Computational and Theoretical Chemistry 1003 (2013) 32–36

Contents lists available at SciVerse ScienceDirect

Computational and Theoretical Chemistry

journal homepage: www.elsevier.com/locate/comptc

The sharp-*G* *N*-representability condition

Paul A. Johnson [a,*], Paul W. Ayers [a], Brecht Verstichel [b], Dimitri Van Neck [b], Helen van Aggelen [c]

[a] Department of Chemistry & Chemical Biology, McMaster University, Hamilton, Ontario, Canada
[b] Ghent University, Center for Molecular Modelling, Technologiepark 903, 9052 Zwijnaarde, Belgium
[c] Ghent University, Department of Inorganic and Physical Chemistry, Krijgslaan 281 (S3), 9000 Gent, Belgium

ARTICLE INFO

Article history:
Received 4 September 2012
Received in revised form 26 September 2012
Accepted 26 September 2012
Available online 8 October 2012

Keywords:
N-representability conditions
Reduced density matrix
Exactly solvable model Hamiltonians

ABSTRACT

The *G*-condition for the *N*-representability of the two-electron reduced density matrix is tightened by replacing the semidefiniteness constraint with the true upper and lower bounds of the *G*-type Hamiltonian operator. The lower bound is not easily computed (in contrast to the sharp *P*- and *Q*-conditions), but maps onto a well-known integer programming problem. The sharp-*G*, sharp-*P*, and sharp-*Q* conditions are just three members of a much broader class of conditions based on exactly solvable model Hamiltonians.

1. Motivation

Directly solving the *N*-electron Schrödinger equation is impractical for all but the smallest systems because the cost of solving a partial differential equation in 3*N* spatial coordinates to a specified accuracy ε typically grows exponentially, as ε^N. This scaling can be avoided, in principle, by recognizing that the *N*-electron wavefunction contains more information than is necessary for computing the energy: the 2-electron reduced density matrix (2DM) suffices [1–6]. (One can simplify even further and target the 1-electron reduced density matrix [7–9], the electron pair density [10–13], or the electron density [9,14,15]. However, these descriptors do not explicitly determine the energy, and functionals for remaining energy components must be approximated.) Our goal is to use the 2DM as the fundamental descriptor of molecules [16–18].

In principle, the 2DM is determined quite simply using the variational principle,

$$E_{g.s.} = \underbrace{\min}_{N-\text{representable}\Gamma} \quad \mathrm{Tr}[K_2^{(N)}\Gamma] \tag{1}$$

Here $K_2^{(N)}$ is the 2-electron reduced Hamiltonian of the *N*-electron system. This problem is more difficult than it looks for two reasons. First of all, the variational search must be restricted to 2DM that correspond to some ensemble,

$$\Gamma_{ijkl} = \sum_p w_p \left\langle \Psi_p^{(N)} | a_k^\dagger a_l^\dagger a_j a_i | \Psi_p^{(N)} \right\rangle$$
$$0 \leqslant w_p \leqslant 1 \quad 1 = \sum_p w_p \tag{2}$$

Such states are said to be *N*-representable. Here $\{\Psi_p^{(N)}\}$ is an arbitrary set of *N*-electron wavefunctions. Unfortunately, the *N*-representability constraints are not known in any practical form. In principle, the necessary and sufficient conditions are known: Γ is *N*-representable if and only if, for every possible *N*-electron Hamiltonian, $\mathrm{Tr}[K_2^{(N)}\Gamma]$ is greater than the true ground-state energy [19]. I.e., we can rewrite Eq. (1) as

$$E_{g.s.} = \underbrace{\min}_{\left\{\Gamma \middle| \begin{array}{l}\text{for every } \widetilde{K}_2^{(N)}, \\ Tr[\widetilde{K}_2^{(N)}\Gamma] \geqslant E_{g.s.}[\widetilde{K}_2^{(N)}, N]\end{array}\right\}} \mathrm{Tr}[K_2^{(N)}\Gamma] \tag{3}$$

In practice, one considers only a small subset of Hamiltonians [1,19], and so one has a lower bound,

$$E_{g.s.} \geqslant \underbrace{\min}_{\left\{\Gamma \middle| \begin{array}{l}\text{for a few specific } \widetilde{K}_2^{(N)}, \\ Tr[\widetilde{K}_2^{(N)}\Gamma] \geqslant E_{g.s.}[\widetilde{K}_2^{(N)}, N]\end{array}\right\}} \mathrm{Tr}[K_2^{(N)}\Gamma] \tag{4}$$

There has been progress towards deriving better *N*-representability constraints in recent years [13,20–33]; this paper is a contribution in that direction.

