Solving Condensed-Matter Ground-State Problems by Semidefinite Relaxations

Thomas Barthel and Robert Hübener

Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin,
Germany and Institute for Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany
(Received 22 June 2011; revised manuscript received 7 January 2012; published 17 May 2012)

We present a generic approach to the condensed-matter ground-state problem which is complementary to variational techniques and works directly in the thermodynamic limit. Relaxing the ground-state problem, we obtain semidefinite programs (SDP). These can be solved efficiently, yielding strict lower bounds to the ground-state energy and approximations to the few-particle Green's functions. As the method is applicable for all particle statistics, it represents, in particular, a novel route for the study of strongly correlated fermionic and frustrated spin systems in $D > 1$ spatial dimensions. It is demonstrated for the *XXZ* model and the Hubbard model of spinless fermions. The results are compared against exact solutions, quantum Monte Carlo calculations, and Anderson bounds, showing the competitiveness of the SDP method.

Introduction.—Prominent simulation techniques for condensed-matter systems are sampling algorithms like the quantum Monte Carlo (QMC) method [1–4] and variational algorithms like the density-matrix renormalization group [5,6], other tensor-network-state approaches [7–10], or variational Monte Carlo methods [11–14]. For a number of interesting classes of systems, like frustrated or fermionic systems in $D > 1$ spatial dimensions, the powerful QMC technique is inefficient, due to the sign problem [15–17]. Such systems are then often studied with variational techniques by minimizing the energy within a certain class of states. The energy expectation value of the obtained state is necessarily an upper bound to the exact ground-state energy.

In this Letter, a complementary approach is presented. By relaxations of the ground-state problem, we obtain semidefinite programs (SDP) [18,19], which can be solved efficiently on classical computers. This yields lower bounds to the ground-state energy and corresponding approximations to few-particle Green's functions. The obtained Green's functions allow, e.g., for the study of phase diagrams. As the presented SDP method works irrespective of the particle statistics, it provides, in particular, a novel route for the study of strongly correlated fermionic and frustrated spin systems for $D > 1$. The method can also be used to judge the quality of variational algorithms in situations where exact or QMC results are not available. This is especially important for variational Monte Carlo calculations [13,14] and the recently developed variational tensor-network-state techniques for fermions in $D > 1$ [20–24].

The idea is to specify the system by its equal-time k-point Green's functions $G^{(k)}$. For systems of fermions, bosons, or hard-core bosons (being equivalent to spins-1/2) in a normalized state $\hat{\rho}$, they are defined as the correlation functions

$$G_{i,j}^{(k)} := \mathrm{Tr}\,(\hat{\rho}\,\hat{a}_{i_1} \ldots \hat{a}_{i_m} \hat{a}_{j_n}^{\dagger} \ldots \hat{a}_{j_1}^{\dagger}), \qquad k = m + n, \quad (1)$$

for ladder operators $\hat{a}_i$ and some single-particle basis states $|i\rangle$ [25]. The energy expectation value $E = \mathrm{Tr}\,\hat{\rho}\,\hat{H}$ is a function of the (few-particle) Green's functions, i.e., $E = E(G)$. The exact ground-state energy is obtained by minimization among all representable Green's functions G, i.e., those for which a density operator $\hat{\rho}$ exists, such that Eq. (1) is obeyed. However, to determine whether a given Green's function G is representable turns out to be a computationally hard problem, the famous N-representability problem [26–29], which is quantum Merlin Arthur (QMA) complete [30]. Nevertheless, an efficient minimization of E is possible if we relax the constraints on the Green's function, then, yielding not the exact ground-state energy but a lower bound and not the exact ground-state Green's function but an approximation. Note that minimizing $E(G)$ without any constraints is doomed to fail, as the energy is linear in G. Manageable constraints on G can be constructed by imposing the positivity of the expectation values of certain positive-definite observables, an example being the particle density operator $\hat{a}_i^{\dagger}\hat{a}_i$. Such an approach for fermionic $G^{(1)}$ and $G^{(2)}$ has been successfully applied to finite systems in quantum chemistry; see, e.g., Ref. [31] and references therein.

