})$	6/0	2/0	6/0	2/2	2/0	6/2	1/0	1/0	2/0	2/0	1/0	1/0	1/0	5/0	0/0	0/0	0/2	1/0
$\alpha\hat{O}(i\bar{j}k\bar{l}m\bar{n})+\beta\hat{O}(\bar{i}j\bar{k}l\bar{m}n)$	2/2	0/0	2/0	0/0	0/0	2/0	0/0	0/0	0/0	0/0	0/0	0/0	0/1	2/0	0/0	1/0	1/1	2/0
$\alpha\hat{O}(i\bar{j}k\bar{l}\bar{m}n)+\beta\hat{O}(\bar{i}j\bar{k}lm\bar{n})$	2/2	0/0	2/0	0/0	0/0	2/0	1/0	1/0	1/0	1/0	1/1	0/0	0/1	2/0	0/1	0/1	1/1	1/0
$\alpha\hat{O}(i\bar{j}\bar{k}lmn)+\beta\hat{O}(\bar{i}jk\bar{l}\bar{m}\bar{n})$	6/0	2/0	6/0	2/2	2/0	6/2	0/0	2/1	3/1	3/1	1/0	0/0	1/0	3/0	0/0	0/0	0/3	1/2
$\alpha\hat{O}(i\bar{j}\bar{k}lm\bar{n})+\beta\hat{O}(\bar{i}jk\bar{l}\bar{m}n)$	2/2	0/0	2/0	0/0	0/0	2/0	0/1	1/1	1/1	1/1	1/1	0/1	0/1	1/1	1/1	1/0	0/1	1/1
$\alpha\hat{O}(i\bar{j}\bar{k}l\bar{m}n)+\beta\hat{O}(\bar{i}jk\bar{l}m\bar{n})$	2/2	0/0	2/0	0/0	0/0	2/0	0/0	1/0	1/0	1/0	0/0	0/1	0/1	1/1	0/1	0/1	0/1	0/1
$\alpha\hat{O}(i\bar{j}\bar{k}\bar{l}mn)+\beta\hat{O}(\bar{i}jkl\bar{m}\bar{n})$	2/2	0/0	2/0	0/0	0/0	2/0	0/1	1/1	1/0	1/1	1/1	0/1	0/1	1/1	0/1	0/0	0/1	0/0
$\alpha\hat{O}(\bar{i}jklmn)+\beta\hat{O}(i\bar{j}\bar{k}\bar{l}\bar{m}\bar{n})$	12/0	6/2	6/0	2/2	6/2	2/0	5/3	3/2	3/1	3/0	3/1	6/3	6/1	6/0	5/3	3/3	0/3	1/2
$\alpha\hat{O}(\bar{i}jklm\bar{n})+\beta\hat{O}(i\bar{j}\bar{k}\bar{l}\bar{m}n)$	6/0	2/0	2/0	0/0	2/0	0/0	2/1	1/1	0/0	1/0	2/1	3/1	3/0	3/0	3/1	2/1	0/1	0/0
$\alpha\hat{O}(\bar{i}jkl\bar{m}n)+\beta\hat{O}(i\bar{j}\bar{k}\bar{l}m\bar{n})$	6/0	2/0	2/0	0/0	2/0	0/0	3/1	2/1	2/1	2/0	2/1	3/1	3/0	3/0	2/1	1/2	0/1	0/1
$\alpha\hat{O}(\bar{i}jk\bar{l}mn)+\beta\hat{O}(i\bar{j}\bar{k}l\bar{m}\bar{n})$	6/0	2/0	2/0	0/0	2/0	0/0	2/1	1/1	1/0	1/0	1/0	3/1	3/0	3/0	3/2	1/1	0/1	1/1
$\alpha\hat{O}(\bar{i}j\bar{k}lmn)+\beta\hat{O}(i\bar{j}k\bar{l}\bar{m}\bar{n})$	6/0	2/0	2/0	0/0	2/0	0/0	1/1	1/1	1/0	1/0	1/0	1/0	3/0	1/0	2/1	1/1	1/3	1/3
$\alpha\hat{O}(\bar{i}\bar{j}klmn)+\beta\hat{O}(ij\bar{k}\bar{l}\bar{m}\bar{n})$	6/0	2/0	2/0	0/0	0/0	0/0	1/0	1/0	1/0	1/0	1/0	0/0	0/0	3/0	1/1	0/1	0/2	0/1