The other problem is that the optimization in Eq. (4) is a semidefinite programming problem. There has been progress towards better semidefinite programming algorithms [31,32,34–39], but

* Corresponding author.
E-mail address: johnsopa@mcmaster.ca (P.A. Johnson).

2210-271X/$ - see front matter
http://dx.doi.org/10.1016/j.comptc.2012.09.029

the woeful inefficiency of those methods is still the primary stumbling block in this field.

2. The sharp-*G* condition

In practice, the variational determination of the 2DM uses constraints *even weaker* than those in Eq. (4). Typically one chooses a manifestly positive semidefinite Hamiltonian of the form [1,19,40],

$$P_2^{(N)} = \sum_p w_p \widehat{B}_p^\dagger \widehat{B}_p \tag{5}$$

and then replaces the ground-state energy with its lower bound, zero, even though this lower bound is rarely achieved. I.e., almost all variational 2DM algorithms use

$$E_{g.s} \geqslant \underbrace{\min}_{\left\{\Gamma \middle| \begin{array}{l}\text{for a few specific } P_2^{(N)} \succeq 0, \\ Tr[P_2^{(N)}\Gamma] \geqslant 0\end{array}\right\}} \mathrm{Tr}[K_2^{(N)}\Gamma] \tag{6}$$

which gives an even weaker lower bound than Eq. (4).

This is not mandatory. There are two examples in the literature where operators were chosen for which *sharp* lower bounds could be computed analytically; in these cases Eq. (3) is in fact the appropriate variational procedure [20,29]. This paper can be considered an extension to Ref. [29]. That paper considers two of the most popular *N*-representability conditions, which are obtained by inserting

$$\widehat{B} = \sum_{i,j} p_{ij} a_j a_i \quad p_{ij} = -p_{ji} \tag{7}$$

or

$$\widehat{B} = \sum_{i,j} q_{ij} a_j^\dagger a_i^\dagger \quad q_{ij} = -q_{ji} \tag{8}$$

into Eq. (5). These are called the *P* (or *D*) and *Q* conditions, respectively [1]. The upper and lower bounds to the resulting Hamiltonian can be determined analytically in these cases, by solving a set of nonlinear equations [29,41–44]. Unfortunately, these conditions do not seem to be very forceful for molecular systems [45]. For example, from full-configuration interaction calculations of the 2DM of atomic and molecular systems we learn that the true lower bound of the *P*-condition and *Q*-condition Hamiltonians is typically 10^{-8}, which is so close to zero that imposing the "sharp *P*" and "sharp *Q*" conditions is unhelpful. The universal upper bound on the *P* matrix (i.e., not dependent on the specific p_{ij}) was first derived by Sasaki [46].

The only other *N*-representability constraint whose simplicity is comparable to the *P* and *Q* conditions is the so-called *G*-condition, which is obtained by inserting

$$\widehat{B} = \sum_{i,j} g_{ij} a_j^\dagger a_i \tag{9}$$

into Eq. (5). The upper and lower bounds of the resulting *G*-Hamiltonian

$$\widehat{G} = \sum_{i,j,i',j'} g_{ij} g^*_{j'i'} a_i^\dagger a_{j'} a_j^\dagger a_i \tag{10}$$

were addressed by Garrod and Rosina [47], but explicit results for the upper and lower bounds have not be derived. The practical importance of the *G* condition is clear when g_{ij} is Hermitian: the *G*-condition implies that any 2-electron Hamiltonian that is the square of a 1-electron Hamiltonian is positive semidefinite. The *G*-type Hamiltonian has been analyzed previously by Garrod and Rosina, Erdahl and Grudzinski, and Nakata et al. [47–49]. The universal (independent of the specific g_{ij}) upper bound on the *G*-Hamiltonian was first derived by Garrod and Rosina [47]. They also noted that the lowest eigenvalue of the *G*-Hamiltonian is zero when there is an appropriate symmetry in the Hamiltonian [47]. The goal of this paper is to derive the sharp-*G* conditions in the most general case; our main assumption (which does not seem to be essential) is that the (possibly asymmetric) matrix of g_{ij}'s is diagonalizable.