Here, we present a systematic method for the construction and solution of relaxed ground-state problems for condensed-matter systems. As in the approach known from quantum chemistry, our constraints enforce positive expectation values for operators of the form $\hat{C}^{\dagger}\hat{C}$ with respect to the Green's functions G. More generally than before, we (a) choose the constraint operators $\hat{C}$ to be arbitrary polynomials of degree $\leq K \in \mathbb{N}$ in the ladder operators, which (b) act on suitably chosen subsets of the lattice. This makes it possible to address large systems and to control the precision and the computation cost. We (c) exploit the translation invariance of the condensed-matter systems to (d) work effectively with an infinite number of degrees of freedom and describe the systems

directly in the thermodynamic limit. The method yields coupled constraints for $G^{(1)}, \ldots, G^{(2K)}$ such that the energy optimization problem attains the form of an SDP. On the basis of the bipolar theorem [32], we further elucidate the mathematical background of the method and further possible reductions to the number of constraints.

An alternative method for calculating lower bounds to the ground-state energy is due to Anderson. Anderson bounds [33,34] are obtained by splitting the Hamiltonian $\hat{H}$ into a sum of subsystem Hamiltonians $\hat{H}_m$ that are accessible by exact diagonalization. The Anderson bound for the ground-state energy E^0 is then given by the sum of the ground-state energies E^0_m of the $\hat{H}_m$,

$$\hat{H} = \sum_m \hat{H}_m \Rightarrow E^0 \geq \sum_m E^0_m. \tag{2}$$

The computation cost for this bound scales exponentially in the sizes of the spatial supports of the operators $\hat{H}_m$ [35]. A generalization of this approach to finite temperatures is presented in Ref. [36].

In contrast, the computation cost for the SDP method scales only polynomially in the support of the constraint operators. In the prominent systems that we studied with moderate computer resources, the SDP method outperforms the Anderson bound substantially. The SDP method has the additional advantage of giving access to the Green's functions, which can be used to study phase diagrams, etc.

Ground-state problem.—The following description applies to lattice systems of fermions, bosons, and hard-core bosons—each corresponding to a certain algebra for the ladder operators $\{\hat{a}_i, \hat{a}^\dagger_i\}$ [25]. Spins-$1/2$ can be treated by mapping them to hard-core bosons via the identifications $\hat{a}_i = \hat{S}^-_i$, $\hat{a}^\dagger_i = \hat{S}^+_i$, and $\hat{S}^z_i = \hat{a}^\dagger_i \hat{a}_i - \frac{1}{2}$. The generalization to higher spins is straightforward. For each subset Ω of the single-particle modes $\{|i\rangle\}$, let $\mathcal{A}^k_\Omega$ denote the operator basis of normal-ordered monomials of degree k in the ladder operators for subsystem Ω,

$$\mathcal{A}^k_\Omega := \{\hat{a}_{i_1} \ldots \hat{a}_{i_m} \hat{a}^\dagger_{i_{m+1}} \ldots \hat{a}^\dagger_{i_k} | 0 \leq m \leq k, i_\ell \in \Omega\}. \tag{3}$$

Each density operator $\hat{\rho}$ corresponds to a representable Green's function $\mathcal{G}$, with its k-point component given by

$$\mathcal{G}^{(k)}_{\hat{\sigma}} := \mathrm{Tr}\hat{\rho}\,\hat{\sigma} \quad \text{for } \hat{\sigma} \in \mathcal{A}^k_\Omega. \tag{4}$$

For the moment, let us choose Ω to be the full system. Every linear operator $\hat{B}$ on the Hilbert space can be expanded in the basis $\mathcal{A} := \bigcup_k \mathcal{A}^k$ as $\hat{B} = \sum_{\hat{\sigma} \in \mathcal{A}} B_{\hat{\sigma}} \hat{\sigma}$. Its expectation value with respect to a state $\hat{\rho}$ is then

$$\mathrm{Tr}\,\hat{\rho}\,\hat{B} = \sum_{\hat{\sigma} \in \mathcal{A}} \mathcal{G}_{\hat{\sigma}} B_{\hat{\sigma}} =: \mathcal{G}[\hat{B}], \tag{5}$$

where $\mathcal{G}$ is the Green's function of $\hat{\rho}$. In this sense, Green's functions are linear functionals on the operators.

For a Hamiltonian $\hat{H}$, the ground-state problem reads

$$E^0 = \min_{\hat{\rho} \in \mathcal{S}} \mathrm{Tr}\hat{\rho}\,\hat{H} = \min_{\mathcal{G} \in \mathcal{R}} \mathcal{G}[\hat{H}], \tag{6}$$

where $\mathcal{S}$ denotes the set of all density operators and $\mathcal{R}$ denotes the set of all representable Green's functions,

$$\begin{aligned}\mathcal{R} &:= \{\mathcal{G} | \exists \hat{\rho} \in \mathcal{S} : \mathcal{G}_{\hat{\sigma}} = \mathrm{Tr}\hat{\rho}\,\hat{\sigma} \;\, \forall_{\hat{\sigma} \in \mathcal{A}}\} \\ &= \{\mathcal{G} | \mathcal{G}[\mathrm{Id}] = 1, \mathcal{G}_{\hat{\sigma}^\dagger} = \mathcal{G}^*_{\hat{\sigma}}, \mathcal{G}[\hat{B}] \geq 0 \;\, \forall_{\hat{B} \geq 0}\}. \end{aligned} \tag{7}$$

This equality follows from the fact that the only constraints on a valid density operator $\hat{\rho}$ are $\mathrm{Tr}\hat{\rho} = 1$, $\hat{\rho} = \hat{\rho}^\dagger$, and its positivity $\hat{\rho} \succeq 0$, which is equivalent to requiring $\mathrm{Tr}\hat{\rho}\hat{B} \geq 0$ for all positive-semidefinite operators $\hat{B} \succeq 0$.

Variational methods proceed from Eq. (6) by choosing some accessible subset of $\mathcal{S}$. Each variational state from such a subset yields an upper bound to the ground-state energy E^0. In contrast, for the SDP method, described in the following, one chooses an accessible superset $\mathcal{F}$ of the set $\mathcal{R}$ of representable Green's functions, i.e., relaxes the constraints. Minimizing the energy in such a superset yields a lower bound to E^0. A decisive feature of the SDP method is that the minimum energies for the chosen supersets $\mathcal{F}$ can be found certifiably.

SDP method.—Solving the ground-state problem (6) in general is known to be a computationally hard problem; it is QMA-complete [37]. Similarly, determining whether given Green's functions are representable, i.e., elements of $\mathcal{R}$ in Eq. (7), is also a QMA-complete problem [30]. A straightforward way to relax the—apparently too demanding—constraints represented by $\mathcal{R}$ is to require the Green's functional $\mathcal{G}[\hat{B}]$ to be non-negative, not for all $\hat{B} \succeq 0$ but only for operators $\hat{B}$ of the form $\hat{B} = \hat{C}^\dagger \hat{C}$ with constraint operators $\hat{C}$ from some suitable set $\mathcal{C}$. Minimizing the energy $\mathcal{G}[\hat{H}]$ with respect to Green's functions $\mathcal{G}$ from the set

$$\mathcal{F}_\mathcal{C} := \{\mathcal{G} | \mathcal{G}[\mathrm{Id}] = 1, \mathcal{G}_{\hat{\sigma}^\dagger} = \mathcal{G}^*_{\hat{\sigma}}, \mathcal{G}[\hat{C}^\dagger \hat{C}] \geq 0 \;\, \forall_{\hat{C} \in \mathcal{C}}\} \tag{8}$$

yields a lower bound to the ground-state energy (6),

$$E^0 \geq \min_{\mathcal{G} \in \mathcal{F}_\mathcal{C}} \mathcal{G}[\hat{H}] \equiv \min_{\mathcal{G} \in \mathcal{F}_\mathcal{C}} \sum_{\hat{\sigma}} \mathcal{G}_{\hat{\sigma}} H_{\hat{\sigma}}, \tag{9}$$

as $\mathcal{R} \subset \mathcal{F}_\mathcal{C}$. Imposing more and more constraints by enlarging the operator set $\mathcal{C}$, the bound approaches E^0 and the optimal $\mathcal{G}$ approaches the ground-state Green's function. Determining the optimum in Eq. (9) is a semidefinite programming problem for the variables $\mathcal{G}_{\hat{\sigma}}$, as $\mathcal{G}[\hat{H}] \equiv \sum_{\hat{\sigma}} \mathcal{G}_{\hat{\sigma}} H_{\hat{\sigma}}$ is linear in $\mathcal{G}$, and the constraints $\mathcal{G}[\hat{C}^\dagger \hat{C}] \geq 0 \;\forall\, \hat{C} \in \mathcal{C}$ can be written in the form

