

Benchmarking the variational reduced density matrix theory in the doubly-occupied configuration interaction space with integrable pairing models

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Abstract

The variational reduced density matrix theory has been recently applied with great success to models within the truncated doubly-occupied configuration interaction space, which corresponds to the seniority zero subspace. Conservation of the seniority quantum number restricts the Hamiltonians to be based on the $SU(2)$ algebra. Among them there is a whole family of exactly solvable Richardson-Gaudin pairing Hamiltonians. We benchmark the variational theory against two different exactly solvable models, the Richardson-Gaudin-Kitaev and the reduced BCS Hamiltonians. We obtain exact numerical results for the so-called $\mathcal{P}QGT$ N -representability conditions in both cases for systems that go from 10 to 100 particles. However, when random

single-particle energies as appropriate for small superconducting grains are considered, the exactness is lost but still a high accuracy is obtained.

1 Introduction

One of the main problems in many-body quantum mechanics, which includes condensed matter, nuclear physics, and quantum chemistry, is the so-called exponential wall problem,¹ namely, the exponential growth of the dimension of the Hilbert space with the number of particles composing the studied system. A complete diagonalization of the corresponding Hamiltonian in the many-particle space provides the exact answer but at a prohibitively expensive computational cost. Therefore, research efforts have been focused on the development of approximate methods capturing the relevant degrees of freedom present in the wavefunction at a feasible computational cost, i.e., with a polynomial increase.

A great variety of such approximate methods that have been developed over the years can be broadly classified into approximations that improve over a reference state and variational theories. In the former case, a standard approach is to start from a mean-field reference state and improve on this by adding perturbative corrections² or excitations with increasing complexity within Coupled Cluster Theory.^{3,4} However, these methods break down in strong correlation regimes where multi-reference approximations are needed. New variational methods overcoming this issue were developed in the last decades. For instance, variational algorithms like tensor-network-state approaches,⁵⁻⁸ variational Monte Carlo methods,⁹⁻¹² or stochastic techniques¹³⁻¹⁶ can be made, in principle, as accurate as the exact diagonalizations while extending its computational limits beyond. Some of these many-body methods were recently benchmarked in the hydrogen chain.¹⁷

A very different approach to tackle the exponential wall problem that is applicable to any correlation regime concentrates on the second-order reduced density matrix (2RDM),^{18,19} while dispensing with the wavefunction altogether. The 2RDM is a much more compact

object than the wavefunction and it holds all the necessary information to evaluate the expectation values of one- and two-particle observables of physical interest. As the energy of any pairwise-interacting system can be written as an exact but simple linear function of the 2RDM, it can be used to variationally optimize this matrix at polynomial cost.²⁰ This optimization should be constrained to the class of 2RDMs that can be derived from a wavefunction (or an ensemble of wavefunctions), the so-called N -representable 2RDMs.^{21,22} Since the complete characterization of this class of 2RDMs is known to be a quantum Merlin Arthur (QMA) complete problem,²³ one has to use an incomplete set of necessary but not (in general) sufficient constraints on the 2RDM. The optimization thus finds a lower bound to the exact ground-state energy and an approximation to the exact ground-state 2RDM. Such an approach, known as the variational second-order reduced density matrix (v2RDM) method has been applied with different degrees of success in quantum-chemistry problems,^{24–27} nuclear-physics,^{28,29} and condensed-matter.^{30–32}

Recently, the computational efficiency of the v2RDM method has been substantially improved for systems whose states can be accurately described in terms of doubly-occupied single-particle states only. This lies at the heart of the doubly-occupied configuration interaction (DOCI) method, widely used in quantum chemistry to reduce the dimension of the configuration interaction Hilbert space. DOCI corresponds to the subspace of the Hilbert space of seniority zero, where the seniority quantum number³³ counts the number of unpaired particles. It has been recognized that the DOCI subspace captures most of the static correlations, serving as the first rung on a seniority ladder leading to the exact full configuration interaction (CI) solution.^{34–37} The assumptions in DOCI drastically simplify the structure of the 2RDM^{38,39} and reduce the scaling of the v2RDM method^{40–42} while, expectedly, retain most of the correlation. Several applications of the v2RDM for seniority nonconserving Hamiltonians were already implemented and their accuracy tested against exact diagonalizations for small systems.^{40,42,43} Here we will take advantage of the seniority-zero nature of DOCI space that restricts the Hamiltonians to be seniority conserving and therefore, to

be based on the SU(2) algebra. An important class of SU(2) Hamiltonians are the pairing Hamiltonians, where the fundamental physics lies in the specific form of the paired states. The quantum integrable and exactly solvable Richardson-Gaudin pairing models^{44–46} are ideal Hamiltonians to test the performance of the v2RDM method within the DOCI space. In this paper, we will benchmark the method for two different integrable Richardson-Gaudin models: the Richardson-Gaudin-Kitaev model⁴⁷ describing a chain of spinless fermions with p-wave pairing, and the constant pairing or reduced BCS Hamiltonian with uniform⁴⁸ and random single-particle energies.⁴⁹ We will also explore the behavior of the method for increasingly large systems addressing its extensivity properties

2 Theory

In second quantization, an N -particle Hamiltonian with pairwise interactions can be written as⁵⁰

$$H = \sum_{ij} t_{ij} c_i^\dagger c_j + \frac{1}{4} \sum_{ijkl} V_{ijkl} c_i^\dagger c_j^\dagger c_l c_k \quad (1)$$

where t and V are the one-body energy and the two-body interaction terms, respectively. c_i^\dagger and c_j are the standard fermion creation and annihilation operators in a given orthonormal single-particle basis $\{i, j, k, l, \dots\}$.

According to Eq. (1), the ground-state energy can be expressed solely in terms of the second-order reduced density matrix, 2RDM, ${}^2\Gamma$ ¹⁸

$$E_0[{}^2\Gamma] = \frac{1}{4} \sum_{ijkl} H_{ijkl}^{(2)} {}^2\Gamma_{ijkl} \quad (2)$$

where

$${}^2\Gamma_{ijkl} = \langle \psi | c_i^\dagger c_j^\dagger c_l c_k | \psi \rangle \quad (3)$$

and

$$H_{ijkl}^{(2)} = \frac{1}{N-1} (t_{ik}\delta_{jl} - t_{jk}\delta_{il} - t_{il}\delta_{jk} + t_{jl}\delta_{ik}) + V_{ijkl} \quad (4)$$

is the two-particle reduced Hamiltonian with $|\psi\rangle$ the ground-state wavefunction and N the number of particles.

The idea behind the variational 2RDM methodology is to minimize the energy functional (2) by varying the coefficients of ${}^2\Gamma$. However, direct application of this procedure yields unrealistic energies^{19,20,51} as ${}^2\Gamma$ must be constrained to the class of N -representable 2RDMs.²² N -representability of a 2RDM implies there must exist an N -particle wavefunction (or an ensemble of wavefunctions) from where it derives. The necessary and sufficient conditions to assure the N -representability of a p RDM are formally known:⁵²⁻⁵⁴ A p RDM is N -representable if and only if for every p -body Hamiltonian H_ξ the following inequality is satisfied

$$\frac{1}{(p!)^2} \sum_{i_1 i_2 \dots i_{2p}} H_\xi^{(p)}_{i_1 i_2 \dots i_{2p}} {}^p\Gamma_{i_1 i_2 \dots i_{2p}} \geq E_0(H_\xi) \quad (5)$$

with $H_\xi^{(p)}$ and $E_0(H_\xi)$ being the p -particle reduced Hamiltonian and the exact ground-state energy of H_ξ , respectively. Unfortunately, this theorem cannot be used in practice since it would require knowledge of the ground-state energy of every possible p -body Hamiltonian H_ξ . However, it can be relaxed using a set of Hamiltonians for which a lower bound for the ground-state energy is known. This is the case of the group of all semidefinite Hamiltonians, which are completely defined by its extreme elements

$$H = B^\dagger B \quad (6)$$

yielding the well-known \mathcal{P} , \mathcal{Q} and \mathcal{G} two-index N -representability conditions^{22,52} on the ${}^2\Gamma$ matrix if B is restricted to the forms $B = \sum_{ij} p_{ij} c_i c_j$, $B = \sum_{ij} q_{ij} c_i^\dagger c_j^\dagger$, and $B = \sum_{ij} g_{ij} c_i^\dagger c_j$, respectively. It has been shown that these conditions are the necessary and sufficient conditions to assure the N -representability for one-body Hamiltonians,^{22,55} as well as for two-body

Hamiltonians with an exact antisymmetric geminal power (AGP) ground state.^{55,56} We will demonstrate this last assertion analytically and numerically in Section 3.1 for the case of the Richardson-Gaudin-Kitaev Hamiltonian.

Hamiltonians of the class

$$H = B^\dagger B + B B^\dagger \quad (7)$$

with $B = \sum_{ijk} t_{ijk}^1 c_i^\dagger c_j^\dagger c_k^\dagger$, and $B = \sum_{ijk} t_{ijk}^2 c_i^\dagger c_j^\dagger c_k$ yield the \mathcal{T}_1 and \mathcal{T}_2 three-index N -representability conditions^{27,57,58} coming from the 3RDM on the ${}^2\Gamma$ matrix, respectively. As these conditions are in general necessary but not sufficient, the v2RDM will always find a lower bound to the exact ground-state energy and an approximation to the exact ground-state 2RDM.

In this work we will focus our attention on Hamiltonians with pairing interactions in the seniority zero subspace. Assuming time-reversal symmetry, the single-particle levels are doubly degenerate in the spin degree of freedom. The seniority quantum number classifies the Hilbert space into subspaces with a given number of singly occupied levels. The most general pairing Hamiltonian conserving seniority is

$$H = \frac{1}{2} \sum_{i=1}^L \epsilon_i N_i + \sum_{ij=1}^L V_{ij} c_i^\dagger c_i^\dagger c_j c_j \quad (8)$$

where ϵ_i are the energies of L doubly degenerate single-particle levels, $N_i = c_i^\dagger c_i + c_i^\dagger c_i$ is the number operator, and V_{ij} is the pairing interaction. The (i, \bar{i}) pair defines the pairing scheme, which can involve two particles with either opposite spins ($i \uparrow, i \downarrow$), momenta ($i, -i$), or in general any classification of conjugate quantum numbers in doubly degenerate single-particle levels. For these Hamiltonians the seniority number is an exact quantum number, as unpaired particles do not interact with the rest of the system and the pairing Hamiltonian does not allow for pair breaking. The Hamiltonian thus becomes block diagonal in sectors labeled by the seniority quantum number.

The pairing Hamiltonian (8) is based on the SU(2) pair algebra with generators

$$K_i^+ = c_i^\dagger c_i^\dagger = (K_i^-)^\dagger, \quad K_i^z = \frac{1}{2}(N_i - 1) \quad (9)$$

and commutation relations

$$[K_i^+, K_j^-] = 2\delta_{ij}K_i^z, \quad [K_i^z, K_j^\pm] = \pm\delta_{ij}K_i^\pm \quad (10)$$

We note that in the seniority zero subspace $N_i = 2K_i^+K_i^-$ and therefore, the Hamiltonian (8) can be written in terms of the ladder SU(2) operators as

$$H = \sum_{ij=1}^L J_{ij}K_i^+K_j^- \quad (11)$$

where $J_{ij} = \delta_{ij}\epsilon_i + V_{ij}$. The ground-state energy is thus given by

$$E_0 = \sum_{ij=1}^L J_{ij}P_{ij} \quad (12)$$

where the P matrix is

$$P_{ij} = \langle \psi | c_i^\dagger c_i^\dagger c_j^- c_j^- | \psi \rangle = \langle \psi | K_i^+ K_j^- | \psi \rangle \quad (13)$$

