

Atomic ground states in strong magnetic fields: Electron configurations and energy levels

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Using a combination of a fast two-dimensional-Hartree-Fock-Roothaan method and highly accurate fixed-phase diffusion quantum Monte Carlo simulations, we analyze the electronic structure and calculate the energy of the ground states of atoms with nuclear charges $Z = 2\text{--}26$ in very strong magnetic fields $B = 10^7\text{--}5 \times 10^8$ T, relevant for astrophysical problems, e.g., the thermal emission of strongly magnetized isolated neutron stars.

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I. INTRODUCTION

Over the past decade, continuing effort has gone into calculating, with ever-increasing accuracy and with various methods, the energies of atoms and ions in neutron star magnetic fields. The motivation comes largely from the fact that features discovered [1–3] in the thermal emission spectra of isolated neutron stars may be due to the absorption of photons by heavy atoms in the hot thin atmospheres of these strongly magnetized cosmic objects [4]. Also, features of heavier elements may be present in the spectra of magnetic white dwarf stars [5,6].

Although comprehensive and precise data for hydrogen in strong magnetic fields have been available for some time (cf. Refs. [7–10]), this is less the case for atoms and ions with more than one electron. Accurate ground-state energies of atoms up to nuclear charge $Z = 10$ in the high-field regime were first determined by Ivanov and Schmelcher [11], who solved the two-dimensional- (2D-) Hartree-Fock equations on a flexible mesh. By means of a specific multiconfigurational perturbative hybrid Hartree-Hartree-Fock method, Mori and Hailey [12] computed the energies of low-lying states in strong magnetic fields for atoms up to $Z = 26$. In another Hartree-Fock approach, Thirumalai and Heyl [13] obtained quite accurate values for the low-lying levels of helium, whereas, Becken *et al.* [14] and Becken and Schmelcher [15–17] used a highly precise full configuration-interaction (CI) method to analyze a large amount of helium states and transitions in a wide range of magnetic-field strengths. Low-lying states of lithium and beryllium have been studied with high accuracy using modified freezing full-core methods [18,19], configuration-interaction methods [20,21], and methods based on an anisotropic Gaussian basis set [22–24].

Along a different line of approach, Monte Carlo methods from *ab initio* quantum chemistry [25] have also been proven to be a powerful tool for the very accurate computation of the energy values of the ground states of all elements up to iron ($Z = 26$) in magnetic fields $B = 10^7\text{--}5 \times 10^8$ T [26]. For helium, they have also been used for the computation of low-lying excited states [27,28]. These methods use precalculated Hartree-Fock wave functions enhanced by Jastrow factors as guiding wave functions for the diffusion quantum Monte Carlo step.

In Ref. [26], the guiding wave functions were determined using the adiabatic approximation, which amounts to taking

single-particle orbitals as products of a Landau wave function for the quantum-mechanical description of the (fast) motion of the electron perpendicular to the direction of the magnetic field, and a longitudinal wave function for the (slow) motion along the field. This approximation limits the applicability of the method to magnetic fields where the nuclear charge scaled magnetic-field parameter $\beta_Z = B/(B_0 Z^2)$ (with $B_0 = 4.701\,03 \times 10^5$ T) is much larger than 1. (At B_0 , the electron's Larmor radius becomes equal to the Bohr radius of the hydrogen atom.)

The purpose of this paper is to abandon this approximation and, in this way, to extend the range of applicability of quantum Monte Carlo calculations for atoms in strong magnetic fields down towards the regime of intermediate-field strengths. We perform this by choosing a more sophisticated Ansatz for the single-particle orbitals in the Hartree-Fock step, which yields enhanced guiding wave functions for the quantum Monte Carlo procedure.

In very strong magnetic fields, the spin of all electrons can be assumed to be aligned opposite to the direction of the magnetic field because of the large spin-flip energies. This is no longer true when the magnetic field decreases. We also include states without full spin alignment and can, indeed, demonstrate that, for $Z > 10$ in a field with $B = 10^7$ T and for $Z > 21$ at $B = 5 \times 10^7$ T, the ground-state configurations contain an electron with spin parallel to the magnetic field, contrary to the assumptions made in earlier calculations [26].

The paper is organized as follows. In Sec. II, we give a brief summary of the 2D-Hartree-Fock-Roothaan (2DHFR) method and recapitulate the fixed-phase diffusion quantum Monte Carlo (FPDQMC) method in Sec. III. Section IV contains a comparison of our results for ground-state energies and oscillator strengths with previous work in the literature. We conclude with a summary and an outlook in Sec. V.

II. THE 2DHFR METHOD

A. Two-dimensional-Hartree-Fock-Roothaan equations

Since we restrict ourselves to strong magnetic fields $\beta_Z \geq 0.1$, we use cylindrical coordinates and atomic Rydberg units for the many-particle Hamiltonian,

$$\hat{H} = \sum_{i=1}^N \left(-\Delta_i - 2i\beta\partial_{\varphi_i} + \beta^2\rho_i^2 + 4\beta m_{s_i} - 2\frac{Z}{|\mathbf{r}_i|} + \sum_{j=i+1}^N \frac{2}{|\mathbf{r}_i - \mathbf{r}_j|} \right), \quad (1)$$

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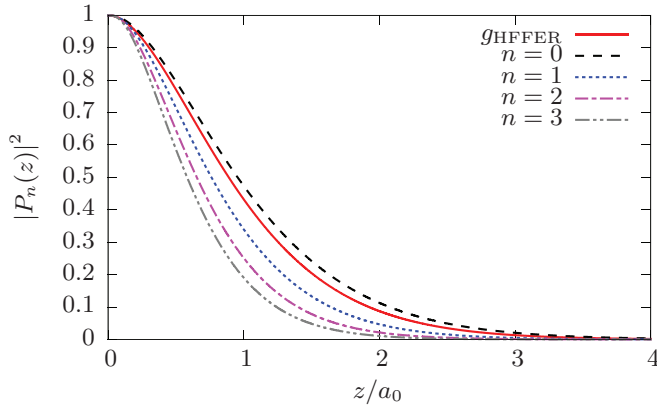


FIG. 1. (Color online) Squared z -wave functions $|P_n(z)|^2$ (maxima normed to one) corresponding to the first four Landau channels for the hydrogen ground state at $B = 10^5$ T compared to $|P(z)|^2$ (g_{HFFER}) obtained with our previous Ansatz (2).

of a nonmoving N -electron atomic system in a magnetic field pointing in the z direction with infinite mass of the nucleus of charge Z . Flipping a single-electron spin m_s equals 4β in Rydberg energies, so for very high magnetic fields, we expect full spin-down polarization, whereas, for intermediate-field strengths, the spin of a few electrons may point “up” to gain access to low-lying single-particle orbitals that are already occupied with spin-down electrons.