it represents an N-electron density function. A solution to the diagonal problem was developed in the context of both the Boole 0-1 programming problem and the maximum cut problem of graph theory [37,53]. The recent constructive solution of the N-representability problem for fermionic density matrices extends the classical solution to the more general quantum case. All of the quantum conditions can be cast in the form of restricting the trace of two-body operators (model Hamiltonians) against the 2-RDM to be non-negative. In the limit that all tensors in the model Hamiltonians are decomposed into products of orthogonal rank 1 (one-index) tensors, the quantum conditions reduce to the classical (diagonal) conditions for all unitary transformations of the one-electron basis set. The quantum (2,6) conditions presented here reduce in the classical limit to the complete set of classical (2,6) conditions [36,37], which were shown to be complete by Grishukhin [52].

A significant difference between the classical and the quantum conditions is the orthogonality (classical) or nonorthogonality (quantum) of the rank 1 tensors. Consequently, in the classical case the creation and annihilation operators form a commutative algebra, while in the quantum case they form a noncommutative algebra. The nonorthogonality leads to active N-representability conditions on the 2-RDM that lack a classical analog. For example, all classes of lifting conditions that we presented are inactive in the classical limit. Because the creation and annihilation operators commute, each class of classical $(2,q)$-lifting conditions reduces to a class of classical $(2,p)$-pure conditions where $p < q$. Furthermore, typically more than one pure quantum condition reduces to each classical condition in the classical limit. Table III lists four pure (2,4) conditions that reduce to the same classical condition. These quantum conditions differ only in the ordering of the creation and annihilation operators—

a difference that disappears in the classical, commutative limit.

The conic combination of the extreme two-body operators in the N-representability conditions forms a convex set (cone) of model Hamiltonians for which the N-representability conditions are exact. From the perspective of quantum information the computational complexity of enforcing all N-representability conditions on the 2-RDM can be shown to be nondeterministic polynomial-time complete, meaning that in the worst-case scenario, enforcing exact N representability scales nonpolynomially with system size. Despite this complexity, however, many realistic quantum systems are much more tractable than the worst-case scenario implies. For example, the 2-positivity conditions, particularly the G condition, are exact for pairing Hamiltonians whose ground states are antisymmetrized geminal power wave functions. Such pairing Hamiltonians have been employed to model the Cooper pairing and long-range order associated with superconductivity. For any strength of interaction the ground-state energy for this class of Hamiltonians can be computed in polynomial time.

More generally, for fixed q the $(2,q)$-positivity conditions, which contain the lower positivity conditions, cover a large class of model Hamiltonians whose ground states are computable in polynomial time—in a time that scales polynomially with system size. Even when the Hamiltonian of interest is not rigorously contained in this class, the associated N-representability conditions, which intrinsically are not constrained by the approximations of perturbation theory, may produce an accurate lower bound on the ground-state energy. Computational experience with the variational calculation of the 2-RDM in atoms and molecules [3,14,15,18,25,26,54,55] shows that sufficiently accurate lower-bound ground-state energies are often produced with $(2,q)$-positivity conditions where $q \leqslant 3$.

The practical implementation of the variational 2-RDM method requires that the energy be minimized as a functional of the 2-RDM constrained by its N-representability conditions. Both the 2-positivity conditions and the T1 and T2 conditions can be expressed as positive semidefinite constraints (also known as linear matrix inequalities) in which metric matrices are constrained to be positive semidefinite. These constraints on the 2-RDM can be imposed during the minimization of the ground-state energy through a genre of constrained optimization known as semidefinite programming [14–16,21,23,24,47–49]. The remaining $(2,q)$-positivity conditions, however, cannot be expressed as a traditional semidefinite constraint because the coefficients in the $\hat{C}_i$ operators must be tensor decomposed to remove the dependence of the constraints on the higher RDMs. Practically, as described in Sec. II B, these constraints can be added to the semidefinite program through recursively generated linear inequalities, similar to those described in Ref. [50] for T2.