This matrix together with the D matrix

$$D_{ij} = \frac{1}{4} \langle \psi | N_i N_j | \psi \rangle = \langle \psi | \left(K_i^z + \frac{1}{2} \right) \left(K_j^z + \frac{1}{2} \right) | \psi \rangle \quad (14)$$

define the seniority blocks of the ${}^2\Gamma$ matrix. Notice that the diagonal elements of both matrices are equal ($D_{ii} = P_{ii}$). According to these definitions, it follows that the P and D

matrices are hermitian and fulfill

$$\sum_{i=1}^L P_{ii} = \sum_{i=1}^L D_{ii} = M \quad (15)$$

$$\sum_{j=1}^L D_{ij} = MP_{ii} \quad (16)$$

where M is the number of particle pairs in a system with L doubly degenerate single-particle levels and total $\langle \psi | K^z | \psi \rangle = M - \frac{L}{2}$. The \mathcal{P} , \mathcal{Q} , \mathcal{G} , \mathcal{T}_1 and \mathcal{T}_2 N -representability conditions can thus be written in terms of the seniority blocks of the 2RDM as,³⁸⁻⁴³

- The \mathcal{P} condition:

$$P \succeq 0 \quad (17)$$

$$D_{ij} \geq 0, \quad \forall i, j \quad (18)$$

- The \mathcal{Q} condition:

$$Q \succeq 0 \quad (19)$$

$$q_{ij} \geq 0, \quad \forall i, j \quad (20)$$

where

$$Q_{ij} = P_{ij} + \delta_{ij}(1 - 2P_{ii}) \quad (21)$$

$$q_{ij} = D_{ij} + 1 - P_{ii} - P_{jj} \quad (22)$$

- The \mathcal{G} condition:

$$G_{ij} \succeq 0, \quad \forall i > j \quad (23)$$

$$g \succeq 0 \quad (24)$$

where

$$G_{ij} = \begin{pmatrix} P_{ii} - D_{ij} & -P_{ij} \\ -P_{ji} & P_{jj} - D_{ij} \end{pmatrix} \quad (25)$$

$$g_{ij} = D_{ij} \quad (26)$$

- The \mathcal{T}_1 condition:

$$T_1^i \succeq 0, \quad \forall i \quad (27)$$

$$t_{1ijk} \geq 0, \quad \forall i > j > k \quad (28)$$

where

$$(T_1)_{jk}^i = \delta_{jk}(1 - 2P_{jj} - P_{ii} + 2D_{ij}) + P_{jk}, \quad \forall j, k \neq i \quad (29)$$

$$t_{1ijk} = 1 - P_{ii} - P_{jj} - P_{kk} + D_{ij} + D_{jk} + D_{ki} \quad (30)$$

- The \mathcal{T}_2 condition:

$$T_2^i \succeq 0, \quad \forall i \quad (31)$$

$$T_2^{ijk} \succeq 0, \quad \forall i > j > k \quad (32)$$

where

$$T_2^i = \begin{pmatrix} D_{jk} & -\delta_{jk}P_{ik} & D_{ik} \\ -\delta_{jk}P_{ki} & \delta_{jk}(P_{ii} - 2D_{ik}) + P_{jk} & P_{ik} \\ D_{ji} & P_{ji} & P_{ii} \end{pmatrix} \quad (33)$$

$$T_2^{ijk} = \begin{pmatrix} P_{ii} - D_{ij} - D_{ik} + D_{jk} & P_{ij} & P_{ik} \\ P_{ji} & P_{jj} - D_{ij} - D_{jk} + D_{ik} & P_{jk} \\ P_{ki} & P_{kj} & P_{kk} - D_{ik} - D_{jk} + D_{ij} \end{pmatrix} \quad (34)$$

where the symbol $\succeq 0$ denotes that a matrix is positive semidefinite.

The variational optimization of the 2RDM subject to conditions (15)-(34) can be formulated as a semidefinite problem (SDP) in which the energy, being a linear function of the 2RDM, is minimized over the intersection of a linear affine space and the convex cone of block-diagonal positive semidefinite matrices.⁵⁹⁻⁶² As discussed in,⁴⁰⁻⁴² the SDP in the seniority subspace computationally scales as $O(L^3)$ for the \mathcal{PQG} conditions and as $O(L^4)$ for the \mathcal{PQGT} conditions. This will allow us to treat without excessive computational efforts systems of sizes up to $L = 100$. In our numerical calculations we use the semidefinite programming algorithm (SDPA) code.^{63,64} This code solves semidefinite problems at several precision levels by means of the Mehrotra-type predictor-corrector primal-dual interior-point method, providing ground-state energies and the corresponding 2RDM.

We programmed our v2RDM method as a dual problem in the SDPA code, which does not allow for the equality constraints (15)-(16). These are included by relaxing them into inequality constraints with a sufficiently small summation error δ .^{27,65} In our work we have set $\delta = 10^{-7}$, which effectively fixes the precision of the ground-state energies.

3 Richardson-Gaudin integrable models

The Richardson-Gaudin (RG) models are based on a set of integrals of motion (IM) or quantum invariants that are linear and quadratic combinations of the generators of the $SU(2)$ algebra. By requiring the IM to commute with the total spin operators $K^z = \sum_i K_i^z$, the most general expression for the IM is

$$R_i = K_i^z + G \sum_{j(\neq i)} \frac{X_{ij}}{2} (K_i^+ K_j^- + K_j^+ K_i^-) + Z_{ij} K_i^z K_j^z \quad (35)$$

where X_{ij} and Z_{ij} are antisymmetric matrices and G is the pairing strength. The operators R_i must commute among themselves to constitute a set of IM. Imposing these conditions leads to two families of integrable models:

1. The hyperbolic or XXZ family

$$X_{ij} = \frac{2\eta_i \eta_j}{\eta_i^2 - \eta_j^2}, \quad Z_{ij} = \frac{\eta_i^2 + \eta_j^2}{\eta_i^2 - \eta_j^2} \quad (36)$$

2. The rational or XXX family

$$X_{ij} = Z_{ij} = \frac{1}{\eta_i^2 - \eta_j^2} \quad (37)$$

where the η 's are an arbitrary set of real parameters.

The common eigenstates of IM (35) are determined by the solution of the set of M non-linear coupled RG equations

$$1 + \frac{G}{2} \sum_{i=1}^L Z_{i\alpha} - G \sum_{\beta \neq \alpha}^M Z_{\beta\alpha} = 0, \quad \forall \alpha = 1, \dots, M \quad (38)$$

with $Z_{i\alpha} = Z(\eta_i^2, E_\alpha)$ in terms of the M spectral parameters E_α .

Defining the new L variables

$$\Lambda_i = \sum_{\alpha=1}^M Z(\eta_i^2, E_\alpha) \quad (39)$$

we can write the RG equations as a set of L coupled quadratic equations⁶⁶ in the Λ variables

$$\Lambda_i^2 = M(L - M)C - \frac{2}{G}\Lambda_i + \sum_{j \neq i}^L Z_{ij}(\Lambda_i - \Lambda_j) \quad (40)$$

where C is a constant that depends on the Gaudin algebra, 0 for the rational family and -1 for the hyperbolic family. This new system of equations is free of the divergences that plague the original set of RG equations (38), and it can be solved numerically with the Levenberg-Marquardt algorithm. Once we have determined the set of Λ_i for a particular eigenstate, the eigenvalues of the IM are

$$r_i = \frac{1}{2} \left(-1 - G\Lambda_i + \frac{G}{2} \sum_{j \neq i}^L Z_{ij} \right) \quad (41)$$

If the Hamiltonian is an arbitrary linear combination of the IM, $H = \sum_{i=1}^L \varepsilon_i R_i$, the corresponding eigenvalue is

$$E = \sum_{i=1}^L \varepsilon_i r_i \quad (42)$$

3.1 The Richardson-Gaudin-Kitaev model

The Richardson-Gaudin-Kitaev (RGK) model⁴⁷ is a variation of the celebrated Kitaev wire⁶⁷ proposed as a toy model to understand topological superconductivity. While the Kitaev wire is a non-number-conserving one-body Hamiltonian for spinless fermions in a 1D chain, the RGK Hamiltonian is two-body and number conserving. Moreover, it is exactly solvable for closed boundary conditions, either periodic or antiperiodic. Hence, this interacting many-body Hamiltonian allows to obtain precise answers for the characterization of topological superconductivity.

The RGK Hamiltonian is a particular realization of the hyperbolic family of RG models describing p-wave pairing⁶⁸⁻⁷⁰

$$H = \frac{1}{2} \sum_{i \in I+} \varepsilon_i N_i - G \sum_{ij \in I+} \eta_i \eta_j c_i^\dagger c_i^\dagger c_j c_j \quad (43)$$

where $\eta_i = \sin(i/2)$ and $\varepsilon_i = \eta_i^2$, such that the one-body term describes near-neighbor hoppings in a 1D chain. For simplicity we will assume antiperiodic boundary conditions. In this

case, the allowed values of i in a 1D chain of length $2L$ are $I+ = \{\pi, 3\pi, \dots, (2\pi L - \pi)\} / (2L)$.

The complete set of eigenstates in the seniority zero subspace is given by a product pair ansatz

$$|\Psi\rangle = \prod_{\alpha=1}^M \left(\sum_{i=1}^L \frac{\eta_i}{\varepsilon_i - E_\alpha} c_i^\dagger c_i^\dagger \right) |0\rangle \quad (44)$$

where the set of M spectral parameters (pair energies) E_α are a particular solution of a set of M non-linear coupled RG equations and $|0\rangle$ is the vacuum state.

The ground state solution has two critical values of G with peculiar properties: the Moore-Read point $G_{MR} = \frac{1}{L-M+1}$,⁷¹ and the Read-Green point $G_{RG} = \frac{1}{L-2M+2}$.⁷²

For the ground state solution at the Moore-Read point G_{MR} , and independently of the definition of the η 's, all pair energies E_α collapse at 0 energy ($E_\alpha = 0, \forall \alpha$). Therefore, the RGK ground state for G_{MR} is a pair condensate also known as number projected BCS (PBCS) wavefunction in nuclear physics or antisymmetric geminal power, AGP, in quantum chemistry

$$|\Psi_{MR}\rangle = \left(\sum_{i=1}^L \frac{1}{\eta_i} c_i^\dagger c_i^\dagger \right)^M |0\rangle \quad (45)$$

The PBCS or AGP wavefunction, being exact at G_{MR} , will display important consequences for the v2RDM approach. As mentioned above, the \mathcal{PQG} conditions are sufficient to produce the exact v2RDM result at this point. This statement can be independently proven starting from the set of killers of an AGP wavefunction

$$B_{ij} = \eta_j c_i^\dagger c_j - \eta_i c_j^\dagger c_i \quad (46)$$

such that

$$B_{ij} |\Psi_{MR}\rangle = 0 \quad (47)$$

from which the Moore-Read Hamiltonian derives as the positive semidefinite operator

$$H_{MR} = \frac{1}{[2(L+1) - 2M]} \sum_{ij} B_{ij}^\dagger B_{ij} \quad (48)$$

$$= \frac{1}{2} \sum_i \eta_i^2 N_i - \frac{1}{L - M + 1} \sum_{ij} \eta_i \eta_j c_i^\dagger c_i^\dagger c_j^- c_j \quad (49)$$

with 0 ground-state energy.

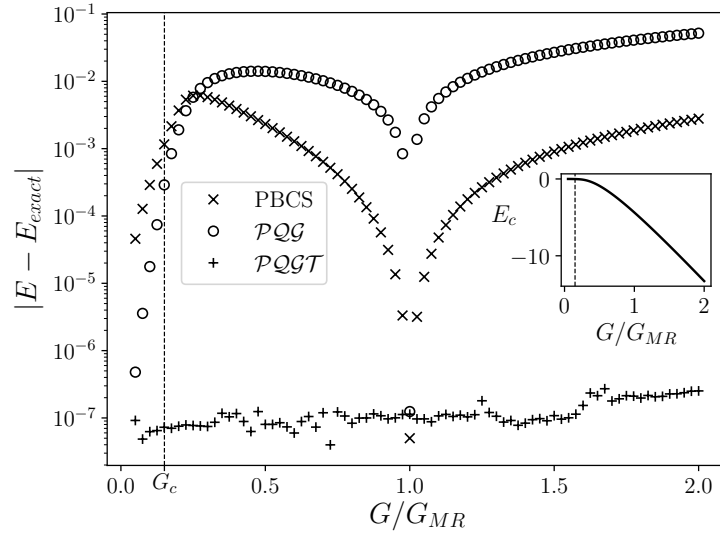


Figure 1: Absolute energy difference of v2RDM and PBCS with respect to the exact ground-state energy of the RGK Hamiltonian at different interaction strengths for a system with $L = 50$ doubly degenerate levels. The v2RDM results are computed with the PQG and the $PQGT$ conditions. Inset: exact correlation energy.

The Read-Green point G_{RG} signals the topological quantum phase transition. In the thermodynamic limit the scaled pairing strength is $g_{RG} = G_{RG}L = 1/(1 - 2\rho)$ implying that there is no phase transition for densities $\rho \geq 1/2$. Since we are interested in testing the accuracy of the v2RDM specifically around the Moore-Read point, we will consider systems of different sizes at half filling for several values of the pairing strength in units of G_{MR} .

In addition to the ground-state energies we will test another magnitude that characterizes

the pair mixing across the Fermi level, the canonical gap defined as

$$\begin{aligned}\Delta_c &= G \sum_{i=1}^L \eta_i \sqrt{\langle c_i^\dagger c_i^\dagger c_i c_i \rangle - \langle c_i^\dagger c_i \rangle \langle c_i^\dagger c_i \rangle} \\ &= G \sum_{i=1}^L \eta_i \sqrt{P_{ii} (1 - P_{ii})}\end{aligned}\tag{50}$$

It turns out that Δ_c coincides with the BCS gap Δ when it is evaluated with a number non-conserving BCS wavefunction. In this case the BCS gap equation reduces to

$$\frac{1}{G} = \sum_{i=1}^L \frac{\eta_i}{\sqrt{(\varepsilon_i - \mu)^2 + \eta_i^2 \Delta^2}}, \quad \mu = \frac{\varepsilon_M + \varepsilon_{M+1}}{2}\tag{51}$$

As a function of G the system has a phase transition from a metallic state characterized by $\Delta = 0$ to a superconducting state with finite gap. The critical value of G is obtained from the gap equations as

$$G_c = \left[\sum_i \frac{\eta_i}{|\varepsilon_i - \mu|} \right]^{-1}\tag{52}$$

Even though BCS predicts a non-superconducting state for $G < G_c$ ($\Delta = 0$), for correlated number conserving wavefunctions like PBCS or AGP the gap is always greater than zero.⁷³

We have now all the tools for testing the different variational approximations with the exact solution of the RGK model. We start with a system of $L = 50$ doubly degenerate levels at half filling corresponding to $M = 25$ fermion pairs. The size of the Hilbert space is 1.26×10^{14} , well beyond the limits of an exact diagonalization. Note that for finite size systems at half-filling, the Read-Green point lies at very large values of G , $G_{RG} = 1/2$ as compared to the Moore-Read point ($G_{MR} = 1/26$). Therefore, we assume G_{MR} as a characteristic value of the pairing strength, at which PBCS and the \mathcal{PQG} v2RDM approximations must be exact. Thus, we will study the behavior of the different approximations as a function of

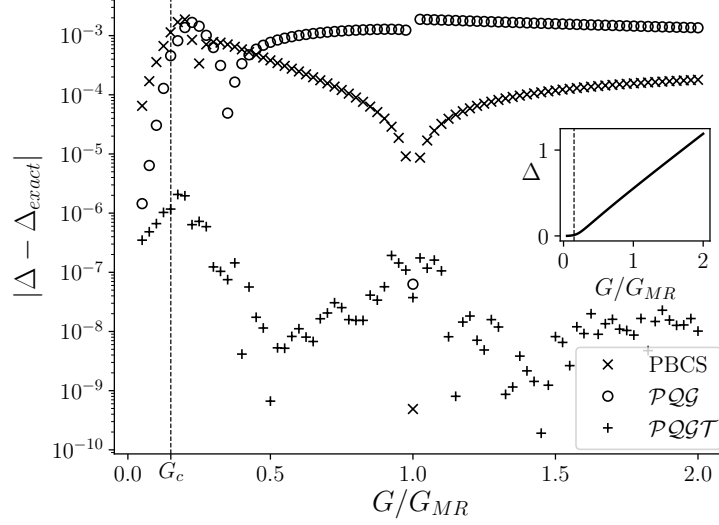


Figure 2: Absolute canonical gap difference of the v2RDM and the PBCS with respect to the exact canonical gap of the RGK Hamiltonian at different interaction strengths. The v2RDM results are computed with the \mathcal{PQG} and the \mathcal{PQGT} conditions. Computations are for a system with $L = 50$ doubly degenerate levels. Inset: exact canonical gap.

G in units of G_{MR} .

Fig. 1 shows the absolute value of the difference between the approximated and the exact ground-state energy. We display here the absolute value in order to compare PBCS and v2RDM. However, we should keep mind that this difference is positive for PBCS due to its Ritz variational character, while it is negative for v2RDM because it provides lower bounds. The inset displays the behavior of the correlation energy, which stays flat for weak pairing, and starts to decrease linearly with G entering the superconducting region. The correlation energy is defined as

$$E_c = \langle \psi | H | \psi \rangle - \langle \psi(0) | H | \psi(0) \rangle \quad (53)$$

where $|\psi(0)\rangle$ is the ground state of the noninteracting Hamiltonian.

As it was expected, the \mathcal{PQG} and PBCS are indeed exact at the Moore-Read point G_{MR} . While both approximations have a comparable accuracy in the weak coupling region, PBCS is two orders of magnitude better in the superconducting region. In contrast, the addition of constraints coming from the 3RDM in the \mathcal{PQGT} approximation makes the formalism

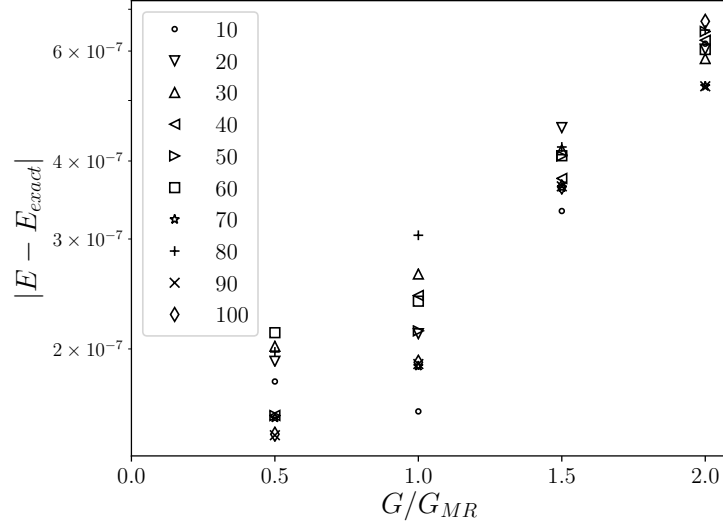


Figure 3: Absolute energy difference of the v2RDM with the \mathcal{PQGT} conditions with respect to the exact ground-state energy of the RGK Hamiltonian with different number of doubly degenerate levels as specified in the legend)

numerically exact within the accuracy limit imposed by the semidefinite programming code SDPA.

Fig. 2 shows the comparison of the canonical gap (50) computed with PBCS and the v2RDM with the exact one. As the gap is not determined from a variational principle, we plot the absolute value of the differences between approximated and exact gaps. Again, the PBCS and \mathcal{PQG} gaps are exact at the Moore-Read point, providing a second numerical confirmation of the exactness of both approaches. The \mathcal{PQG} approximation manages to give a fairly good description of the gap but the PBCS again provides at least one order of magnitude approximation better in the superconducting region. The computations with the \mathcal{PQGT} conditions give again a numerically exact approximation to the canonical gap. The inset in the figure shows the behavior of the exact canonical gap, which remains small at weak interactions due to pairing fluctuations, until it opens at around the critical interaction strength G_c , where the system enters a superconducting phase. The gaps in the PBCS and \mathcal{PQG} approximations show some structure for $G/G_c \sim 1.7$ and 2.3 for which we could not find an explanation. However, this structure disappears with the \mathcal{PQGT} conditions.

To ensure that the v2RDM method is extensible to systems of arbitrary sizes we show in Fig. 3 the comparison of the total ground-state energy under the \mathcal{PQGT} conditions with the exact energy for systems with sizes ranging from $L = 10$ to 100 levels. To compute systems of such larger sizes we have relaxed the summation error to $\delta = 3 \cdot 10^{-7}$, which is marginally lower than the previous computations. Our results show that the exact ground-state energies are numerically exact to the required precision independently of the system sizes. The relative energy errors are of the same order of magnitude taking into account that the correlation energy (inset of Fig. 1) increases by one order of magnitude along the horizontal axis.

3.2 The reduced BCS Hamiltonian

The reduced BCS or constant pairing Hamiltonian has been widely employed in condensed matter and nuclear physics to study superconducting properties of extensive as well as finite size systems in the BCS approximation. Few years after the celebrated BCS paper, Richardson solved this Hamiltonian exactly.⁷⁴ More recently, the exact solution has been generalized to families of exactly solvable pairing models.⁴⁴ In this subsection we will resort to the constant pairing Hamiltonian in the form used to describe ultrasmall superconducting grains⁷⁵

$$H_{BCS} = \sum_{i=1}^L \frac{\varepsilon_i}{2} N_i - G \sum_{ij=1}^L c_i^\dagger c_i^\dagger c_j c_j \quad (54)$$

Richardson proposed a product pair ansatz for the exact eigenstates of the BCS Hamiltonian

$$|\Psi\rangle = \prod_{\alpha=1}^M \left(\sum_{i=1}^L \frac{c_i^\dagger c_i^\dagger}{\varepsilon_i - E_\alpha} \right) |0\rangle \quad (55)$$

As in the RGK case, the pair energies, E_α , are obtained from the solution of a set of M nonlinear coupled equations and the total eigenvalues are the sum of the pair energies $E = \sum_{\alpha=1}^M E_\alpha$.

Note the slight difference with the eigenstates of the RGK Hamiltonian. In spite of the

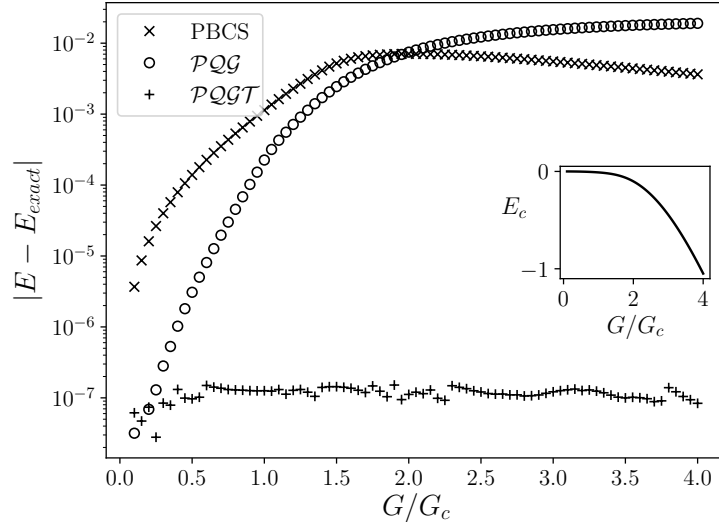


Figure 4: Absolute energy difference of the v2RDM and the PBCS with respect to the exact ground-state energy of the constant pairing Hamiltonian at different interaction strengths for a system with $L = 50$ doubly degenerate levels. The v2RDM results are computed with the PQG and the $PQGT$ conditions. Inset: exact correlation energy.

similarities in the wavefunction, the physics of these two Hamiltonians is completely different. While the BCS Hamiltonian describes fermions interacting through an attractive s-wave pairing, the RGK Hamiltonian describes a p-wave interaction. In the former case there is a smooth crossover from a superconducting BCS state to a Bose-Einstein condensate.⁷⁶ In the latter case there is a third-order quantum phase transition from a topological superconducting phase to a trivial superconducting phase or Bose-Einstein condensate of p-wave molecules.⁶⁹

In small grains it is customary to assume equidistant levels and to express all quantities in units of the mean level spacing d , which in turn is inversely proportional to the volume of the grain. However, due to presence of disorder, the level spacing in small metallic grains follows a Wigner-Dyson distribution obtained from random matrix theory. We will take advantage of the two standard descriptions of small grains to benchmark the v2RDM. First, we will test it with uniformly distributed equidistant levels, and then investigate how robust is the method in the presence of random disorder.

In order to quantify pairing fluctuations around the Fermi level we make use of the

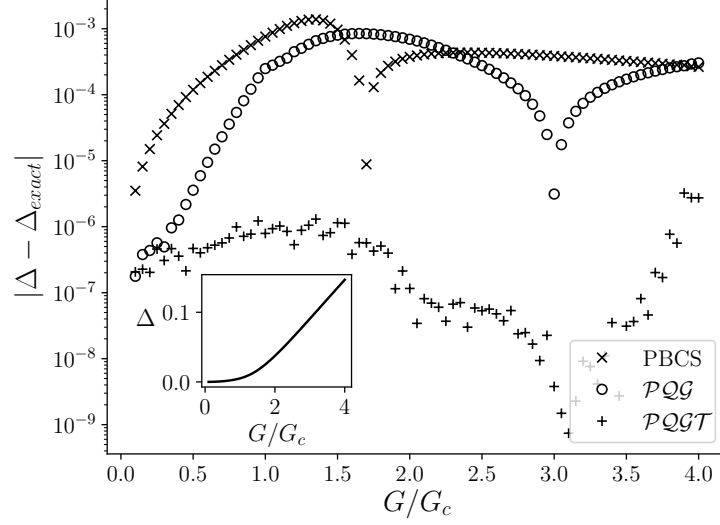


Figure 5: Absolute canonical gap difference of the v2RDM and the PBCS with respect to the exact canonical gap of the constant pairing Hamiltonian at different interaction strengths. The v2RDM results are computed with the \mathcal{PQG} and the \mathcal{PQGT} conditions. Computations are for a system with 50 doubly degenerate levels.

canonical gap Δ_c

$$\begin{aligned}
\Delta_c &= G \sum_{i=1}^L \sqrt{\langle c_i^\dagger c_i^\dagger c_{\bar{i}} c_i \rangle - \langle c_i^\dagger c_i \rangle \langle c_{\bar{i}}^\dagger c_{\bar{i}} \rangle} \\
&= G \sum_{i=1}^L \sqrt{P_{ii} (1 - P_{ii})}
\end{aligned} \tag{56}$$

For finite systems the BCS approximation has a metallic phase with no gap, and a superconducting phase with finite gap. The critical value of G is

$$G_c = \left[\sum_i \frac{1}{|\varepsilon_i - \mu|} \right]^{-1} \tag{57}$$

Since G_c is a sensible value to assess the degree of superconducting correlations, we will study the BCS Hamiltonian for different system sizes as a function of G in units of G_c .

Fig. 4 shows the absolute value of the differences between the ground-state energy in the different approximations and the exact one for a system of $M = 25$ fermion pairs in $L = 50$

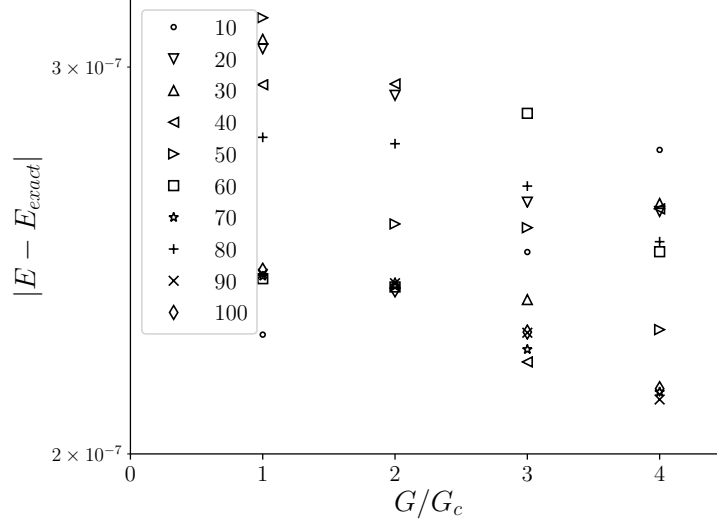


Figure 6: Absolute energy difference of the v2RDM with the \mathcal{PQGT} conditions with respect to the exact ground-state energy of the constant pairing Hamiltonian with different number of doubly degenerate levels as specified in the legend.

equidistant single-particle levels with spacing $d = 1/L$ as a function of the pairing strength G in units of G_c . As in the case of the RGK model, the \mathcal{PQGT} conditions are sufficient enough to reproduce the exact results within the numerical error of the computing program. Ref.²⁹ found the same conclusion for a system of $M = 12$ pairs. \mathcal{PQG} and PBCS are significantly less precise with a complementary behavior. \mathcal{PQG} starts with a good description of the system at weak pairing, but it quickly degrades approaching the critical region. On the contrary, PBCS is less accurate in weak pairing but tends to improve towards the strong superconducting region. The inset displays the exact correlation energy as a function of G , exhibiting a change in curvature around the critical BCS value of G that separates a regime dominated by pairing fluctuations from a superconducting phase characterized by a condensation of Cooper pairs. A similar picture is described in the inset of Fig. 5 with small but nonzero values of the canonical gap below G_c changing to a linear behavior above G_c .

Fig. 5 confirms the remarkable accuracy of the \mathcal{PQGT} approximation. Curiously, the gaps in the PBCS and \mathcal{PQG} approximations show a similar behavior for $G/G_c \sim 1.7$ and 3.0 respectively as in the RGK model.

Fig. 6 explores the accuracy of the \mathcal{PQGT} method as a function of the system size in a similar way as it has been done for the RGK Hamiltonian. As seen in the figure, the v2RDM energies are numerically exact within the accepted tolerance. The relative errors are comparable since the correlation energy is of the same order of magnitude for the whole range of interactions (inset of Fig. 4). As in the RGK example, we have relaxed the summation error to $\delta = 3 \cdot 10^{-7}$.

It is known that the energy levels of small metallic grains follow a Gaussian orthogonal ensemble distribution. For simplicity, most of the studies have been carried out assuming a uniform level spacing. However, the exact solution of the BCS Hamiltonian (54) is valid for arbitrary single-particle levels ε_i . This feature has been exploited to study in an exact manner the interplay between randomness and interaction in the crossover from metal to superconductor as a function of the grain size.⁴⁹ Here, we will use this ability of the exact solution to test the robustness of the \mathcal{PQGT} conditions against disorder in the single-particle levels spectrum. For each value of G/G_c in Fig. 7 we generate 70 symmetric random matrices of size $2L \times 2L$. Upon diagonalization, we select the central L eigenvalues to avoid edge effects. In order to assure an average constant level spacing we rescale them as $\varepsilon \rightarrow (1/2\pi)[4L \sin^{-1}(\varepsilon/\sqrt{4L}) + \varepsilon\sqrt{4L - \varepsilon^2}]$.

Fig. 7 shows the results obtained in the \mathcal{PQGT} approximation for each random ensemble as compared with the uniform level spacing case. Interestingly enough, the transition from metallic to superconductor reveals a clear cut distinction in the accuracy of the v2RDM method. While the method is completely accurate for all instances below the critical G_c value, it starts to deviate from the exact ground-state energy crossing this point and loosing three orders of magnitude in accuracy. In spite of this loss, errors of 10^{-4} in the correlation energy are quite acceptable for many standards. However, the reason of this deviation cannot be attributed the loss of integrability since the random Hamiltonian (54) is always exactly solvable and the exact eigenstates are given by the ansatz (55). It might be attributed to the complexity of the wavefunction (55) with random energy levels ε_i .

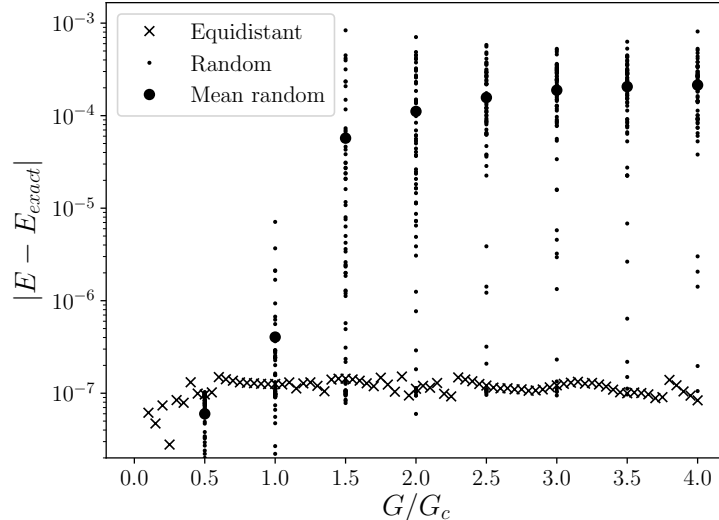


Figure 7: Absolute energy differences of the v2RDM with the \mathcal{PQGT} conditions of 70 samples of random single-particle energies with respect to the exact ground-state for selected values of G/G_c . The big solid circle signals the mean value of the ensemble. For comparison we display the \mathcal{PQGT} energies of the equidistant single-particle case. Computations are for a system with 50 doubly degenerate levels.

4 Summary

In this work we have explored the performance of the v2RDM within the seniority zero subspace for two classes of integrable RG models with different characteristics. The RGK model has a particular value of the pairing strength $G_{MR} = \frac{1}{L-M+1}$, obtained by Moore and Read,⁷¹ at which the exact ground-state wavefunction is a pair condensate (PBCS or AGP). From the exact solution, at this point the M pair energies E_α converge to zero transforming the product of geminals (44) into the AGP (45). From the other side, starting with the AGP and making use of the killers we derived the Moore-Read Hamiltonian (49) that is contained in the \mathcal{G} condition, and therefore the v2RDM with the \mathcal{PQG} conditions should provide the exact solution. Fig. 1 gives the numerical proof of this statement in a highly non-trivial problem. This figure also shows that the variational method with the \mathcal{PQGT} conditions gives the exact numerical ground-state energy from weak to strong pairing. Additional confirmation of the exactness of the \mathcal{PQGT} conditions comes from the canonical gaps in Fig. 2, which also shows an exact value for \mathcal{PQG} at the Moore-Read point. Similar results

for the ground-state energies and gaps were obtained for the reduced BCS Hamiltonian with equidistant single-particle levels. We then tested the robustness of the \mathcal{PQGT} N -representability conditions against disorder in the single-particle levels as in the case of small metallic grains (see Fig. 7). Surprisingly, and even though the systems are always quantum integrable, the exactness of the numerical results was lost in the superconducting region ($G > G_c$). This fact might be explained by the complexity of the ground-state wavefunctions in most of the random instances, as can be deduced from the distribution of pair energies E_α in the complex plane when the system enters the superconducting phase. However, relative errors of 10^{-4} are still competitive with DMRG calculations⁷⁷ for equidistant levels, and with more recent approaches tested in the Richardson model for small size systems.^{78,79}

The exact solvability of these models allowed us to test the v2RDM method for large systems in order to assess its extensive properties. Fig. 3 and 6 demonstrate that the high accuracy of the \mathcal{PQGT} is independent of the system size in the studied range from $L = 10$ to $L = 100$.

Before closing, we would like to point out that $SU(2)$ Hamiltonians encompass the area of quantum magnetism with Heisenberg type Hamiltonians. The formalism developed in⁴² and tested in this work could be directly applied to the study of spin systems. Due to the non-perturbative nature of v2RDM, it might be possible to describe with high accuracy exotic phases and quantum phase transitions.

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