$$\sum_{\hat{\sigma}} \mathcal{G}_{\hat{\sigma}} M_{\hat{\sigma}} \succeq 0, \tag{10}$$

where the Hermitian matrices $M_{\hat{\sigma}}$ are completely determined by the underlying algebra of the ladder operators $\hat{a}_i$ and the choice for the constraint operator set $\mathcal{C}$. Equations (9) and (10) correspond to a standard

form for an SDP [18,19,35]. Equation (10) results from expanding the constraint operators in the basis $\mathcal{A}$, $\hat{C} = \sum_{\hat{\sigma}} C_{\hat{\sigma}} \hat{\sigma}$. This yields the constraints in the form $\sum_{\hat{\sigma}'\hat{\sigma}''} C_{\hat{\sigma}'}^* G[(\hat{\sigma}')^\dagger \hat{\sigma}''] C_{\hat{\sigma}''} \geq 0 \; \forall_C$. Expanding the operators $(\hat{\sigma}')^\dagger \hat{\sigma}''$ in the operator basis $\mathcal{A}$ (by bringing them into normal-ordered form) and using $G[\hat{\sigma}] \equiv G_{\hat{\sigma}}$ yields the matrices $[M_{\hat{\sigma}}]_{\hat{\sigma}',\hat{\sigma}''}$ and the constraints

$$\sum_{\hat{\sigma}\hat{\sigma}'\hat{\sigma}''} G_{\hat{\sigma}} C_{\hat{\sigma}'}^* [M_{\hat{\sigma}}]_{\hat{\sigma}',\hat{\sigma}''} C_{\hat{\sigma}''} = \sum_{\hat{\sigma}} G_{\hat{\sigma}} \mathbf{C}^\dagger M_{\hat{\sigma}} \mathbf{C} \geq 0 \quad \forall_C,$$

from which Eq. (10) follows. See the Supplemental Material [35] for explicit examples.

Thermodynamic limit and constraint operators.—Let us now turn to the specific case of condensed-matter systems in the thermodynamic limit. Let the Hamiltonian be translation-invariant $\hat{H} = \sum_r \mathcal{T}_r(\hat{h})$ with finite-range interaction terms $\hat{h}$ and the lattice translation operator $\mathcal{T}_r$. We denote the spatial support of the κ-point terms in $\hat{h}$ by Λ_κ. Because of the translation invariance of $\hat{H}$, we can restrict ourselves to translation-invariant density matrices and Green's functions. A constraint operator set can be constructed by choosing, for each operator degree k, a subsystem Ω_k of the full lattice such that

$$\Omega_{k'} \subset \Omega_k \quad \forall_{k'>k} \quad \text{and} \quad \Lambda_\kappa \subset \Omega_{\lceil \kappa/2 \rceil} \quad \forall_\kappa. \quad (11)$$

Every such choice of subsystems and the corresponding set of constraint operators

$$\mathcal{C}_\mathbf{\Omega} := \text{span}\mathcal{A}_\mathbf{\Omega} \quad \text{with} \quad \mathcal{A}_\mathbf{\Omega} := \bigcup_k \mathcal{A}_{\Omega_k}^k \quad (12)$$

defines with Eq. (8) a set $\mathcal{F}_{\mathcal{C}_\mathbf{\Omega}} \supset \mathcal{R}$ of Green's functions. The number of Green's function elements $G_{\hat{\sigma}}$ occurring as degrees of freedom in the SDP is then given by the size $|\mathcal{A}_\mathbf{\Omega}|$ of the operator basis. We always choose some K so that $\Omega_k = \varnothing \; \forall_{k>K}$. Enlarging the subsystems Ω_k systematically improves the solution of Eq. (9) and increases the computation cost polynomially. For given model and computer resources, the optimal choice for the subsystems Ω_k depends on the position in the phase diagram.