The constructive solution of N representability establishes 2-RDM theory as a fundamental theory for many-particle quantum mechanics for particles with pairwise interactions. Lower bounds on the ground-state energy can be computed and improved systematically within the theory. While not all of the 2-RDM conditions will be imposed in practical calculations, a complete knowledge of the conditions—their form and function—can be invaluable in devising and testing approximate N-representability conditions for different types of quantum systems and interactions. Like Feynman diagrams, the positivity conditions represent different physical interactions of the electrons. Adding positivity conditions to the 2-RDM calculation expands the class of exactly describable model Hamiltonians. Just as classes of Feynman diagrams differ in importance according to the nature of the interaction, for a given system some positivity conditions will be significantly more important than others. For example, both the G and the T2 conditions have proven to be especially important in calculations of many-electron atoms and molecules [14,15,17], while the T1 condition has rarely been of any significance. Similar evaluations must be performed in a variety of many-electron quantum systems for the conditions resulting from the constructive solution.

Previous variational 2-RDM computations on metallic hydrogen chains [55], polyaromatic hydrocarbons [25,26], and firefly luciferin [54] show that they can capture strong, multireference correlation effects for which appropriate ansätze for the wave function are difficult to construct. With a suitable choice of N-representability conditions, therefore, strong electron correlation effects can be computed at a computational cost that scales polynomially with the system size. Although the exploration of the conditions following from the constructive solution is still in its earliest stages, a 2-RDM-based theory with systematically improvable accuracy promises fresh theoretical and computational possibilities for treating strong correlation in quantum many-electron systems.

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[1] D. A. Mazziotti, ed., *Reduced-Density-Matrix Mechanics: With Application to Many-Electron Atoms and Molecules*, *Advances in Chemical Physic*, Vol. 134 (Wiley, New York, 2007).
[2] A. J. Coleman and V. I. Yukalov, *Reduced Density Matrices: Coulson's Challenge* (Springer, New York, 2000).
[3] D. A. Mazziotti, Chem. Rev. **112**, 244 (2012).
[4] A. J. Coleman, Rev. Mod. Phys. **35**, 668 (1963).
[5] C. Garrod and J. Percus, J. Math. Phys. **5**, 1756 (1964).
[6] H. Kummer, J. Math. Phys. **8**, 2063 (1967).
[7] J. E. Harriman, Phys. Rev. A **17**, 1257 (1978).
[8] R. M. Erdahl, Int. J. Quantum Chem. **13**, 697 (1978).
[9] J. K. Percus, Int. J. Quantum Chem. **13**, 89 (1978).
[10] R. M. Erdahl and B. Jin, in *Many-electron Densities and Density Matrices*, edited by J. Cioslowski (Kluwer, Boston, 2000) .