To derive the spectral bounds for the *G*-Hamiltonian, consider a basis set containing *K* spin orbitals and decompose the g_{ij} matrix using its eigenvalues $\{\lambda_k\}_{k=1}^K$ and the matrices containing its left (V_{mn}) and right (V^{-1}_{mn}) eigenvectors,

$$\sum_{i,j=1}^K g_{ij} a_j^\dagger a_i = \sum_{i,j,k,l=1}^K V_{jk}(\lambda_k \delta_{kl}) V^{-1}_{li} a_j^\dagger a_i \tag{11}$$

In the special case where $g_{ij} = g^*_{ji}$, this can be rewritten as,

$$\sum_{i,j=1}^K g_{ij} a_j^\dagger a_i = \sum_{k=1}^K \lambda_k \tilde{a}_k^\dagger \tilde{a}_k \tag{12}$$

where $\tilde{a}_k = \sum_{i=1}^K U_{ki}^\dagger a_i$ denotes annihilation operators in the eigenvector basis of g_{ij}.

Because Eq. (11) (similarly, Eq. (12)) is a one-body operator, its *N*-electron eigenvectors are Slater determinants, and its *N*-electron eigenvalues are

$$\Lambda^{(N)} = \sum_{k=1}^K n_k \lambda_k, \tag{13}$$

where $n_k \in \{0,1\}$ are the occupation numbers in the Slater determinant. The left-eigenvectors of $\sum_{i,j=1}^K g^*_{ji} a_i^\dagger a_j = (\sum_{i,j=1}^K g_{ij} a_j^\dagger a_i)^\dagger$ are the complex conjugates of the right-eigenvectors of $\sum_{i,j=1}^K g_{ij} a_j^\dagger a_i$; they are also Slater determinants. The *N*-electron eigenvectors of the *G* Hamiltonian are therefore Slater determinants that are eigenvectors of Eq. (11) and the eigenvalues are the squared magnitudes of the sum of occupied orbital energy eigenvalues,

$$\widehat{G}|\Phi\rangle = \left|\sum_{k=1}^K n_k \lambda_k\right|^2 |\Phi\rangle. \tag{14}$$

The spectral bounds, $G^{(N)}_{\min} \preceq \widehat{G} \preceq G^{(N)}_{\max}$ are obtained as solutions to the integer programming problems,

$$G^{(N)}_{\min} = \underbrace{\min}_{\left\{n_k \in \{0,1\} \middle| N = \sum_{k=1}^K n_k\right\}} \left|\sum_{k=1}^K n_k \lambda_k\right|^2 \tag{15}$$

$$G^{(N)}_{\max} = \underbrace{\max}_{\left\{n_k \in \{0,1\} \middle| N = \sum_{k=1}^K n_k\right\}} \left|\sum_{k=1}^K n_k \lambda_k\right|^2 \tag{16}$$

or as the optimization of a quadratic objective function subject to linear and quadratic constraints,

$$G^{(N)}_{\min} = \underbrace{\min}_{\left\{n_k \in \mathbb{R} \middle| \begin{array}{l} N = \sum_{k=1}^K n_k \\ n_k^2 = n_k \end{array}\right\}} \mathbf{n}^T \mathbf{L} \mathbf{n} \tag{17}$$

$$G^{(N)}_{\max} = \underbrace{\max}_{\left\{n_k \in \mathbb{R} \middle| \begin{array}{l} N = \sum_{k=1}^K n_k \\ n_k^2 = n_k \end{array}\right\}} \mathbf{n}^T \mathbf{L} \mathbf{n} \tag{18}$$

where $\mathbf{n}$ is the vector of occupation numbers and $\mathbf{L}$ is the positive semidefinite matrix (with *K*-1 zero eigenvalues),

$$\mathbf{L} = \begin{bmatrix} |\lambda_1|^2 & \lambda_1^*\lambda_2 & \cdots & \lambda_1^*\lambda_K \\ \lambda_2^*\lambda_1 & |\lambda_2|^2 & \cdots & \lambda_2^*\lambda_K \\ \vdots & & \ddots & \vdots \\ \lambda_K^*\lambda_1 & \lambda_K^*\lambda_2 & \cdots & |\lambda_K|^2 \end{bmatrix} \tag{19}$$

Notice that the spectral bounds are strongly dependent on the number of electrons; this distinguishes them from conventional N-representability conditions.

Determining $G^{(N)}_{\max}$ is not difficult. For example, if we assume that the eigenvalues are real and listed in increasing order, $\lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_K$, the upper bound will be caused by either the sum of the smallest (most-negative) or largest eigenvalues,

$$G^{(N)}_{\max} = \max\left[\left(\sum_{k=N-K+1}^{K}\lambda_k\right)^2, \left(\sum_{k=1}^{N}\lambda_k\right)^2\right] \tag{20}$$

More generally, one needs to find the vector sum of complex numbers with the largest magnitude. Like the upper bounds to the P- and Q-Hamiltonians, in our tests the upper bound to the G-Hamiltonian was ineffective.

Determining the lower bounds is *NP* hard. The problem is closely related to the minimum sum-of-squares clustering problem [50], maximizing the expectation value of a positive-definite quadratic form using 0–1 vectors (PosDef-0-1-Max) [51], and the p-dispersion problem [52–55] which is known to be NP-hard [54]. The connection to the p-dispersion problem is especially direct. Assuming real eigenvalues, one can compute the lower bound by solving the problem,

$$-G^{(N)}_{\min} = \underbrace{\max}_{\left\{n_k\in\{0,1\}\middle|N=\sum_{k=1}^{K}n_k\right\}} \mathbf{n}^T(-\mathbf{L})\mathbf{n} \tag{21}$$

which is equivalent to the N-dispersion problem

$$-G^{(N)}_{\min} + N|\lambda|^2_{\max} = \underbrace{\max}_{\left\{n_k\in\{0,1\}\middle|N=\sum_{k=1}^{K}n_k\right\}} \mathbf{n}^T(|\lambda|^2_{\max}\mathbf{1} - \mathbf{L})\mathbf{n} \tag{22}$$

where $\mathbf{1}$ is a matrix whose entries are all ones and $|\lambda|_{\max} = \max_{k=1,2\ldots K}|\lambda_k|$ is the magnitude of whichever eigenvalue of g_{ij} has highest magnitude. The matrix in Eq. (22) has only positive entries, so this is a N-dispersion problem.

This problem is *NP*-hard because, in general, the sum of positive and negative eigenvalues with very different magnitude can be close to zero. In cases where there are too few positive or negative eigenvalues for this sort of pernicious cancelation to occur, the $G_{\min}$ is easily computed. In particular: (1) if $\sum_{k=1}^{N}\lambda_k > 0$, then the lowest eigenvalue of the G Hamiltonian is $(\sum_{k=1}^{N}\lambda_k)^2$ and (2) if $\sum_{k=K}^{K-N+1}\lambda_k < 0$ then the lowest eigenvalues of the G Hamiltonian is $(\sum_{k=K}^{K-N+1}\lambda_k)^2$. Bounds for the p-dispersion problem could be adapted to form lower bounds on $G_{\min}$ [52]. For smaller basis sets, explicit enumeration of the possible solutions is feasible; this is what we did in our computational tests. In general, this type of 0–1 integer programming problem is usually solved by relaxing the restriction to integer solutions (this conventional optimization problem provides a lower bound to the desired solution) and then adding constraints until the optimal integer solution is obtained. Near-optimal solutions to the p-dispersion problem can be found in $O(K^3)$ time, and rigorously optimal solutions to the p-dispersion problems with up to $K = 100$ are routinely accessible [52]. The actual computational cost depends strongly on the structure of the problem; much larger problems can be solved when the estimate of a greedy algorithm is accurate.

The preceding analysis assumes that g_{ij} are the elements of a diagonalizable matrix. If this is not true, then, instead of Eq. (11), one would need to analyze the corresponding Jordan canonical form,

$$\sum_{i,j=1}^{K} g_{ij}a_j^\dagger a_i = \sum_{k,l=1}^{K} T_{jk}J_{kl}T^{-1}_{li}a_j^\dagger a_i \tag{23}$$

where $\mathbf{J}$ is a Jordan matrix [56]. Our results appear to extend to non-diagonalizable matrices, but we have not meticulously confirmed this.

3. Summary

The goal of this paper is to present sharp upper and lower bounds for the G-Hamiltonian. This allows one to replace the condition that the G-matrix be positive semidefinite with the condition that the spectrum of G be contained within the correct spectral bounds. When combined with the results in Ref. [29], this allows one to reformulate the variational optimization of the 2DM subject to the sharp-2-positivity conditions as

$$E_{g.s} \geqslant \underbrace{\min}_{\left\{\Gamma\middle|\begin{array}{l} P^{(N)}_{\min} \preceq \mathrm{Tr}[P\Gamma] \preceq P^{(N)}_{\max} \\ Q^{(N)}_{\min} \preceq \mathrm{Tr}[Q\Gamma] \preceq Q^{(N)}_{\max} \\ G^{(N)}_{\min} \preceq \mathrm{Tr}[G\Gamma] \preceq P^{(N)}_{\max} \end{array}\right\}} \mathrm{Tr}[K_2^{(n)}\Gamma]. \tag{24}$$

While the P, Q, and G-type Hamiltonians are the most conventional constraints for the variational 2DM method, *any* readily solvable Hamiltonian can be used. In addition to the cases previously considered in the literature on N-representability [20,29], other possibilities are the (one-dimensional) Heisenberg model [57,58], the t–J model [59] and the supersymmetric U-model [60,61]. The Hubbard model [62–69] (known in chemistry as the Pariser–Parr–Pople model Hamiltonian [70–72]) in one dimension is exactly solvable by a coordinate Bethe ansatz [73]. Exact solutions for the model Hamiltonians of Richardson [42,43,74], Gaudin [44], and many of their generalizations are also available [41,75–77].

We have not found any cases where the sharp-P or sharp-Q conditions significantly improved the results beyond a conventional calculation subject to the 2-positivity conditions,

$$E_{g.s.} \geqslant \underbrace{\min}_{\left\{\Gamma\middle|\begin{array}{l} 0 \leqslant \mathrm{Tr}[P\Gamma] \\ 0 \leqslant \mathrm{Tr}[Q\Gamma] \\ 0 \leqslant \mathrm{Tr}[G\Gamma] \end{array}\right\}} \mathrm{Tr}[K_2^{(N)}\Gamma] \tag{25}$$

$G^{(N)}_{\min}$ is exactly zero for any singlet state (zero spin-angular momentum) and any spherically-symmetric pure state (zero orbital-angular momentum). Our preliminary investigations indicate that the violations of the sharp-G condition (specifically, $G^{(N)}_{\min}$) in other atoms and molecules is very small ($G^{(N)}_{\min} \sim 10^{-8}$). However, we found significant violations for a 3-electron 4-site Hubbard model with a strong on-site repulsion ($G^{(N)}_{\min} \approx .07$), which suggests that the sharp-G conditions may be important for strongly-correlated electronic materials. The sharp-G condition is *strongly* violated in the systems considered by Nakata et al. because optimizing a G-type Hamiltonian subject to the sharp-G conditions will always give the exact ground state energy [49].

Acknowledgements

P.A.J. acknowledges funding from the Vanier Canada Graduate Scholarships. P.W.A. was supported by NSERC and the Canada Research Chairs. We gratefully acknowledge FWO-Flanders and the research council of Ghent University for financial support.

References

[1] J. Coleman, Structure of fermion density matrices, Rev. Mod. Phys. 35 (1963) 668–687.
[2] A.J. Coleman, V.I. Yukalov, Reduced Density Matrices: Coulson's Challenge, Springer, Berlin, 2000.
[3] E.R. Davidson, Reduced Density Matrices in Quantum Chemistry, Academic Press, New York, 1976.
[4] D.A. Mazziotti, Two-electron reduced density matrix as the basic variable in many-electron quantum chemistry and physics, Chem. Rev. 112 (2012) 244–262.
[5] D.A. Mazziotti, Variational two-electron reduced-density-matrix theory, in: D.A. Mazziotti (Ed.) Reduced-Density-Matrix Mechanics –With Application to Many-Electron Atoms and Molecules, 2007, pp. 21–59.
[6] D.A. Mazziotti, Quantum chemistry without wave functions: two electron reduced density matrices, Acc. Chem. Res. 39 (2006) 207–215.
[7] T.L. Gilbert, Hohenberg–Kohn theorem for nonlocal external potentials, Phys. Rev. B 12 (1975) 2111–2120.
[8] R.A. Donnelly, R.G. Parr, Elementary properties of an energy functional of the first order density matrix, J. Chem. Phys. 69 (1978) 4431–4439.
[9] M. Levy, Universal variational functionals of electron-densities, 1st-order density-matrices, and natural spin–orbitals and solution of the V-representability problem, Proc. Natl. Acad. Sci. 76 (1979) 6062–6065.
[10] P. Ziesche, Attempts toward a pair density functional theory, Int. J. Quantum Chem. 60 (1996) 1361–1374.
[11] P. Ziesche, Pair density-functional theory – a generalized density-functional theory, Phys. Lett. A 195 (1994) 213–220.
[12] P.W. Ayers, Using classical many-body structure to determine electronic structure: an approach using *k*-electron distribution functions, Phys. Rev. A 74 (2006) 042502.
[13] P.W. Ayers, E.R. Davidson, Linear inequalities for diagonal elements of density matrices, Adv. Chem. Phys. 134 (2007) 443–483.
[14] P. Hohenberg, W. Kohn, Inhomogeneous electron gas, Phys. Rev. 136 (1964) B864–B871.
[15] E.H. Lieb, Density functionals for Coulomb systems, Int. J. Quantum Chem. 24 (1983) 243–277.
[16] H. van Aggelen, B. Verstichel, P. Bultinck, D. Van Neck, P.W. Ayers, D.L. Cooper, Chemical verification of variational second-order density matrix based potential energy surfaces for the N-2 isoelectronic series, J. Chem. Phys. 132 (2010) 114112.
[17] B. Verstichel, H. van Aggelen, D. Van Neck, P.W. Ayers, P. Bultinck, Variational determination of the second-order density matrix for the isoelectronic series of beryllium, neon, and silicon, Phys. Rev. A 80 (2009) 032508.
[18] H. Van Aggelen, P. Bultinck, B. Verstichel, D. Van Neck, P.W. Ayers, Incorrect diatomic dissociation in variational reduced density matrix theory arises from the flawed description of fractionally charged atoms, PCCP 11 (2009) 5558–5560.
[19] C. Garrod, J.K. Percus, Reduction of the *N*-particle variational problem, J. Math. Phys. 5 (1964) 1756–1776.
[20] N. Shenvi, A.F. Izmaylov, Active-space *N*-representability constraints for variational two-particle reduced density matrix calculations, Phys. Rev. Lett. 105 (2010) 213003.
[21] B. Verstichel, H. van Aggelen, D. Van Neck, P.W. Ayers, P. Bultinck, Subsystem constraints in variational second order density matrix optimization: curing the dissociative behavior, J. Chem. Phys. 132 (2010) 114113.
[22] B.J. Braams, J.K. Percus, Z.J. Zhao, The T1 and T2 representability conditions, in: D.A. Mazziotti (Ed.) Reduced-Density-Matrix Mechanics – With Application to Many-Electron Atoms and Molecules, 2007, pp. 93–101.
[23] Z.J. Zhao, B.J. Braams, M. Fukuda, M.L. Overton, J.K. Percus, The reduced density matrix method for electronic structure calculations and the role of three-index representability conditions, J. Chem. Phys. 120 (2004) 2095–2104.
[24] J.R. Hammond, D.A. Mazziotti, Variational two-electron reduced-density-matrix theory: partial 3-positivity conditions for *N*-representability, Phys. Rev. A 71 (2005) 062503.
[25] D.A. Mazziotti, R.M. Erdahl, Uncertainty relations and reduced density matrices: mapping many-body quantum mechanics onto four particles, Phys. Rev. A 63 (2001) 042113.
[26] T. Juhasz, N. Shenvi, D.A. Mazziotti, Recursively generated linear constraints for variational two-particle reduced-density-matrix theory, Chem. Phys. Lett. 445 (2007) 79–83.
[27] G. Gidofalvi, D.A. Mazziotti, Variational reduced-density-matrix theory: strength of Hamiltonian-dependent positivity conditions, Chem. Phys. Lett. 398 (2004) 434–439.
[28] B. Verstichel, H. van Aggelen, W. Poelmans, D. Van Neck, Variational two-particle density matrix calculation for the hubbard model below half filling using spin-adapted lifting conditions, Phys. Rev. Lett. 108 (2012) 213001.
[29] D. Van Neck, P.W. Ayers, Necessary conditions for the *N*-representability of the second-order reduced density matrix: upper bounds on the *P* and *Q* matrices, Phys. Rev. A 75 (2007) 032502.
[30] E.R. Davidson, Linear inequalities for density matrices: III, Int. J. Quantum Chem. 91 (2003) 1–4.
[31] D.A. Mazziotti, Significant conditions for the two-electron reduced density matrix from the constructive solution of *N* representability, Phys. Rev. A 85 (2012) 062507.
[32] D.A. Mazziotti, Structure of fermionic density matrices: complete *N*-representability conditions, Phys. Rev. Lett. 108 (2012) 263002.
[33] H. Grudzinski, J. Hirsch, Searching for new conditions for fermion N-representability, Rep. Math. Phys. 53 (2004) 331–338.
[34] M. Fukuda, B.J. Braams, M. Nakata, M.L. Overton, J.K. Percus, M. Yamashita, Z.J. Zhao, Large-scale semidefinite programs in electronic structure calculation, Math. Prog. 109 (2007) 553–580.
[35] K. Fujisawa, M. Fukuda, K. Nakata, Preprocessing sparse semidefinite programs via matrix completion, Optim. Method. Soft. 21 (2006) 17–39.
[36] M. Nakata, H. Nakatsuji, M. Ehara, M. Fukuda, K. Nakata, K. Fujisawa, Variational calculations of fermion second-order reduced density matrices by semidefinite programming algorithm, J. Chem. Phys. 114 (2001) 8282–8292.
[37] E. Cances, G. Stoltz, M. Lewin, The electronic ground-state energy problem: a new reduced density matrix approach, J. Chem. Phys. 125 (2006) 064101.
[38] D.A. Mazziotti, Realization of quantum chemistry without wave functions through first-order semidefinite programming, Phys. Rev. Lett. 93 (2004) 213001.
[39] B. Verstichel, H. van Aggelen, D. Van Neck, P. Bultinck, S. De Baerdemacker, A primal-dual semidefinite programming algorithm tailored to the variational determination of the two-body density matrix, Comput. Phys. Commun. 182 (2011) 1235–1244.
[40] R.M. Erdahl, Representability, Int. J. Quantum Chem. 13 (1978) 697–718.
[41] J. Dukelsky, S. Pittel, G. Sierra, Colloquium: exactly solvable richardson-gaudin models for manybody quantum systems, Rev. Mod. Phys. 76 (2004) 643–662.
[42] R.W. Richardson, N. Sherman, Exact eigenstates of the pairing-force Hamiltonian, Nucl. Phys. 52 (1964) 221–238.
[43] R. Richardson, A restricted class of exact eigenstates of the pairing-force Hamiltonian, Phys. Lett. 3 (1963) 277–279.
[44] M. Gaudin, Diagonalisation d'une classe d'hamiltoniens de spin, J. Phys. 37 (1976) 1087–1098.
[45] Brecht Verstichel. Ph.D. Thesis, Ghent University, 2012.
[46] F. Sasaki, Eigenvalues of fermion density matrices, Phys. Rev. 138 (1965) B1338–B1342.
[47] C. Garrod, M. Rosina, Particle-hole matrix: it's connection with the symmetries and collective features of the ground state, J. Math. Phys. 10 (1969) 1855–1861.
[48] R.M. Erdahl, H. Grudzinski, Spectral properties of cones of approximately representable reduced density matrices, Rep. Math. Phys. 14 (1978) 405–418.
[49] M. Nakata, B.J. Braams, M. Fukuda, J.K. Percus, M. Yamashita, Z.J. Zhao, Simple Hamiltonians which exhibit drastic failures by variational determination of the two-particle reduced density matrix with some well known *N*-representability conditions, J. Chem. Phys. 125 (2006) 244109.
[50] A.K. Jain, M.N. Murty, P.J. Flynn, Data clustering, a review, ACM Comput. Surv. 31 (1999) 264–323.
[51] P. Gritzmann, V. Klee, On the 0–1-maximization of positive definite quadratic forms, in: Operations Research Proceedings, Springer, Berlin, 1988, pp. 222–227.
[52] D. Pisinger, Upper bounds and exact algorithms for p-dispersion problems, Comput. Oper. Res. 33 (2006) 1380–1398.
[53] S.S. Ravi, D.J. Rosenkrantz, G.K. Tayi, Facility dispersion problems – Heuristics and special cases, Lect. Notes Comput. Sci. 519 (1991) 355–366.
[54] S.S. Ravi, D.J. Rosenkrantz, G.K. Tayi, Heuristic and special case algorithms for dispersion problems, Oper. Res. 42 (1994) 299–310.
[55] D.J. Rosenkrantz, G.K. Tayi, S.S. Ravi, Facility dispersion problems under capacity and cost constraints, J. Comb. Optim. 4 (2000) 7–33.
[56] G.H. Golub, C.F. Van Loan, Matrix Computations, third ed., Johns Hopkins UP, Baltimore, MD, U.S.A., 1996.
[57] W. Heisenberg, Zur Theorie des Ferromagnetismus, Z. Phys. 49 (1928) 619–636.
[58] H. Bethe, Zur Theorie der Metalle, Zeitschrift für Physik 71 (1931) 205–226.
[59] F. Zhang, T. Rice, Effective Hamiltonian for the superconducting Cu oxides, Phys. Rev. B 37 (1988) 3759–3761.
[60] A.J. Bracken, M.D. Gould, J.R. Links, Y.Z. Zhang, New supersymmetric and exactly solvable model of correlated electrons, Phys. Rev. Lett. 74 (1995) 2768–2771.
[61] I.N. Karnaukhov, Model of fermions with correlated hopping (integrable cases), Phys. Rev. Lett. 73 (1994) 1130–1133.
[62] J. Kanamori, Electron correlation and ferromagnetism of transition metals, Prog. Theor. Phys. 30 (1963) 275–289.
[63] M. Gutzwiller, Effect of correlation on the ferromagnetism of transition metals, Phys. Rev. Lett. 10 (1963) 159–162.
[64] J. Hubbard, Electron correlations in narrow energy bands. VI. The connexion with many-body perturbation theory, Proc. Roy. Soc. A: Math., Phys. Eng. Sci. 296 (1967) 100–112.
[65] J. Hubbard, Electron correlations in narrow energy bands. V. A perturbation expansion about the atomic limit, Proc. Roy. Soc. A: Math., Phys. Eng. Sci. 296 (1967) 82–99.
[66] J. Hubbard, Electron correlations in narrow energy bands. IV. The atomic representation, Proc. Roy. Soc. A: Math., Phys. Eng. Sci. 285 (1965) 542–560.
[67] J. Hubbard, Electron correlations in narrow energy bands. III. An improved solution, Proc. Roy. Soc. A: Math., Phys. Eng. Sci. 281 (1964) 401–419.
[68] J. Hubbard, Electron correlations in narrow energy bands. II. The degenerate band case, Proc. Roy. Soc. A: Math., Phys. Eng. Sci. 277 (1964) 237–259.