The many-particle wave function Ψ is constructed from a Slater determinant of single-particle orbitals for each electron i . These orbitals are products of a spatial wave function $\psi^i(\mathbf{r})$ and a spin function $\chi^i(s)$. In a previous version of the Hartree-Fock-Roothaan method [29,30], the single-electron wave functions were taken in the form of a product,

$$\tilde{\psi}^i(\rho_i, \varphi_i, z_i) = P^i(z_i) \sum_{n=0}^{N_L} t_n^i \Phi_{nm_i}(\rho_i, \varphi_i), \quad (2)$$

a sum over the $N_L + 1$ Landau states $\Phi_{nm_i}(\rho, \varphi)$, weighted by an occupation vector t_n^i and a Landau quantum number independent longitudinal wave function $P^i(z_i)$.

In this paper, we go beyond the product Ansatz in Eq. (2) and proceed to a full 2D description of the problem with individual longitudinal wave functions $P_n^i(z_i)$ for each Landau level,

$$\psi^i(\rho_i, \varphi_i, z_i) = \sum_{n=0}^{N_L} P_n^i(z_i) \Phi_{nm_i}(\rho_i, \varphi_i). \quad (3)$$

As an example, Fig. 1 shows that the longitudinal wave functions $P_n^i(z_i)$ corresponding to the Landau levels Φ_{nm_i} differ considerably for magnetic-field strengths $\beta_Z \lesssim 1$, thus, our Ansatz (3) will allow for a much better description of the wave functions.

The z -wave functions,

$$P_n^i(z_i) = \sum_v \alpha_{nv}^i B_v^i(z_i) \quad (4)$$

are expanded using individual B -spline [31] bases $B_v^i(z_i)$ for each electron as described in Refs. [29,30]. The variation in the energy functional with respect to the B -spline coefficients α_{nv}^i

yields two-dimensional-Hartree-Fock-Roothaan equations,

$$\sum_{n'\mu} F_{nvn'\mu}^i \alpha_{n'\mu}^i = \varepsilon_i \sum_{n'\mu} S_{nvn'\mu}^i \alpha_{n'\mu}^i, \quad (5)$$

with $F_{nvn'\mu}^i$ and $S_{nvn'\mu}^i$ being the Fock matrix and the overlap matrix, respectively. The Fock matrix is the sum of the longitudinal and transverse kinetic energies, the nuclear potential energy, as well as the direct and exchange electron-electron energy matrices,

$$\text{long} F_{nvn'\mu}^i = -\delta_{n,n'} \int_{-\infty}^{\infty} B_v^i(z_i) \frac{\partial^2}{\partial z_i^2} B_{\mu}^i(z_i) dz_i, \quad (6)$$

$$\text{tran} F_{nvn'\mu}^i = 4n\beta \delta_{n,n'} \int_{-\infty}^{\infty} B_v^i(z_i) B_{\mu}^i(z_i) dz_i, \quad (7)$$

$$\text{nucl} F_{nvn'\mu}^i = \int_{-\infty}^{\infty} B_v^i(z_i) V_{nn'}^i(z_i) B_{\mu}^i(z_i) dz_i, \quad (8)$$

$$\begin{aligned} \text{dir} F_{nvn'\mu}^i &= \sum_{j=1}^N \frac{1}{\xi_j} \sum_{k,k'}^{N_{\text{int}}^j} \int_{-\infty}^{\infty} B_v^i(z_i) B_{\mu}^i(z_i) \\ &\times \int_{-\infty}^{\infty} P_k^j(z_j) U_{nn'kk'}^{ij}(z_i, z_j) P_{k'}^j(z_j) dz_j dz_i, \end{aligned} \quad (9)$$

$$\begin{aligned} \text{ex} F_{nvn'\mu}^i &= -\sum_{j=1}^N \delta_{m_{s_i}, m_{s_j}} \frac{1}{\xi_j} \sum_{k,k'}^{N_{\text{int}}^j} \int_{-\infty}^{\infty} B_v^i(z_i) P_k^j(z_j) \\ &\times \int_{-\infty}^{\infty} B_{\mu}^i(z_i) A_{nn'kk'}^{ij}(z_i, z_j) P_{k'}^j(z_j) dz_j dz_i. \end{aligned} \quad (10)$$

Explicit forms of the effective potentials $V_{nn'}^i(z_i)$, $U_{nn'kk'}^{ij}(z_i, z_j)$, and $A_{nn'kk'}^{ij}(z_i, z_j)$ can be found in Ref. [29] along with a description of their computation. They are precalculated to a precision of eight digits to speed up the evaluation of the integrals. The parameters ξ_j and N_{int}^j will be explained in detail in the next subsection. The overlap matrix can be calculated using

$$S_{nvn'\mu}^i = \delta_{n,n'} \int_{-\infty}^{\infty} B_v^i(z_i) B_{\mu}^i(z_i) dz_i. \quad (11)$$

To avoid convergence problems and to reduce the number of iterations, we use the results obtained with our Hartree-Fock-finite-element-Roothaan II (HFFER II) code [30] as the initial wave functions and solve equations (5) self-consistently.

B. Interaction cutoff and convergence

In the regime of intermediate magnetic-field strengths $\beta_Z \lesssim 1$, single-electron states close to the nucleus and its spherically symmetric Coulomb potential are not easily described using only a few Landau states in the cylindrically symmetric expansion (3). This problem occurs for states with magnetic quantum numbers $|m| \lesssim 5$ and, especially, for states with $m = 0$, whose probability distributions have a finite cusp at $\rho = 0$. Entering this regime, therefore, requires blowing up the Landau expansion considerably.

We increased the number of included Landau levels from $N_L = 7$ in the previous application of the Hartree-Fock-Roothaan method to $N_L = 30$ in this paper. However, a complete evaluation of the energy functional would require

the calculation of roughly $N(N_L)^4$ electron interaction terms in (9) and (10), causing an unacceptable loss of efficiency. We bypass this problem by introducing the cutoff parameters N_{int}^i , dropping higher Landau-level interaction terms in Eqs. (9) and (10) between electrons i and j with $k, k' > N_{\text{int}}^j$ or $n, n' > N_{\text{int}}^i$ but include all N_L Landau levels in Eq. (8). We, thereby, induce a new cutoff error in our energy functional, lowering its minimum value and depriving it of its variational nature since the repulsive Coulomb interactions are not fully taken into account anymore.

To reduce this error, we compensate for the loss of the energy contributions due to the repulsive electron-electron interaction by renormalizing the lower Landau-levels' interaction terms in (9) and (10) with a factor,

$$\xi^j = \sum_{k=0}^{N_{\text{int}}^j} \int_{-\infty}^{\infty} |P_k^j(z_j)|^2 dz_j. \quad (12)$$

We implemented a simple Monte Carlo integration algorithm (not the FPDQMC method discussed later) with a correct evaluation of the electron-electron interaction terms ($N_{\text{int}}^i = N_{\text{int}}^j = N_L$) to double-check the results obtained with this modified energy functional. With the help of this algorithm, we are able to show that the new cutoff-induced energy error is negligible as long as the occupation of the higher Landau expansion terms stays small. This is the case for all single-particle wave functions when $\beta_Z \gtrsim 0.1$.

Choosing a proper interaction cutoff parameter N_{int}^i for each electron is crucial, both for the speed of the algorithm and for the quality of the results. The optimal N_{int}^i strongly depends on β_Z and the quantum numbers of the wave function ψ^i . By the use of the Landau-level occupation vector t_n^i from the initial wave functions obtained with our previous implementation [30], we can predict reasonable parameters N_{int}^i for each electron. We found $(t_{N_{\text{int}}}^i)^2 \approx 10^{-6}$ to be a reliable criterion for the cutoff parameter.

Figure 2 shows the change in the computed ground-state energy of neutral iron at $B = 5 \times 10^7$ T when the Landau

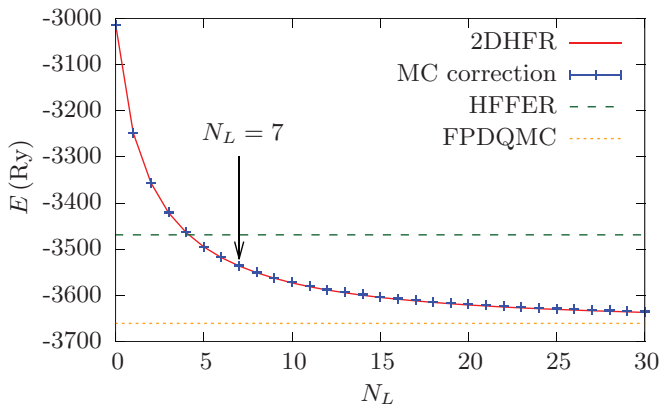


FIG. 2. (Color online) Ground-state energy of neutral iron at $B = 5 \times 10^7$ T calculated with the 2DHFR method for different orders N_L of the Landau expansion. Simple Monte Carlo calculations confirm the smallness of the energy error induced by the reduced electron-electron interactions. Results of our previous method (HFFER) with $N_L = 7$ and of the accurate FPDQMC procedure are shown as well.

expansion order N_L of the single-particle wave functions is increased (solid red line). The convergence of our Ansatz (3) is clearly visible. The simple Monte Carlo corrected energies (blue points with error bars) correspond to the unmodified energy functionals and are, at most, 2.2 Ry or 0.6% above the 2DHFR results. The statistical error of these Monte Carlo results is very small, thus, the error bars are hardly visible. At $N_L = 30$, the gap to the FPDQMC result (dotted orange line) has decreased to less than 7%, which means an improvement compared to our previous HFFER result (dashed green line) of about 166 Ry or 46%. Since the electron-electron interaction potentials are precalculated only up to $N_{\text{int}}^i = 7$, the small cutoff error is unavoidable, unless we restrict ourselves to $N_L = 7$. However, this yields a result 100 Ry off the current method's value as indicated by the black arrow.

III. ESSENTIALS OF THE FPDQMC METHOD

For the reader's convenience, we briefly recapitulate the essentials of the FPDQMC method. More detailed discussions of the DQMC method can be found, e.g., in Refs. [32,33].

The DQMC method is a projector method based on the simulation of the importance-sampled imaginary-time ($\tau = it$) Schrödinger equation,

$$\frac{\partial f(\mathbf{R}, \tau)}{\partial \tau} = \frac{1}{2} \Delta f(\mathbf{R}, \tau) - \frac{1}{2} \nabla \cdot [f(\mathbf{R}, \tau) \mathbf{F}_Q(\mathbf{R})] - [E_L(\mathbf{R}) - E_{\text{off}}] f(\mathbf{R}, \tau). \quad (13)$$

Here, $\mathbf{R} = (\mathbf{r}_1, \dots, \mathbf{r}_N)$ is a position vector in full configuration space, the sampled density,

$$f(\mathbf{R}, \tau) \equiv \Psi_G(\mathbf{R}) \Psi(\mathbf{R}, \tau) \quad (14)$$

is a product of an arbitrary function $\Psi(\mathbf{R}, \tau)$ and the guiding function $\Psi_G(\mathbf{R})$, whereas, $\mathbf{F}_Q(\mathbf{R}) = 2\nabla \Psi_G(\mathbf{R}) / \Psi_G(\mathbf{R})$ is the quantum force and $E_L(\mathbf{R}) = \hat{H} \Psi_G(\mathbf{R}) / \Psi_G(\mathbf{R})$ is the local energy. The energy offset E_{off} is introduced to increase the stability of the simulation and is continuously adapted to the current best estimate of the true ground-state energy. By expanding the function Ψ in the basis of eigenfunctions $\{\Psi_i\}$ of $\hat{H}$, i.e.,

$$\Psi(\mathbf{R}, \tau) = \sum_{i=0}^{\infty} c_i \Psi_i(\mathbf{R}) e^{-(E_i - E_{\text{off}})\tau}, \quad (15)$$

one sees that contributions of excited states are exponentially suppressed with increasing τ , and only low-lying state contributions remain after a sufficient number of steps in imaginary time. Equation (13) is rewritten in integral form

$$f(\mathbf{R}', \tau + \Delta\tau) = \int G(\mathbf{R}', \mathbf{R}, \Delta\tau) f(\mathbf{R}, \tau) d^3N \mathbf{R}, \quad (16)$$

and the Green's function is written in short-time approximation as $G = G_D G_B + O(\delta\tau^2)$, where

$$G_D(\mathbf{R}', \mathbf{R}; \delta\tau) = \frac{\exp\left[-\frac{(\mathbf{R}' - \mathbf{R} - \delta\tau \mathbf{F}_Q(\mathbf{R})/2)^2}{2\delta\tau}\right]}{(2\pi \delta\tau)^{3N/2}}, \quad (17)$$

and

$$G_B(\mathbf{R}', \mathbf{R}; \delta\tau) = \exp \left[- \left(\frac{E_L(\mathbf{R}) + E_L(\mathbf{R}')}{2} - E_{\text{off}} \right) \delta\tau \right]. \quad (18)$$