Symmetries.—Hamiltonian symmetries, like translation or rotation invariance, imply that several Green's function elements $G_{\hat{\sigma}}$ can be chosen to be identical (e.g., $G_{\hat{a}_x \hat{a}_y^\dagger} \equiv G_{\hat{a}_0 \hat{a}_{y-x}^\dagger} \; \forall_{xy}$) and it is sufficient to use in the SDP only one representative for each of the corresponding equivalence classes. Further, several Green's function elements can be zero (e.g., $G_{\hat{a}_x \hat{a}_y} = 0$ for particle-number-conserving models). A corresponding block structure in $\sum_{\hat{\sigma}} G_{\hat{\sigma}} M_{\hat{\sigma}}$ can be exploited to further reduce the computation cost.

Exemplary applications.—We demonstrate the capabilities of our SDP approach with three example systems. Let us first address the spin-1/2 *XXZ* model $\hat{H} = \sum_{\langle i,j \rangle} (\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y + J_z \hat{S}_i^z \hat{S}_j^z)$ in one spatial dimension (1D). Using comparable (moderate) computer resources, the energy bound obtained from the SDP method (9)
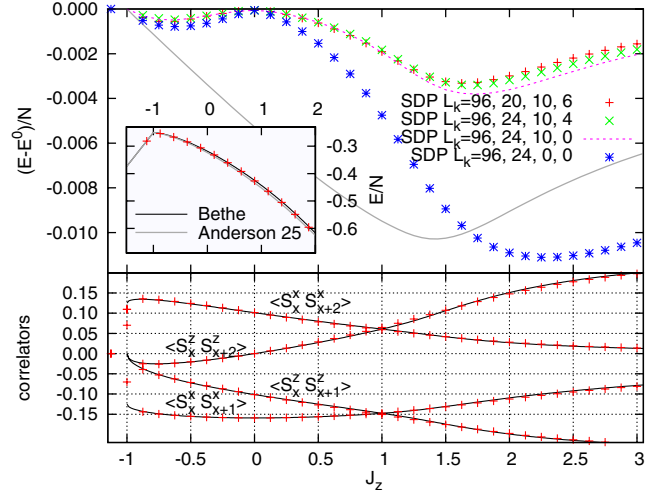

FIG. 1 (color online). Lower bounds E to the ground-state energy and approximations to correlators for the *XXZ* chain. The Anderson bound (2) was calculated with clusters of 25 sites. The subsystems Ω_k for the SDP method (12) are chosen to be clusters of contiguous sites with sizes L_1, L_2, L_3, and L_4 for constraint operators of polynomial degree 1, 2, 3, and 4, respectively, as specified in the legend ($K = 4$). The Bethe ansatz yields the exact ground-state energy E^0 and short-range correlators [38,39].

improves substantially on the Anderson bound (2); see Fig. 1. Employing higher-order Green's functions tends to improve bounds at larger J_z. The obtained short-range correlators coincide very well with the exact Bethe ansatz results [38,39].
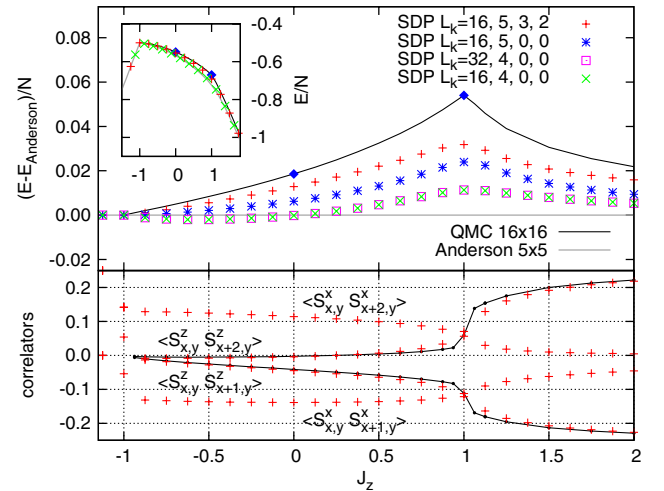

FIG. 2 (color online). Lower energy bounds and correlators for the 2D *XXZ* model, complemented by QMC data calculated for a square lattice of 16×16 sites with periodic boundary conditions and inverse temperature $\beta = 96$. The QMC energies for $J_z = 0, 1$ coincide with earlier results ($\blacklozenge$) from Refs. [43,44]. As SDP constraint subsystems Ω_k [Eq. (12)], we chose $L_k \times L_k$ squares with $K = 4$ and L_1, L_2, L_3, and L_4, as specified in the legend.

Let us now consider the spin-1/2 *XXZ* model on a square lattice. With the identifications $\hat{a}_i = \hat{S}_i^-$, $\hat{a}_i^\dagger = \hat{S}_i^+$, and $\hat{S}_i^z = \hat{a}_i^\dagger \hat{a}_i - \frac{1}{2}$, it maps to a model of interacting hard-core bosons obeying the algebra $\hat{a}_i \hat{a}_j^\dagger - (-1)^{\delta_{ij}} \hat{a}_j^\dagger \hat{a}_i = \delta_{ij}$. As displayed in Fig. 2, the SDP method yields much better lower bounds to the ground-state energy than the Anderson bound. As there is no exact solution available, we also simulated the model with QMC calculations based on the stochastic series expansion with directed loops [3]. It is again established that the SDP method gives access to the correlation functions.

Finally, Fig. 3 shows results of the SDP method for the 2D $t - V$ Hubbard model of spinless fermions $\hat{H} = -\frac{1}{2}\sum_{\langle i,j\rangle}(\hat{a}_i^\dagger \hat{a}_j + \text{H.c.}) + V\sum_{\langle i,j\rangle}(\hat{n}_i - \frac{1}{2})(\hat{n}_j - \frac{1}{2})$ on a square lattice. In this case, except for $V = 0$, no exact results are available. The QMC approach is in this case hampered by the sign problem [15–17]. It is hence inefficient and only applicable for small system sizes. The exact diagonalization results for small lattices show strong finite-size effects. The SDP method, however, is applicable just as well as for the other models, outperforms the Anderson bound, and reproduces the exact result for $V = 0$. Hence, we have a completely new and promising route to easily and controlledly study frustrated magnets and fermionic systems in $D \geq 2$, which theorists have laboriously tried to address for decades while being confronted with big methodological hurdles. Note that the SDP method employing the full single- and two-particle Green's functions, as developed in the context of quantum chemistry, has been applied to finite Hubbard chains of up to 14 sites [40–42].

Bipolar theorem.—Often, one is only interested in the single- and two-particle Green's functions. However, in the presented SDP approach, we also introduce higher Green's functions to improve the approximation. On the basis of the bipolar theorem, one can understand that such higher Green's functions represent slack variables. The set of representable ($k \leq P$)-point Green's functions
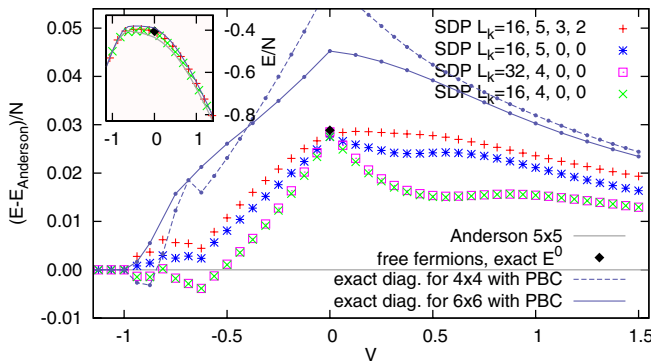

FIG. 3 (color online). Lower energy bounds for the 2D $t - V$ Hubbard model of spinless fermions on a square lattice, compared to exact energies for 4×4 and 6×6 lattices with periodic boundary conditions (PBC) as well as the thermodynamic limit at $V = 0$.

$$\tilde{\mathcal{R}}_P := \{\mathcal{G} | \exists \hat{\rho} \in \mathcal{S}: \mathcal{G}_{\hat{\sigma}}^{(k)} = \text{Tr}\hat{\rho}\,\hat{\sigma} \ \forall_{k \leq P, \hat{\sigma} \in \mathcal{A}^k}\}$$

is convex, as $\mathcal{G}$ is linear in $\hat{\rho}$ and $\mathcal{S}$ is convex. Giving up on the (inessential) normalization of the Green's functions, the set $\mathcal{R}_P := \{\alpha\mathcal{G} | \mathcal{G} \in \tilde{\mathcal{R}}_P, \alpha \in \mathbb{R}_+\}$ becomes a convex cone. For a given scalar product, $\langle \cdot, \cdot \rangle$, the bipolar theorem [32] states that $(\mathcal{R}_P^*)^* = \mathcal{R}_P$, where $\mathcal{R}_P^* := \{\hat{B} | \langle B, \mathcal{G}\rangle \geq 0 \ \forall_{\mathcal{G} \in \mathcal{R}_P}\}$ is the polar cone of $\mathcal{R}_P$. With the choice $\langle B, \mathcal{G}\rangle := \sum_k \sum_{\hat{\sigma} \in \mathcal{A}^k} \mathcal{G}_{\hat{\sigma}}^{(k)} B_{\hat{\sigma}} \equiv \mathcal{G}[\hat{B}]$, the polar $\mathcal{R}_P^*$ is the convex cone of all positive-semidefinite operators from $\mathcal{B}_P := \text{span} \bigcup_{k=0}^{P} \mathcal{A}^k$. Because of the bipolar theorem, $\mathcal{R}_P$ is hence characterized by $\mathcal{R}_P^*$ as

$$\mathcal{R}_P = \{\mathcal{G} | \mathcal{G}_{\hat{\sigma}^\dagger} = \mathcal{G}_{\hat{\sigma}}^* \ \forall_{\hat{\sigma}}, \mathcal{G}[\hat{B}] \geq 0 \ \forall_{\hat{B} \in \mathcal{B}_P, \hat{B} \geq 0}\}. \quad (13)$$

So, to obtain (or approximate) the ($k \leq P$)-point Green's functions, one needs to consider only ($k \leq P$)-point operators $\hat{B} \succeq 0$. In this sense, higher Green's functions are slack variables, which are only employed in order to bring the ground-state problem into the form of an SDP; see Eqs. (9) and (10). We showed how constraints $G[\hat{B}] \geq 0$ can be enforced in the SDP, for the case that $\hat{B} = \hat{C}^\dagger \hat{C}$ with constraint operators $\hat{C}$ that are polynomials of degree $\leq P/2$. However, there are also subspaces of operators $\hat{C}$ of polynomial degree $> P/2$ such that $G[\hat{C}^\dagger \hat{C}]$ can be evaluated with the ($k \leq P$)-point Green's functions. They can hence be taken into account without introducing higher Green's functions. A particularly simple space of such operators for a particle-number-conserving system is given by $\hat{C} = \sum_i c_i \hat{a}_{i_1} \dots \hat{a}_{i_m} + \text{H.c.}$: For every odd m, $G[\hat{C}^\dagger \hat{C}]$ can be evaluated without requiring $G^{(2m)}$.

Conclusion.—We have presented an SDP method for calculating lower bounds to the ground-state energy of condensed-matter systems and approximations to the ground-state Green's functions. It can be used for arbitrary particle statistics by employing the corresponding operator algebra. Our generic considerations on the SDP method carry over to quantum chemistry problems. An advantage in condensed-matter applications is that translation invariance and locality can be exploited to systematically balance the precision and the computation cost. Still, the idea of restricting the set of constraint operators to a physically motivated subset is also applicable to quantum chemistry problems.

[1] M. Suzuki, S. Miyashita, and A. Kuroda, Prog. Theor. Phys. **58**, 1377 (1977).

[2] N. V. Prokof'ev, B. V. Svistunov, and I. S. Tupitsyn, JETP Lett. **64**, 911 (1996).

[3] O. F. Syljuåsen and A. W. Sandvik, Phys. Rev. E **66**, 046701 (2002).

[4] F. Alet, S. Wessel, and M. Troyer, Phys. Rev. E **71**, 036706 (2005).

[5] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).

[6] U. Schollwöck, Rev. Mod. Phys. **77**, 259 (2005).

[7] H. Niggemann, A. Klümper, and J. Zittartz, Z. Phys. B **104**, 103 (1997).

[8] T. Nishino, K. Okunishi, Y. Hieida, N. Maeshima, and Y. Akutsu, Nucl. Phys. **B575**, 504 (2000).

[9] F. Verstraete and J. I. Cirac, arXiv:cond-mat/0407066.

[10] G. Vidal, Phys. Rev. Lett. **99**, 220405 (2007).

[11] W. L. McMillan, Phys. Rev. **138**, A442 (1965).

[12] D. Ceperley, G. V. Chester, and M. H. Kalos, Phys. Rev. B **16**, 3081 (1977).

[13] F. Mezzacapo, N. Schuch, M. Boninsegni, and J. I. Cirac, New J. Phys. **11**, 083026 (2009).

[14] H. J. Changlani, J. M. Kinder, C. J. Umrigar, and G. K.-L. Chan, Phys. Rev. B **80**, 245116 (2009).

[15] J. E. Hirsch, R. L. Sugar, D. J. Scalapino, and R. Blankenbecler, Phys. Rev. B **26**, 5033 (1982).

[16] M. Takasu, S. Miyashita, and M. Suzuki, Prog. Theor. Phys. **75**, 1254 (1986).

[17] M. Troyer and U.-J. Wiese, Phys. Rev. Lett. **94**, 170201 (2005).

[18] L. Vandenberghe and S. Boyd, SIAM Rev. **38**, 49 (1996).

[19] F. Alizadeh, SIAM J. Optim. **5**, 13 (1995).

[20] C. V. Kraus, N. Schuch, F. Verstraete, and J. I. Cirac, Phys. Rev. A **81**, 052338 (2010).

[21] P. Corboz, G. Evenbly, F. Verstraete, and G. Vidal, Phys. Rev. A **81**, 010303(R) (2010).

[22] C. Pineda, T. Barthel, and J. Eisert, Phys. Rev. A **81**, 050303(R) (2010).

[23] T. Barthel, C. Pineda, and J. Eisert, Phys. Rev. A **80**, 042333 (2009).

[24] P. Corboz and G. Vidal, Phys. Rev. B **80**, 165129 (2009).

[25] J. W. Negele and H. Orland, *Quantum Many-Particle Systems* (Perseus, Reading, MA, 1988).

[26] R. H. Tredgold, Phys. Rev. **105**, 1421 (1957).

[27] C. A. Coulson, Rev. Mod. Phys. **32**, 170 (1960).

[28] A. J. Coleman, Rev. Mod. Phys. **35**, 668 (1963).

[29] M. Deza and M. Laurent, J. Comput. Appl. Math. **55**, 217 (1994).

[30] Y.-K. Liu, M. Christandl, and F. Verstraete, Phys. Rev. Lett. **98**, 110503 (2007).

[31] D. A. Mazziotti, Acc. Chem. Res. **39**, 207 (2006).

[32] R. T. Rockafellar, *Convex Analysis*, Princeton Mathematical Series Vol. 28 (Princeton University Press, Princeton, NJ, 1970).

[33] P. W. Anderson, Phys. Rev. **83**, 1260 (1951).

[34] T. Wittmann and J. Stolze, Phys. Rev. B **48**, 3479 (1993).

[35] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.108.200404 for a short description of semidefinite programming and more related work, and a derivation for the Anderson bounds.

[36] D. Poulin and M. B. Hastings, Phys. Rev. Lett. **106**, 080403 (2011).

[37] J. Kempe, A. Kitaev, and O. Regev, SIAM J. Comput. **35**, 1070 (2006).

[38] J. D. Cloizeaux and M. Gaudin, J. Math. Phys. (N.Y.) **7**, 1384 (1966).

[39] G. Kato, M. Shiroishi, M. Takahashi, and K. Sakai, J. Phys. A **36**, L337 (2003).

[40] J. R. Hammond and D. A. Mazziotti, Phys. Rev. A **73**, 062505 (2006).

[41] M. Nakata, B. J. Braams, K. Fujisawa, M. Fukuda, J. K. Percus, M. Yamashita, and Z. Zhao, J. Chem. Phys. **128**, 164113 (2008).

[42] N. Shenvi and A. F. Izmaylov, Phys. Rev. Lett. **105**, 213003 (2010).

[43] A. W. Sandvik, Phys. Rev. B **56**, 11 678 (1997).

[44] A. W. Sandvik and C. J. Hamer, Phys. Rev. B **60**, 6588 (1999).