[69] J. Hubbard, Electron correlations in narrow energy bands, Proc. Roy. Soc. A: Math., Phys. Eng. Sci. 276 (1963) 238–257.
[70] R. Pariser, R.G. Parr, A semi-empirical theory of the electronic spectra and electronic structure of complex unsaturated molecules. II, J. Chem. Phys. 21 (1953) 767.
[71] R. Pariser, R.G. Parr, A semi-empirical theory of the electronic spectra and electronic structure of complex unsaturated molecules. I, J. Chem. Phys. 21 (1953) 466–472.
[72] J.A. Pople, Electron interaction in unsaturated hydrocarbons, Trans. Faraday Soc. 49 (1953) 1375.
[73] E. Lieb, F. Wu, Absence of mott transition in an exact solution of the short-range, one-band model in one dimension, Phys. Rev. Lett. 20 (1968) 1445–1448.
[74] R.W. Richardson, Exact eigenstates of the pairing-force Hamiltonian. II, J. Math. Phys. 6 (1965) 1034.
[75] G. Ortiz, R. Somma, J. Dukelsky, S. Rombouts, Exactly-solvable models derived from a generalized Gaudin algebra, Nucl. Phys. B 707 (2005) 421–457.
[76] X.W. Guan, A. Foerster, J. Links, H.Q. Zhou, Integrability and exact solution for coupled BCS systems associated with the su(4) Lie algebra, Nucl. Phys. B 642 (2002) 501–514.
[77] C. Dunning, M. Ibañez, J. Links, G. Sierra, S.-Y. Zhao, Exact solution of the p + ip pairing Hamiltonian and a hierarchy of integrable models, J. Stat. Mech.: Theory Exp. 2010 (2010) P08025.