This integral equation can be simulated in configuration space with an ensemble of random walkers. Each walker moves according to $\mathbf{R}' = \mathbf{R} + \boldsymbol{\eta} + (\delta\tau/2)\mathbf{F}_Q(\mathbf{R})$, where $\boldsymbol{\eta}$ is a vector of Gaussian distributed random numbers (mean $\mu = 0$ and variance $\sigma^2 = \delta\tau$). After each step, $C = \text{trunc}[G_B(\mathbf{R}', \mathbf{R}; \delta\tau) + \chi]$ copies of each walker are created, where $\chi \in [0, 1]$ is a uniform random variate. In all following steps, these C copies move independently.

We note that the FPDQMC method strictly uses two different functions constructed from the Hartree-Fock results. First, the guiding function $\Psi_G(\mathbf{R})$ is used to determine the movement of the ensemble and the creation of walkers as outlined above. Second, the trial function $\Psi_T(\mathbf{R})$ is used to evaluate the energy estimate. As is usual in the FPDQMC method, we take the choice $\Psi_G(\mathbf{R}) = |\Psi_T(\mathbf{R})|$.

In the presence of a magnetic field, the time-reversal invariance of the Hamiltonian is broken, and the ground state may be complex. The fixed-phase variant of the DQMC method introduced in Ref. [34] is designed for the treatment of this situation. The initial function is split into its modulus and its phase via

$$\Psi(\mathbf{R}, \tau) = |\Psi(\mathbf{R}, \tau)| e^{i\phi(\mathbf{R}, \tau)}. \quad (19)$$

With the help of this Ansatz, the Schrödinger equation can be split into two coupled differential equations for the modulus and the phase,

$$\left(\sum_{j=1}^{N_e} -\frac{1}{2} \Delta_j + \frac{1}{2} (\nabla_j \phi + \mathbf{A}_j)^2 + V(\mathbf{r}_j) \right) |\Psi| = E |\Psi|, \quad (20a)$$

$$\sum_{j=1}^{N_e} \nabla_j \cdot [|\Psi|^2 (\nabla_j \phi + \mathbf{A}_j)] = 0. \quad (20b)$$

In the fixed-phase approximation, Eq. (20b) is assumed to be solved by the phase of the trial function Ψ_T , and Eq. (20a) is solved under this assumption.

In recent years, progress has been made in overcoming the fixed-phase approximation, see, e.g., Refs. [35,36]. However, these methods are computationally much more expensive.

A. Properties of the trial functions

The trial function,

$$\Psi_T(\mathbf{R}) = \mathcal{J} \Psi_\downarrow(\mathbf{R}) \Psi_\uparrow(\mathbf{R}) \quad (21)$$

is constructed from two Slater determinants—one for all spin-up electrons $\Psi_\uparrow$ and one for all spin-down electrons $\Psi_\downarrow$ —using the resulting single-particle orbitals of the 2DHFR calculations. This Ansatz does not change the expectation value of any observable [25] and is most simple to implement. In Eq. (21), we also add a Padé-Jastrow factor [25] $\mathcal{J} =$

$\exp(-u)$, with $u = u_{\text{Ne}} + u_{\text{ee}}$, where

$$u_{\text{Ne}} = \sum_{i=1}^N \frac{Z r_i}{1 + b_{\text{Ne}} r_i} \quad (22)$$

is the electron-nucleus part and

$$u_{\text{ee}} = \sum_{i=1}^N \sum_{j < i}^N \frac{a_{ij} r_{ij}}{1 + b_{\text{ee}} r_{ij}} \quad (23)$$

is the electron-electron part with $a_{ij} = -1/4$ for electrons with parallel spin and $a_{ij} = -1/2$ for electrons with antiparallel spin.

The two free parameters b_{Ne} and b_{ee} are optimized in a two-dimensional scheme using a variational quantum Monte Carlo algorithm with correlated sampling [25]. We optimize our guiding function such that the energy is minimal. We found this optimization scheme to be more stable than the usual optimization with respect to the variance. Our results are almost unaffected by small variations in the values of b_{Ne} and b_{ee} , therefore, this rather simple procedure is sufficient. For a detailed discussion of more advanced methods for the optimization of the Jastrow trial functions see, e.g., Refs. [37,38].

B. Control of the time-step error

The short-time approximation yields an error of order $O(\delta\tau^2)$ but with a prefactor that strongly depends on the employed guiding function. As we have to consider many different guiding functions for different elements and several magnetic-field strengths, it is not a trivial task to find step sizes $\delta\tau$ such that the time-step error is negligible on the one hand and, on the other hand, that $\delta\tau$ is as large as possible in order to minimize the correlation of our data.

To minimize the time-step error in all cases, we implemented the modifications to the quantum force proposed by Umrigar *et al.* [39]. In addition to that, we found $\langle |\ln(G_B)| \rangle \lesssim 10^{-3}$ per walker and step to be a good criterion for a suitable step size. This means each walker is copied or is deleted in each step with a probability of approximately 0.1%. We implemented a routine that performs very small FPDQMC test runs to determine a step size such that this condition is fulfilled. An example of the dependence of the time-step error on the value of $\langle |\ln(G_B)| \rangle$ is shown in Fig. 3. Smaller values of $\langle |\ln(G_B)| \rangle$ obviously correspond to smaller time steps.

IV. RESULTS AND DISCUSSION

A. Notation

Throughout the rest of this paper, we will use the high-field notation $(-m, \nu)$ with the magnetic quantum number m and the longitudinal excitation number ν to denote single-particle electronic configurations. Corresponding low-field quantum numbers can be found, e.g., in Ref. [7]. Since the FPDQMC method works in full configuration space, single-particle quantum numbers are replaced by the total wave function's

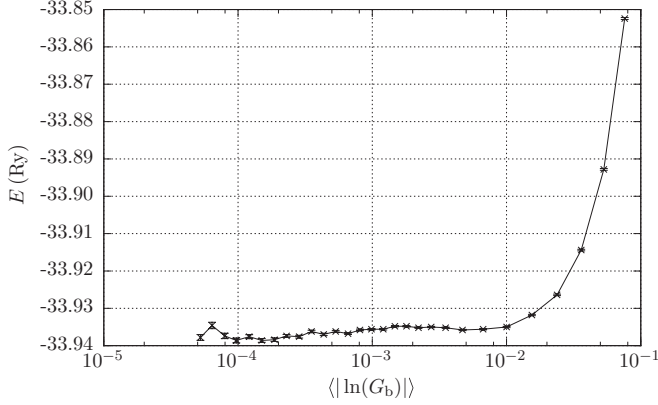


FIG. 3. Time-step error for the helium state ($m = 0, \nu = 0$) ($m = -1, \nu = 0$) at $B = 5 \times 10^7$ T as a function of $|\ln(G_b)|$.

quantum numbers,

$$M = \sum_i m_i \quad \Pi_z = \prod_i \pi_{z_i}, \quad S_z = \sum_i m_{s_i}, \quad (24)$$

namely, the total magnetic quantum number M , the total z parity Π_z , and the total spin projection S_z . The FPDQMC method is limited to the computation of the ground-state energy of a symmetry subspace $(-M, \Pi_z, -S_z)$ defined by the guiding wave function. Thus, a direct comparison of energies obtained with Hartree-Fock calculations to FPDQMC results is restricted to such states.

B. Helium

We begin this discussion introducing results for several helium states. In Tables I and II, we compare our previous results [29] (HFFER) with the ones found by our 2DHFR and FPDQMC methods as well as with one-dimensional Hartree-Fock results from Jones *et al.* [40], who used an anisotropic basis set, and with those from Thirumalai and Heyl [13], who solved 2D Hartree-Fock equations on a grid.

TABLE I. Binding energies of the (0,0)(1,0) state of helium—symmetry subspace $(1, +, 1)$ —in Rydberg units at different magnetic-field strengths calculated with our previous (HFFER) and current (2DHFR and FPDQMC) Ansätze, compared to the results of other groups.

β_z	HFFER	2DHFR	FPDQMC	Ref. [40]	Ref. [13]
0.1	5.049	5.544	5.6667(3)	5.6602	5.6756
0.2	6.173	6.549	6.6145(2)	6.6032	6.6340(1)
0.5	8.268	8.572	8.6101(1)	8.5960	8.6200(9)
0.7	9.273	9.564	9.5980(1)	9.5822	9.6116(6)
1	10.504	10.784	10.8171(1)	10.800	10.810(2)
2	13.455	13.722	13.7545(1)	13.733	13.754(3)
5	18.716	18.969	19.0091(1)	18.976	19.00(2)
7	21.109	21.357	21.4026(2)	21.3632	21.39(3)
10	23.956	24.197	24.2494(2)	24.2022	24.22(4)
20	30.307	30.736	30.8073(2)	30.7380	
50	41.438	41.777	41.8902(4)	41.7752	
70	46.310	46.620	46.7514(5)	46.6132	
100	51.985	52.265	52.4221(6)	52.2528	

TABLE II. Binding energies of the (0,0)(2,0) state of helium—symmetry subspace $(2, +, 1)$ —in Rydberg units at different magnetic-field strengths calculated with our previous (HFFER) and current (2DHFR and FPDQMC) Ansätze, compared to the results of other groups.

β_z	HFFER	2DHFR	FPDQMC	Ref. [40]	Ref. [13]
0.1	4.763	5.245	5.3783(4)	5.3742	5.404(6)
0.2	5.781	6.140	6.2091(3)	6.2010	6.239(3)
0.5	7.667	7.953	7.9908(1)	7.9780	8.00(3)
0.7	8.577	8.849	8.8839(1)	8.8684	8.90(4)
1	9.696	9.957	9.9910(1)	9.9732	9.99(4)
2	12.394	12.642	12.6765(1)	12.654	12.67(4)
5	17.234	17.469	17.5133(1)	17.477	17.50(5)
7	19.445	19.674	19.7241(2)	19.681	19.71(7)
10	22.079	22.302	22.3597(2)	22.3080	22.3(2)
20	27.951	28.406	28.4480(2)	28.3750	
50	38.330	38.683	38.7795(4)	38.6572	
70	42.882	43.202	43.3222(5)	43.1908	
100	48.191	48.478	48.6337(7)	48.4566	

Compared to our previous HFFER method, we achieve large improvements for the energy values, especially at small β_z . Even for very large values of β_z , there is still a small energy correction to the previous values since the (0,0) single-electron state has a nonvanishing probability density at the nucleus, and thus, the wave function always retains a small radial symmetric component. For $\beta_z < 1$, the results from Ref. [13] are better than our FPDQMC results. This might be due to the phase error of the 2DHFR guiding function, which cannot be overcome by the FPDQMC method. For $\beta_z > 1$, our Hartree-Fock results are in good agreement with both Refs. [13] and [40], and our FPDQMC results outmatch them both. We note that the 2DHFR program run time for helium and heliumlike ions is merely about 20 s per state on a single 2.4-GHz AMD Athlon X2 processor.

In a series of papers [14–16], Becken *et al.* [14] and Becken and Schmelcher [15,16] presented very accurate results of full CI calculations for helium for a wide range of magnetic-field strengths. We compare our results for three different helium states to the results from these papers in Tables III–V. In Table III, we investigate state (0,0)(0,1). As this

TABLE III. Binding energies of the real (0,0)(0,1) helium state—symmetry subspace $(0, -, 1)$ —in Rydberg units at different magnetic-field strengths calculated with our current methods and compared to results of Becken *et al.*

β	2DHFR	FPDQMC	Ref. [14]
0.25	4.747	4.959 86(30)	4.960 344
0.40	5.144	5.276 74(22)	5.276 444
0.50	5.360	5.467 64(20)	5.467 626
0.80	5.901	5.975 00(16)	5.974 370
1.00	6.208	6.270 64(14)	6.270 284
2.50	7.882	7.918 54(10)	7.918 470
5.00	9.668	9.697 16(8)	9.697 180
10.00	11.994	12.023 30(8)	12.022 976
25.00	16.093	16.118 60(10)	16.118 932
50.00	20.135	20.160 24(10)	20.159 946

TABLE IV. Same as in Table III but for the complex helium state (0,0)(1,1)—symmetry subspace (1, −, 1).

β	2DHFR	FPDQMC	Ref. [15]
0.25	4.596	4.814 70(28)	4.815 042
0.40	4.985	5.118 08(22)	5.118 01
0.50	5.197	5.301 70(20)	5.301 946
0.80	5.725	5.791 90(16)	5.792 384
1.00	6.025	6.080 66(16)	6.080 608
2.50	7.673	7.703 30(10)	7.703 766
5.00	9.451	9.474 66(10)	9.474 98
10.00	11.780	11.802 66(8)	11.804 22
25.00	15.895	15.915 70(10)	15.918 188
50.00	19.952	19.975 22(10)	19.978 752

state is real, Eq. (20b) is trivially fulfilled because $\nabla_j \phi = 0$ and $\nabla_j \Psi \cdot \mathbf{A}_j = 0$ due to the cylindrical symmetry of ψ . Therefore, no phase errors occur for this state. Indeed, our results are in excellent agreement with the values in Ref. [14] with a maximum deviation of 0.1%.

Unlike the (0,0)(0,1) state, the two configurations (0,0)(1,1) (Table IV) and (0,0)(3,0) (Table V) are complex, and therefore, our results are tainted with a phase error. Still, in Table IV, we come very close to the results of Becken *et al.* with a maximum error of $\sim 0.18\%$, which is only slightly larger than the error for the real state. The situation is slightly worse for the configuration (0,0)(3,0), especially for the highest magnetic-field strengths where our results deviate by 2% from those in Ref. [16].

If we take into account that we use a rather simple single-determinant Ansatz as a guiding function, the accuracy of our results is very satisfying. In addition, an error in the range of 0.1% is already on the same order of magnitude as the expected corrections due to the relativistic effects [41].

C. Ground states for $Z = 2-26$

Ground states are of great importance for many applications, e.g., the calculation of ionization energies or thermal occupation, and, in this paper, we, therefore, focus on the computation of their binding energies. We compare our results to the data of heavier atoms in the strong magnetic fields obtained by Mori and Hailey [12] and Ivanov and Schmelcher [11]. Due to a small error in the code of Ref. [26], their results

TABLE V. Same as in Table III but for the complex helium state (0,0)(3,0)—symmetry subspace (3, +, 1).

β	2DHFR	FPDQMC	Ref. [16]
0.25	4.695	4.915 70(28)	4.916 486
0.40	5.138	5.272 12(22)	5.272 564
0.50	5.381	5.487 62(20)	5.488 218
0.80	5.993	6.061 64(16)	6.063 034
1.00	6.342	6.399 86(14)	6.401 364
2.50	8.279	8.315 70(10)	8.321 110
5.00	10.401	10.433 20(10)	10.444 804
10.00	13.217	13.253 14(10)	13.273 922
25.00	18.259	18.303 40(14)	18.339 400
50.00	23.285	23.342 82(20)	23.394 850

TABLE VI. Ground-state electronic configuration given in the format $(-m, \nu)$ for those electrons that deviate from tightly bound positions. No index corresponds to the all-tightly bound high-field ground state.

i	Configuration
a	(0,1)
$\bar{a}$	(0,0,↑)(0,1)
b	(0,1)(1,1)
$\bar{b}$	(0,0,↑)(0,1)(1,1)
c	(0,1)(1,1)(2,1)
$\bar{c}$	(0,0,↑)(0,1)(1,1)(2,1)
d	(0,1)(1,1)(2,1)(3,1)
D	(0,1)(1,1)(2,1)(0,2)
E	(0,1)(1,1)(2,1)(3,1)(0,2)
F	(0,1)(1,1)(2,1)(3,1)(4,1)(0,2)
$\bar{E}$	(0,0,↑)(0,1)(1,1)(2,1)(3,1)(0,2)
$\bar{F}$	(0,0,↑)(0,1)(1,1)(2,1)(3,1)(4,1)(0,2)

are biased towards lower energies, and we, therefore, exclude them from the comparison.

We list values for the ground states of all atoms from helium to silicon at magnetic-field strength 10^7 T (Table VII) and for all atoms from helium to iron at magnetic-field strengths 5×10^7 T (Table VIII), 10^8 T (Table IX), and 5×10^8 T (Table X) also comparing to our results obtained with the HFFER method. Since those tables display an increasing nuclear charge Z at a fixed magnetic-field strength β , β_Z decreases quadratically from the top to the bottom of the tables, e.g., in Table VIII, β_Z decreases from roughly 27 at $Z = 2$ to about 0.16 at $Z = 26$. In Table VII, we reach the limit of our 2DHFR approach at $Z = 14$ with $\beta_Z \approx 0.11$.

Table VI contains the electronic configurations of all ground states corresponding to the superscripts in Tables VII–X. The quantum numbers listed only correspond to those electrons with $\nu \neq 0$, whereas, the other electrons occupy tightly bound orbitals ($\nu = 0$) with falling magnetic quantum numbers m ,

TABLE VII. Ground-state binding energies in Rydberg units at 10^7 T from helium to silicon calculated with our previous (HFFER) and current (2DHFR and FPDQMC) methods, compared to those of other groups. Superscripts denote electronic configuration (see Table VI).

Z	HFFER	2DHFR	FPDQMC	Ref. [11]	Ref. [12]
2	19.13	19.38	19.42776(14)	19.39	19.21
3	39.07	39.70	39.7824(3)	39.72	39.23
4	64.80	65.97	66.1171(4)	66.03	65.39
5	95.89	97.81	98.0428(6)	97.92	97.53
6	132.07	134.95	135.3104(8)	135.16	136.27
7	173.10	177.21	177.7634(12)	177.58	
8	220.01 ^a	225.94 ^a	226.856(2)	226.56 ^a	
9	272.52 ^a	280.51 ^a	281.796(3)	281.47 ^a	
10	329.86 ^a	340.38 ^a	342.159(4)	341.83 ^a	
11	394.20 ^a	418.13 ^a	422.164(14)		
12	477.41 ^b	508.23 ^b	513.86(2)		
13	566.55 ^b	605.37 ^b	612.96(4)		
14	661.31 ^c	709.66 ^c	719.94(6)		

TABLE VIII. Ground-state binding energies in Rydberg units at 5×10^7 T from helium to iron calculated with our previous (HFFER) and current (2DHFR and FPDQMC) methods, compared to those of other groups. Superscripts denote the electronic configuration (see Table VI).

Z	HFFER	2DHFR	FPDQMC	Ref. [11]	Ref. [12]
2	33.6	33.86	33.9368(3)	33.86	33.6
3	70.1	70.68	70.8405(6)	70.69	70.0
4	117.7	118.77	119.0077(7)	118.79	117.6
5	175.4	177.17	177.4887(8)	177.21	175.7
6	242.6	245.16	245.5660(10)	245.22	243.1
7	318.5	322.17	322.7021(13)	322.28	319.9
8	402.9	407.80	408.4447(13)	407.94	405.5
9	495.4	501.60	502.4218(17)	501.84	500.0
10	595.5	603.30	604.3479(18)	603.69	602.5
11	703.6 ^a	713.46 ^a	714.8493(22)		714.3
12	822.0 ^a	834.03a	835.682(4)		838.6 ^a
13	948.1 ^a	962.61 ^a	964.533(4)		973.9 ^a
14	1081.8 ^a	1099.0 ^a	1101.256(5)		1120.6 ^b
15	1225.1 ^b	1245.6 ^b	1248.356(6)		
16	1376.2 ^b	1400.1 ^b	1403.384(8)		
17	1534.6 ^b	1562.3 ^b	1566.104(8)		
18	1702.4 ^c	1734.5 ^c	1739.008(1)		
19	1877.5 ^c	1914.2 ^c	1919.484(12)		
20	2060.2 ^d	2102.1 ^d	2108.32(4)		
21	2251.3 ^d	2306.6 ^E	2313.72(6)		
22	2452.0 ^E	2549.0 ^E	2563.26(12)		
23	2689.8 ^E	2805.6 ^E	2822.02(14)		
24	2940.4 ^E	3071.9 ^E	3091.4(16)		
25	3200.0 ^F	3348.7 ^F	3370.9(4)		
26	3468.5 ^F	3636.6 ^F	3660.4(6)		

beginning at $m = 0$. Configurations including only quantum numbers $\nu = 1$ are denoted by lowercase letters, and such containing an electron with $\nu = 2$ are denoted by capital letters. All electrons have their spin aligned antiparallel to the magnetic field ($\downarrow$), except for a single electron at (0,0), which may have its spin aligned parallel. If this is the case, it is denoted by (0,0, $\uparrow$). Configurations including this spin-flipped state electron have overlined letters and were found to form the ground state at $B = 10^7$ T for elements with nuclear charge $Z \geq 11$ and at $B = 5 \times 10^7$ T for the heavier elements with nuclear charge $Z = 22$ –26. Thus, our energy values for these ground states, by far, excel any result published before.

Throughout Tables VII–X, one can notice a significant improvement on the results gained by the 2DHFR method presented in this paper compared to the data obtained with the HFFER method. For almost all calculations, the ground-state configuration was found to be the same for both methods. Our results are in good agreement with those of Ref. [11].

It is interesting to note that the relative improvement of the FPDQMC results compared to the 2DHFR values in the case of $B = 5 \times 10^8$ T decreases with rising nuclear charge numbers, although the systems grow more complicated due to the larger number of electrons (e.g., for iron, the FPDQMC method only improves the 2DHFR energy by 0.9‰ at this field strength). This effect also occurs at other field strengths

TABLE IX. Ground-state binding energies in Rydberg units at 10^8 T from helium to iron calculated with our previous (HFFER) and current (2DHFR and FPDQMC) methods, compared to those of other groups. Superscripts denote the electronic configuration (see Table VI).

Z	HFFER	2DHFR	FPDQMC	Ref. [11]	Ref. [12]
2	42.4	42.6	42.7488(6)	42.63	42.4
3	89.5	90.0	90.2140(10)	89.99	89.2
4	151.3	152.4	152.6872(12)	152.37	151.1
5	226.8	228.5	228.9330(12)	228.53	226.7
6	315.0	317.5	318.020(2)	317.51	315.2
7	415.0	418.5	419.147(2)	418.55	415.8
8	526.3	531.0	531.721(3)	531.02	527.4
9	648.3	654.3	655.200(4)	654.40	650.1
10	780.5	788.1	789.160(2)	788.24	783.8
11	922.7	931.9	933.204(3)		927.9
12	1074.4	1085.5	1086.978(4)		1083.7
13	1235.3	1248.5	1250.216(4)		1247.5 ^a
14	1409.6 ^a	1425.6 ^a	1427.764(6)		1426.5 ^a
15	1593.5 ^a	1612.2 ^a	1614.580(6)		1616.0 ^a
16	1786.8 ^a	1808.3 ^a	1811.032(6)		1816.7 ^b
17	1990.9 ^b	2015.9 ^b	2019.118(8)		2029.9 ^b
18	2205.8 ^b	2234.3 ^b	2237.902(8)		2261.3 ^b
19	2429.9 ^b	2462.1 ^b	2466.186(10)		2501.6 ^b
20	2664.1 ^c	2700.7 ^c	2705.37(3)		2756.2 ^c
21	2909.0 ^c	2950.0 ^c	2955.248(3)		
22	3162.7 ^c	3208.5 ^c	3214.16(4)		
23	3426.7 ^d	3477.8 ^d	3484.24(4)		
24	3700.4 ^d	3757.1 ^d	3764.24(6)		
25	3983.3 ^E	4054.4 ^E	4062.54(8)		
26	4277.7 ^E	4357.2 ^E	4366.14(10)		

but is masked by the growing error of the 2DHFR's Landau expansion that starts to dominate as β_Z falls below 1. However, the FPDQMC results are not affected as severely by this error in the wave function, and thus, the relative energy corrections of the FPDQMC method to the 2DHFR method rise again for $\beta_Z \leq 1$ as can be seen in Tables VII–IX.

We performed additional computations at $B = 5 \times 10^8$ T to gain a better understanding of this phenomenon. We compared the influence of the Jastrow factors and the overall correction in the FPDQMC method of the energy values for all heliumlike ions and several iron ions. The results of these computations show a strongly decreasing influence of the electron-electron Jastrow factor with increasing core charge, which can, at least partly, explain this phenomenon.

Compared to the perturbative method of Mori and Hailey [12], we obtain much higher binding energies for small nuclear charges $Z \leq 10$, but for heavier elements and when β_Z falls below 1, their results drop far below even our FPDQMC results with some ground-state configurations differing from the ones found by us. We expect that, in this regime, the method presented in Ref. [12] fails to achieve accurate results as the authors themselves state that its application is limited to $\beta_Z > 2$. We also note that their method is not fully variational and, therefore, need not necessarily produce an upper bound on the energy. Our method, however, is far from its limit $\beta_Z \geq 0.1$, and our results are expected to be very accurate.

TABLE X. Ground-state binding energies in Rydberg units at 5×10^8 T from helium to iron calculated with our previous (HFFER) and current (2DHFR and FPDQMC) methods, compared to those of other groups. Superscripts denote the electronic configuration (see Table VI).

Z	HFFER	2DHFR	FPDQMC	Ref. [11]	Ref. [12]
2	70.6	70.7	70.9782(16)	70.70	70.37
3	153.2	153.6	154.108(4)	153.56	152.73
4	264.6	265.5	266.134(4)	265.35	263.57
5	402.9	404.4	405.210(6)	404.21	402.48
6	566.5	568.7	569.748(6)	568.53	565.57
7	754.0	757.2	758.368(8)	756.98	751.96
8	964.4	968.6	969.962(10)	968.38	962.76
9	1196.4	1202.0	1203.510(8)	1201.70	1195.38
10	1449.4	1456.3	1458.144(8)	1456.06	1448.07
11	1722.3	1730.9	1732.922(10)		1720.31
12	2014.7	2025.1	2027.306(8)		2016.51
13	2325.8	2338.1	2340.490(8)		2328.07
14	2655.0	2669.4	2672.072(8)		2657.27
15	3001.8	3018.4	3021.418(10)		3007.2
16	3365.7	3384.8	3388.112(10)		3372.19
17	3746.3	3768.0	3771.580(14)		3753.36
18	4143.2	4167.7	4171.518(10)		4154.88
19	4555.9	4583.4	4587.51(3)		4570.22
20	4984.3	5014.9	5019.49(2)		5000.19
21	5434.2 ^a	5468.7 ^a	5473.92(4)		5452.42 ^a
22	5901.4 ^a	5939.6 ^a	5945.02(4)		5924.14 ^a
23	6384.3 ^a	6426.3 ^a	6432.08(6)		6413.71 ^a
24	6882.6 ^a	6928.6 ^a	6934.72(6)		6927.91 ^a
25	7401.0 ^b	7451.8 ^b	7458.64(4)		7441.74 ^a
26	7936.3 ^b	7991.7 ^b	7998.84(6)		7984.89 ^b

D. Transitions

Transition energies and oscillator strengths are key prerequisites in the analysis of spectra, the only observable quantity of distant stars. The dimensionless oscillator strength f of a transition from an initial state Ψ_i to a final state Ψ_f can be acquired using the well-known relation (see Ref. [7]),

$$f = \Delta E_{if} |p_{if}^q|^2, \quad (25)$$

with the energy difference $\Delta E_{if} = E_f - E_i$ given in Rydberg units and the total magnetic quantum number difference $q = \Delta M = M_f - M_i$ between the initial and the final states. Since $\Delta M = 0$ transitions are the strongest ones at high magnetic-field strengths, we restrict ourselves to the dipole matrix element p_{if}^0 of a photon with linear polarization,

$$p_{if}^0 = \sum_{a,b=1}^N \langle \psi_a^f | z | \psi_b^i \rangle C_{ab}^{if}. \quad (26)$$

Here, C_{ab}^{if} denotes the cofactor of the single-electron wave-function overlap matrix S_{ab}^{if} of the initial and final states,

$$S_{ab}^{if} = \langle \psi_a^f | \psi_b^i \rangle. \quad (27)$$

In order to separate the energy error and the errors of the wave functions in the transition integrals (26), we will also use the dipole strength $d_{if} = |p_{if}|^2$ instead of the oscillator strength f to characterize the transitions. Since the FPDQMC

TABLE XI. Transition energies in Rydberg energies and dipole strengths of $\Delta M = 0$ bound-bound transitions from state (0,0)(0,2) to state (0,0)(0,1) at different magnetic fields compared to the results of Becken and Schmelcher [17].

β	E		d	
	2DHFR	Ref. [17]	2DHFR	Ref. [17]
0.25	-0.033	-0.051 642	6.165	6.709 04
0.4	-0.110	-0.129 206	6.385	6.617 66
0.5	-0.147	-0.166 316	6.157	6.347 01
0.8	-0.222	-0.239 13	5.362	5.487 00
1	-0.255	-0.270 866	4.954	5.061 34
2.5	-0.370	-0.382 072	3.697	3.731 13
5	-0.432	-0.442 282	3.165	3.167 16
10	-0.464	-0.478 08	2.874	2.857 48
25	-0.475	-0.488 42	2.733	2.692 82
50	-0.462	-0.4738	2.725	2.678 38

method is restricted to the calculation of ground states, we can only obtain transitions with the 2DHFR method, but the small corrections of the FPDQMC method compared to the 2DHFR results for the energy values make us to expect that the results for oscillator strengths are very accurate as well.

In Tables XI and XII, we compare energies and dipole strengths obtained with the 2DHFR program and the full CI Ansatz of Becken and Schmelcher [17]. In their paper, they presented a large compendium of electromagnetic transition energies and dipole strengths for the helium atom. At the lowest-field strength, one can see quite large discrepancies between both methods. Here, we deliberately overstretched our Ansatz towards $\beta_Z \approx 0.06$. Gradually increasing the magnetic-field strength, our energy differences from Ref. [17] fall below 3% at $\beta = 5$ in Table XI. In Table XII, our energy error is below 1% at all field strengths with the exception of $\beta = 0.25$. However, the differences in the dipole strengths are somewhat larger, ranging from -4% to +2% in the first table and -2% to +5% in the second one, ignoring the value for $\beta = 0.25$ in both tables. