

Many Body Diffusion and Interacting Electrons in a Harmonic Confinement

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We present numerically exact energy estimates for two-dimensional electrons in a parabolic confinement. By application of an extension of the recently introduced many-body diffusion algorithm, the ground-state energies are simulated very efficiently. The new algorithm relies on partial antisymmetrization under permutation of particle coordinates. A comparison is made with earlier theoretical results for that system.

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I. INTRODUCTION

In this paper we apply the recently developed quantum Monte Carlo algorithms [1,2] to an important model for interacting charge carriers in quantum dots. The fabrication of novel miniaturized semiconductor structures on nanometer scale has shed light on a variety of advanced physical systems and devices in which the classical description of electronic properties breaks down. The band structure of quantum wells, multiple quantum wells and superlattices [3] makes mobile carriers locate parallel to the semiconductor interfaces and hence induces a quasi-two-dimensional confinement [4]. Electrons in sandwiched semiconductor layer structures can be confined perpendicular to the growth direction [5–7]. If the lateral confinement is of the same order as the electron wavelength, the electrons have essentially no free direction left. The resulting quasi-zero-dimensional structure is addressed as a quantum dot or an artificial atom [6]. Mostly, the confinement effect along the growth direction of the layers is much stronger than perpendicular to it. Accordingly, on the microscopic scale, the electrons form two-dimensional disk-shaped objects [7]. Step-like potential structures, being induced by steps in the conduction band edge, became a popular object of study in the framework of self-assembled quantum dots [8]. In field-effect confined quantum dots, experimental far-infrared transmission spectra indicate the occurrence of parabolic-shaped confinement potentials [9]. Depending on the gate voltage applied, the number of electrons may discretely vary from zero to a large number of electrons [10,11].

Motivated by the fabrication techniques of quantum dots, we here focus on a commonly used model of N interacting electrons in a harmonic confinement potential,

$$H = \frac{\vec{p}^2}{2\mu} + V_c(\vec{r}) + V_{\text{int}}(\vec{r}) \quad (1)$$

where

$$V_c(\vec{r}) = \frac{1}{2} \mu \omega^2 \vec{r}^2, \quad V_{\text{int}}(\vec{r}) = \sum_{i=1}^{N-1} \sum_{j=i}^N \frac{e^2}{2\epsilon |\vec{r}_i - \vec{r}_j|}. \quad (2)$$

Here, ω denotes the frequency of the harmonic confinement potential of the dot, μ the effective mass of the electrons and ϵ the dielectric constant of the material. For convenience, we set $\hbar = \omega = e = \mu = 1$. The only parameter which then enters in (1) is $\gamma = \epsilon^{-1}$. It serves as a parameter to adjust the strength of the electron-electron repulsion for a given dot radius.

The derivation of the energy eigenfunctions and eigenvalues of (1) turns out to be challenging in cases where many particles are involved. Even in the classical case, solutions remain elusive, and the use of analytical approximations

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or computational methods is indispensable to reliably predict the energy spectrum of the system. The consideration of identical particles makes analytical or numerical treatments still more difficult. Much effort with different methods has been pursued to investigate the physical properties of quantum dots [12,13]. Various approaches have been performed using the Thomas-Fermi approximation [14], many-body perturbation theory [15], or the Hartree- and Hartree-Fock Ansatz [16]. Bearing in mind that exact analytical approaches are generally restricted either to the limit of non-interacting quantum-mechanical particles or exclusive cases [17], some methods, as e.g. the Padé approximants [18,19] or the renormalization perturbation theory [20,21], attempt to connect these limits. Exact numerical solutions are possible by diagonalization of the Coulomb interaction [15,16,22–24]. Due to their challenging numerical expense, diagonalization techniques are limited to few-electron systems. In particular for many-particle systems, for which diagonalization techniques quickly exceed the capacities of today’s computers, Monte Carlo techniques turn out to be very useful [25]. Monte Carlo approaches have been applied to electrons in a parabolic potentials in refs. [26–28]. Apart from their simplicity and flexibility, the power of Monte Carlo methods lies in the possibility to obtain estimates which converge to the exact values with a known statistical error. Although the computational effort needed for Monte Carlo techniques to obtain a given accuracy does not necessarily grow exponentially with the particle number, it mostly does if identical fermions are involved. As a consequence, exact fermion Monte Carlo methods are limited to few-particle systems. In what follows, we apply a Monte Carlo method which scales favorably and is nevertheless exact.

The paper is organized as follows. In section II we will discuss the principle of many-body diffusion (MBDF) [29–32]. This formalism is applied to derive random processes to numerically predict some energy eigenvalues of the model Hamiltonian. A feasible implementation scheme is discussed. Section III gives the outcome of our numerical analysis, and a comparison to other work is made. Finally, section IV concludes the present article.

II. THE MANY-BODY DIFFUSION ALGORITHM

The model is approached with a recently developed quantum Monte Carlo method, the many-body diffusion algorithm (MBDA) [1,2]. The MBDA is based on the many-body diffusion formalism (MBDF) [29–32]. Here we will restrict ourselves to a brief outline of the underlying concepts. In the MBDF, the propagator of N interacting identical particles in d spatial dimensions is written as a Feynman-Kac functional [33] over a symmetrized process, i.e., as a Euclidean-time path integral over the diffusion process of N identical free particles with superimposed potential-dependent exponential weights. For a given irreducible symmetry representation S , the propagator

$$K_S(\bar{\mathbf{r}}_f, \tau; \bar{\mathbf{r}}_i) = E_{\bar{\mathbf{r}}_i} \left[I_{(\bar{\mathbf{R}}^S(\tau)=\bar{\mathbf{r}}_f)} \exp \left(- \int_0^\tau V(\bar{\mathbf{R}}^S(\varsigma)) d\varsigma \right) \right] \quad (3)$$

is hence represented as an average over all paths starting in $\bar{\mathbf{r}}_i$, as indicated by the averaging index $E_{\bar{\mathbf{r}}_i}$, and ending a Euclidean time lapse τ later in $\bar{\mathbf{r}}_f$, as denoted by the indicator $I_{(\bar{\mathbf{R}}(\tau)=\bar{\mathbf{r}}_f)}$. The symmetry representation S determines the construction principle for the underlying dN -dimensional diffusion process $\{\bar{\mathbf{R}}^S(\tau); \tau \geq 0\}$.

In the MBDF, a detailed analysis has been performed of the diffusion process of free identical particles, and the role of the potential symmetry has been pointed out. It was found that for coordinate-symmetric potentials, i.e., potentials invariant under the permutation of the Cartesian particle coordinates, and for certain irreducible symmetry representations S , the total propagator separates into a sum of stochastically independent sub-propagators. The importance of this coordinate-symmetry shows two-fold. First, it allows to easily generalize the diffusion process of free identical particles to the process of interacting identical particles. Second, dealing with identical fermions, the sign problem is strictly avoided by numerical procedures based on exclusively positive walkers. The Feynman-Kac formulation (3) indicates the relevance of the free diffusion process. For any coordinate-symmetric potential $V(\bar{\mathbf{r}})$, the symmetry properties of the total diffusion process correspond to those of the free one. Rather than interfering with the role of the potential, different irreducible symmetry representations S do completely determine the structure of the free diffusion process. Correspondingly, one may in principle approach various eigenstates of the system by formulating the free diffusion process in the appropriate symmetry representations.

In [31], the free density matrix of N identical particles is decomposed into corresponding one-dimensional N -particle density matrices. In one dimension (1D), the introduction of an ordered N -particle state space $\tilde{D}_N = \{x_1 \geq x_2 \geq \dots \geq x_N\}$ projects the density matrix on a mathematically well-defined expression for both bosons and fermions. On that basis, the MBDF introduces the *fermion diffusion process* \tilde{X}_f and the *boson diffusion process* \tilde{X}_b as a Brownian motion on the irreducible state space \tilde{D}_N with absorbing respectively reflecting boundary conditions. The processes \tilde{X}_f and \tilde{X}_b serve as key ingredients for the multi-dimensional formulation. With the decomposition into

one-dimensional fermion and boson diffusion processes, a scheme has been introduced to sample the free density matrix for specific symmetric and antisymmetric symmetry representations sign-problem-free.