[11] D. A. Mazziotti and R. M. Erdahl, Phys. Rev. A **63**, 042113 (2001).
[12] M. Nakata, H. Nakatsuji, M. Ehara, M. Fukuda, K. Nakata, and K. Fujisawa, J. Chem. Phys. **114**, 8282 (2001).
[13] D. A. Mazziotti, Phys. Rev. A **65**, 062511 (2002).
[14] D. A. Mazziotti, Phys. Rev. Lett. **93**, 213001 (2004).
[15] Z. Zhao, B. J. Braams, H. Fukuda, M. L. Overton, and J. K. Percus, J. Chem. Phys. **120**, 2095 (2004).
[16] E. Cancés, G. Stoltz, and M. Lewin, J. Chem. Phys. **125**, 064101 (2006).
[17] D. A. Mazziotti, Phys. Rev. A **72**, 032510 (2005).
[18] D. A. Mazziotti, Phys. Rev. A **74**, 032501 (2006).
[19] G. Gidofalvi and D. A. Mazziotti, J. Chem. Phys. **126**, 024105 (2007).
[20] R. M. Erdahl, in *Reduced-Density-Matrix Mechanics: With Application to Many-Electron Atoms and Molecules*, *Advances in Chemical Physic*, edited by D. A. Mazziotti, Vol. 134 (Wiley, New York, 2007) .
[21] B. Verstichel, H. van Aggelen, D. Van Neck, P. W. Ayers, and P. Bultinck, Phys. Rev. A **80**, 032508 (2009).
[22] N. Shenvi and A. F. Izmaylov, Phys. Rev. Lett. **105**, 213003 (2010).
[23] D. A. Mazziotti, Phys. Rev. Lett. **106**, 083001 (2011).
[24] T. Baumgratz and M. B. Plenio, New J. Phys. **14**, 023027 (2012).
[25] G. Gidofalvi and D. A. Mazziotti, J. Chem. Phys. **129**, 134108 (2008).
[26] K. Pelzer, L. Greenman, G. Gidofalvi, and D. A. Mazziotti, J. Phys. Chem. A **114**, 583 (2011).
[27] A. E. Rothman and D. A. Mazziotti, Phys. Rev. A **78**, 032510 (2008).
[28] D. A. Mazziotti, Phys. Rev. Lett. (in press); arXiv:1112.5866v1 [quant-ph].
[29] Z. Huang and S. Kais, Chem. Phys. Lett. **413**, 1 (2005).
[30] M. Mella and J. B. Anderson, J. Chem. Phys. **119**, 8225 (2003).
[31] R. G. Parr and W. Yang, *Density Functional Theory* (Oxford University Press, Oxford, UK, 1994).
[32] A. Chakraborty and S. Hammes-Schiffer, J. Chem. Phys. **129**, 204101 (2008).
[33] M. Fukuda, B. J. Braams, M. Nakata, M. L. Overton, J. K. Percus, M. Yamashita, and Z. Zhao, Math. Program. Ser. B **109**, 553 (2007).
[34] E. B. Wilson and F. Weinhold, J. Chem. Phys. **47**, 2298 (1967).
[35] M. L. Yoseloff and H. W. Kuhn, J. Math. Phys. **10**, 703 (1969).
[36] W. B. McRae and E. R. Davidson, J. Math. Phys. **13**, 1527 (1972).
[37] M. M. Deza and M. Laurent, *Geometry of Cuts and Metrics* (Springer, New York, 1997).
[38] E. Kamarchik and D. A. Mazziotti, Phys. Rev. Lett. **99**, 243002 (2007).
[39] J. R. Hammond and D. A. Mazziotti, Phys. Rev. A **71**, 062503 (2005).
[40] D. A. Mazziotti, Phys. Rev. A **57**, 4219 (1998).
[41] J. E. Mayer, Phys. Rev. **100**, 1579 (1955).
[42] R. H. Tredgold, Phys. Rev. **105**, 1421 (1957).
[43] R. T. Rockafellar, *Convex Analysis* (Princeton University Press, Princeton, NJ, 1970).
[44] J. W. Helton, Ann. Math. **156**, 675 (2002).
[45] L. Vandenberghe and S. Boyd, SIAM Rev. **38**, 49 (1996).
[46] R. S. H. Wolkowicz and L. Vandenberghe, eds., *Handbook of Semidefinite Programming: Theory, Algorithms, and Applications* (Kluwer Academic, Lowell, MA, 2000).
[47] M. Fukuda, M. Nakata, and M. Yamashita, in *Reduced-Density-Matrix Mechanics: With Application to Many-Electron Atoms and Molecules*, *Advances in Chemical Physic,* edited by D. A. Mazziotti, Vol. 134 (Wiley, New York, 2007) .
[48] D. A. Mazziotti, Math. Model. Numer. Anal. **41**, 249 (2007).
[49] R. M. Erdahl, Rep. Math. Phys. **15**, 147 (1979).
[50] T. Juhász, N. Shenvi, and D. A. Mazziotti, Chem. Phys. Lett. **445**, 79 (2007).
[51] W. Slebodzinski, *Exterior Forms and Their Applications* (Polish Scientific, Warsaw, 1970).
[52] V. P. Grishukhin, Eur. J. Combin. **11**, 115 (1990).
[53] I. Pitowsky, Math. Program. **50**, 395 (1991).
[54] L. Greenman and D. A. Mazziotti, J. Chem. Phys. **133**, 164110 (2010).
[55] A. Sinitskiy, L. Greenman, and D. A. Mazziotti, J. Chem. Phys. **133**, 014104 (2010).