The symmetry constraints specified in [1,31] rely on the complete (anti-)symmetrization along the Cartesian coordinates. This scheme addresses a particular excited fermion state. To illustrate this idea, consider N identical free fermions or bosons in two dimensions (2D) with unit mass, for which the density matrix can be expressed as a determinant or a permanent:

$$\rho_f(\bar{\mathbf{r}}_f, \tau; \bar{\mathbf{r}}_i) = \det_{j,k=1,N} \left[\rho \left(\vec{r}_f^j, \tau; \vec{r}_i^k \right) \right] \text{ resp. } \rho_b(\bar{\mathbf{r}}_f, \tau; \bar{\mathbf{r}}_i) = \text{perm}_{j,k=1,N} \left[\rho_d \left(\vec{r}_f^j, \tau; \vec{r}_i^k \right) \right]$$

where

$$\rho_d \left(\vec{r}_f^j, \tau; \vec{r}_i^k \right) = \frac{1}{2\pi\tau} \exp \left(-\frac{(\vec{r}_f^j - \vec{r}_i^k)^2}{2\tau} \right).$$

Complete particle (anti)symmetrization along the Cartesian directions then leads to the following representation for N two-dimensional identical fermions

$$\rho_f(\bar{\mathbf{r}}_f, \tau; \bar{\mathbf{r}}_i) = \det_{j,k=1,N} \left[\rho_d \left(\vec{r}_f^j, \tau; \vec{r}_i^k \right) \right] = \rho_f(\bar{\mathbf{x}}_f, \tau; \bar{\mathbf{x}}_i) \rho_b(\bar{\mathbf{y}}_f, \tau; \bar{\mathbf{y}}_i) + \rho_b(\bar{\mathbf{x}}_f, \tau; \bar{\mathbf{x}}_i) \rho_f(\bar{\mathbf{y}}_f, \tau; \bar{\mathbf{y}}_i).$$

Applying an analogous decomposition for three spatial dimensions, excited state energies of up to 20 harmonically interacting identical fermion oscillators have been efficiently simulated within a statistical accuracy of about 0.1 percent [1]. Quadratic particle interaction has also been considered in the framework of quantum dots [35] but is not studied here. By an extension of the many-body diffusion principle, it is also possible to extract the corresponding ground-state energies. Again, particle (anti)symmetrization along the Cartesian directions plays the central role in that formulation. However, in contrast to [1,31], not all particles are necessarily (anti)symmetrized in the same direction. A detailed discussion of the underlying formalism is beyond the scope of the present paper and will be published elsewhere.

The derivation of the sampled functional separates into two parts, the decomposition of the corresponding free density matrix and symmetry considerations on the potential. The underlying free diffusion principle is best explained for the example of three identical free fermions in two dimensions [34]. In this case, the infinite-time limit of the free density matrix reads

$$\begin{aligned} \lim_{\tau \rightarrow \infty} \frac{\rho_f(\bar{\mathbf{r}}_f, \tau; \bar{\mathbf{r}}_i)}{\rho_d(\bar{\mathbf{r}}_f, \tau; \bar{\mathbf{r}}_i) e^{\bar{\mathbf{r}}_f \cdot \bar{\mathbf{r}}_i / \tau}} &= \frac{1}{\tau^2} \begin{vmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \end{vmatrix} \begin{vmatrix} 1 & x'_1 & y'_1 \\ 1 & x'_2 & y'_2 \\ 1 & x'_3 & y'_3 \end{vmatrix} + O(\tau^{-3}) \\ &= \frac{1}{\tau^2} \left(\begin{aligned} & [(x_1 - x_2)(y_2 - y_3)] [(x'_1 - x'_2)(y'_2 - y'_3)] \\ & + [(x_2 - x_3)(y_1 - y_2)] [(x'_2 - x'_3)(y'_1 - y'_2)] \\ & - [(x_1 - x_2)(y_2 - y_3)] [(x'_2 - x'_3)(y'_1 - y'_2)] \\ & - [(x_2 - x_3)(y_1 - y_2)] [(x'_1 - x'_2)(y'_2 - y'_3)] \end{aligned} \right) + O(\tau^{-3}). \end{aligned} \quad (4)$$

As our concern is the generation of equilibrated samples to derive properties of the (lowest available) eigenstate, the use of this asymptotic limit is justified. Emphasis in our approach –as mostly in random-walk or diffusion Monte Carlo approaches– is thus on the long-term distribution rather than on the equilibration process itself. Eq. (4) involves two interdependent stochastic processes. They both include a Brownian motion, but distinguished by their respective positive domains D_1 and D_2 ,

$$D_1 = \{x_1 \geq x_2; y_2 \geq y_3\} \text{ and } D_2 = \{x_2 \geq x_3; y_1 \geq y_2\},$$

and boundary conditions. Apart from an adapted distinguishable-particle diffusion, a jump process must be realized to take into account the process interdependencies [2]. In practice, during an evolution cycle, a walker associated to a particular type of process might be assigned to the other type of process according to the locally dependent process transition rates. In the present case, in which we are interested in the derivation of the ground-state energy, single-process evolution is sufficient for our needs. Indeed, as long as the time decay rates of the individual processes are identical, the energy eigenvalue predicted by any of the single processes is the same as the one predicted from their combination.

Table 1 shows the symmetry configurations for the numerical simulation of the ground-state energy of three and six two-dimensional non-interacting spin-polarized harmonic fermions. The ground-state energy of three identical

fermions in 2D, e.g., can be simulated by anti-symmetrization of pairs of Cartesian coordinates, namely (x_1, x_2) and (y_2, y_3) . Analogously, one might conglomerate the coordinates (x_2, x_3) and (y_1, y_2) . For six identical fermions in 2D, e.g., one simultaneously anti-symmetrizes (x_1, x_2, x_3) , (x_4, x_6) , (y_3, y_4, y_5) , and (y_2, y_6) , and so forth.

The advantage of the (generalized) many-body diffusion approach lies in the efficient sampling of the required probability densities. As mentioned above, symmetry and anti-symmetry in one spatial dimension can be achieved by the definition of reflecting and absorbing boundary conditions on a distinguishable-particle Brownian motion. Neither do we have to deal with negative transition amplitudes, nor is our approach slowed down by sampling determinants. A detailed description of the algorithmic realization has been reported in [1]. The Euclidean-time evolution according to $K_S(\bar{\mathbf{r}}_f, \tau; \bar{\mathbf{r}}_i)$ is simulated in sufficiently small time steps ϵ by the repeated application of the following two-step procedure: a) given $(2N$ -dimensional) initial system configurations $\bar{\mathbf{r}}_i$ sample final ones $\bar{\mathbf{r}}_f(\tau + \epsilon) = \bar{\mathbf{r}}_i(\tau) + \delta\bar{\mathbf{r}}(\epsilon)$, where $\delta\bar{\mathbf{r}}(\epsilon)$ is randomly drawn according to the free identical-particle propagator, and b) apply the potential-dependent weights $\exp\left[-\int_{\tau}^{\tau+\epsilon} V\left(\bar{\mathbf{R}}^S(\varsigma)\right) d\varsigma\right]$ randomly in a branching and killing procedure. The determination of the weights $\exp\left[-\int_{\tau}^{\tau+\epsilon} V\left(\bar{\mathbf{R}}^S(\varsigma)\right) d\varsigma\right]$ in principle requires infinitesimal time steps $\epsilon \rightarrow 0$. Due to limited computer performance, however, this procedure is not practical, and reliable approximation schemes must be provided. In the present case of harmonic confinement and repulsive Coulomb interaction, the use of the Suzuki-Trotter weights $\exp\left\{-\frac{1}{2}\left[V\left(\bar{\mathbf{R}}^S(\tau)\right) + V\left(\bar{\mathbf{R}}^S(\tau + \epsilon)\right)\right]\right\}$ is satisfactory for realistic time steps of 0.001/Hartree (H). The essential requirement for the efficient approach of many-body systems with the outlined free diffusion construction principles is the coordinate-symmetry of the potential involved. This condition holds for both the confinement and the interaction potential of our model

$$\forall (i, j \in \{1, 2, 3\} \vee \{4, 5, 6\}) : V_{\text{int}}(\bar{\mathbf{r}}) = V_{\text{int}}(\hat{P}_x^{i,j}\bar{\mathbf{r}}) = V_{\text{int}}(\hat{P}_y^{i,j}\bar{\mathbf{r}}) \wedge V_c(\bar{\mathbf{r}}) = V_c(\hat{P}_x^{i,j}\bar{\mathbf{r}}) = V_c(\hat{P}_y^{i,j}\bar{\mathbf{r}}). \quad (5)$$

In (5), the operators $\hat{P}_x^{i,j}$ and $\hat{P}_y^{i,j}$ interchange the i th and the j th x - respectively y -coordinates.

It should be emphasized that this invariance of the Hamiltonian under the interchange of the x and y coordinates of any two particles no longer applies if the confinement potential is replaced for instance by a Coulomb potential. The potential then generates transition rates between different types of walkers, as discussed in detail in [2]. Although the principle of sign-problem free diffusion remains valid for such systems, the detailed analytical analysis of the process interdependencies becomes cumbersome. With our present approach of Cartesian decomposition, more than six electrons become almost intractable in practice. New purely numerical techniques are currently under development to perform the required symmetry decompositions, avoiding the tedious and unpractical analytical bookkeeping of the Cartesian decompositions for the different types of walkers. Preliminary studies reveal that this numerical analysis requires in general the evaluation of $N \times N$ determinants relating the initial and final positions of the walkers. This N^3 cost in computation time is presumably overcompensated by a factor $1/N!$ due to the reduction of the state space. Within the present status of our approach however, closed shell systems with potentials satisfying the symmetry condition (5) are tractable for as many as 20 electrons.

III. RESULTS AND DISCUSSION

Table 2 gives the ground-state energy estimates predicted for closed-shell systems of six, twelve and twenty unpolarized electrons as a function of $\gamma^{1/3}$. The energies obtained are supposed to be exact within the numerically estimated statistical error. In the limit of zero electron Coulomb repulsion, $\gamma \rightarrow 0$, (1) is identical to a system of non-interacting fermion oscillators. The arrangement of single-particle harmonic oscillator solutions into a Slater determinant then induces the energy limits $E_0^{\gamma \rightarrow 0} = 10$ H, $E_0^{\gamma \rightarrow 0} = 28$ H and $E_0^{\gamma \rightarrow 0} = 60$ H for six, twelve and twenty electrons, respectively, whereas the neglect of spin statistics would yield $E_{\text{dist}}^{\gamma \rightarrow 0} = N$ H, with N indicating the particle number. In the opposite limit, for infinitely large electron-electron repulsion, $\gamma \rightarrow \infty$, the electrons behave classically and one expects them to arrange in the form of a Wigner lattice [36]. With increasing γ , the average electron-electron distance grows, and the influence of spin-statistics weakens. Accordingly, as γ grows, the energy gap between different excited states is expected to decrease substantially. This physical behavior is recovered by our numerical data. The limit of zero electron-electron repulsion is accurately simulated, and a smooth transition to high γ is found. A comparison of the numerical energy eigenvalues and the energy of distinguishable particles (see Table 3) indeed indicates the irrelevance of quantum statistics as $\gamma \rightarrow \infty$.

It proves instructive to compare our energy estimates for the ground state of the unpolarized electron systems with the Padé approximants reported in ref. [19]. The relative deviation of the Padé approximants with respect to our numerical estimates E_0 for the case of six unpolarized electrons are also studied. For both zero and very large γ , the Padé approximates $P_{3,2}(\gamma)$ and $P_{4,3}(\gamma)$ match our prediction. For intermediate γ , the Padé approximants $P_{4,3}(\gamma)$

for the ground state energy introduce a systematic error of up to almost 4 per cent. A comparison of our numerical estimates for the twelve and the twenty-particle system with the corresponding Padé approximants [19] indicates an analogous qualitative picture. The extreme relative deviations are of the same order. The lack of an accurate description of the system (1) for intermediate regions of the electron-electron-repulsion parameter γ is typical for a variety of analytical approximations.

IV. CONCLUSIONS

In the present paper, we apply a generalization of the recently reported many-body diffusion formalism to a system of interacting electrons in a parabolic confinement. The method is illustrated explicitly for closed-shell configurations of six, twelve and twenty unpolarized electrons for which the ground-state energy is numerically predicted. The algorithm proceeds without the use of analytical approximations. Apart from a small but controllable systematic error, the energy values are numerically exact within a computed statistical error of a few per mil. The feasibility of our approach is indicated by the comparison of our ground-state energy estimates with the corresponding Padé approximants calculated by A. Gonzales et al. [19]. Analogous results [37] were obtained by another Monte Carlo technique [28,38] that strongly reduces the noise due to the sign problem.

Regarding the methodological aspect, this work introduces an algorithm which allows to efficiently simulate the ground-state energy of closed-shell configurations of electrons exposed to coordinate-symmetric potentials. The scheme strictly avoids the fermion sign problem [39,40] by the definition of a Brownian motion on a state space with the appropriate boundary conditions. The resulting random process can be realized by stable diffusion of purely positive walkers.

The formulation of a sign-problem-free algorithm for the quantum-dot model (1) is remarkable, since almost all quantum Monte Carlo algorithms face massive difficulties with the general description of significantly correlated continuous quantum systems. The reason for this is the fermion sign problem, which generally thwarts reliable stochastic many-fermion treatments. Although potentially exact, the transient estimation of eigen-energies experiences a serious inefficiency due to an exponential decreasing signal-to-noise ratio. On the other hand, even the use of very accurate and efficiently implemented trial wave functions in diffusion or Green's function Monte Carlo variants [41] introduces considerable systematic errors due to the assumption of generally incorrect nodal surfaces. The MBDA avoids these problems by the definition of a diffusion process on a state space with absorbing and/or reflecting boundaries. Its derivation is based on a symmetry analysis of the Hamiltonian only.

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- [34] We limit the discussion to closed shell configurations, not because our method is not applicable for open shells, but for reasons of relative algebraic simplicity. For open shell systems the degeneracy of the ground state induces a state space with linear combinations of possible initial and final states . This degeneracy poses no problems of principle, but the resulting conditions become quite involved. E.g., for 4 particles in two dimensions the degeneracy is threefold, and the subprocesses and their boundary conditions have to be determined from the following infinite-time limit of the free density matrix

$$\lim_{\tau \rightarrow \infty} \frac{\rho_f(\bar{r}_f, \tau; \bar{r}_i)}{\rho_d(\bar{r}_f, \tau; \bar{r}_i) e^{\bar{r}_f \cdot \bar{r}_i / \tau}} = \frac{1}{2\tau^4} \left(\begin{array}{l} \left(\begin{array}{l} \left| \begin{array}{l} 1 \ x'_1 \ y'_1 \ (x'_1)^2 \\ 1 \ x'_2 \ y'_2 \ (x'_2)^2 \\ 1 \ x'_3 \ y'_3 \ (x'_3)^2 \\ 1 \ x'_4 \ y'_4 \ (x'_4)^2 \end{array} \right| \left| \begin{array}{l} 1 \ x_1 \ y_1 \ x_1^2 \\ 1 \ x_2 \ y_2 \ x_2^2 \\ 1 \ x_3 \ y_3 \ x_3^2 \\ 1 \ x_4 \ y_4 \ x_4^2 \end{array} \right| \\ \left| \begin{array}{l} 1 \ x'_1 \ y'_1 \ (y'_1)^2 \\ 1 \ x'_2 \ y'_2 \ (y'_2)^2 \\ 1 \ x'_3 \ y'_3 \ (y'_3)^2 \\ 1 \ x'_4 \ y'_4 \ (y'_4)^2 \end{array} \right| \left| \begin{array}{l} 1 \ x_1 \ y_1 \ y_1^2 \\ 1 \ x_2 \ y_2 \ y_2^2 \\ 1 \ x_3 \ y_3 \ y_3^2 \\ 1 \ x_4 \ y_4 \ y_4^2 \end{array} \right| \\ +2 \left| \begin{array}{l} 1 \ x'_1 \ y'_1 \ x'_1 y'_1 \\ 1 \ x'_2 \ y'_2 \ x'_2 y'_2 \\ 1 \ x'_3 \ y'_3 \ x'_3 y'_3 \\ 1 \ x'_4 \ y'_4 \ x'_4 y'_4 \end{array} \right| \left| \begin{array}{l} 1 \ x_1 \ y_1 \ x_1 y_1 \\ 1 \ x_2 \ y_2 \ x_2 y_2 \\ 1 \ x_3 \ y_3 \ x_3 y_3 \\ 1 \ x_4 \ y_4 \ x_4 y_4 \end{array} \right| \end{array} \right) \end{array} \right).$$

The complexity increases with increasing degeneracy of the fermion ground state, and the bookkeeping of the cartesian decompositions soon becomes very complicated. More appropriate methods for handling open shells are under study.

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| N | antisymmetric constellation |
|----|--|
| 3 | $(x_1, x_2); (y_2, y_3)$ |
| 6 | $(x_1, x_2, x_3); (x_4, x_6); (y_3, y_4, y_5); (y_2, y_6)$ |
| 10 | $(y_1, y_2, y_3, y_4); (y_5, y_8, y_9); (y_6, y_{10})$ $(x_4, x_5, x_6, x_7); (x_3, x_8, x_{10}); (x_2, x_9)$ |

TABLE I. List of configurations used for the ground states of N identical 2D fermions.

| $\gamma^{1/3}$ | 0.2 | 0.4 | 0.6 | 0.8 | 1.0 | 1.2 | 1.4 | 1.6 |
|---------------------------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| $E_0(3\uparrow, 3\downarrow)$ | 10.086(4) | 10.804(3) | 12.632(4) | 15.806(4) | 20.367(3) | 26.158(2) | 33.084(4) | 41.115(5) |
| $E_0(6\uparrow, 6\downarrow)$ | 28.28(4) | 31.00(3) | 37.91(2) | 49.62(2) | 66.45(1) | 87.88(2) | 113.52(2) | 143.45(2) |
| $E_0(10\uparrow, 10\downarrow)$ | 60.99(7) | 67.72(9) | 85.24(3) | 114.98(8) | 157.97(4) | 211.70(8) | 276.72(7) | 351.72(6) |

TABLE II. List of energy eigenvalues (a.u.) for model (1) obtained by the MBDA.

| | $E_0(3\uparrow, 3\downarrow)$ | $E_{\text{dist}}(3\uparrow, 3\downarrow)$ | $E_0(6\uparrow, 6\downarrow)$ | $E_{\text{dist}}(6\uparrow, 6\downarrow)$ | $E_0(10\uparrow, 10\downarrow)$ | $E_{\text{dist}}(10\uparrow, 10\downarrow)$ |
|--------------------|-------------------------------|---|-------------------------------|---|---------------------------------|---|
| $\gamma^{1/3} = 2$ | 60.385(5) | 60.12(1) | 215.21(1) | 214.30(3) | 533.56(3) | 531.44(4) |

TABLE III. List of energy eigenvalues (a.u.) for model (1) obtained by the MBDA.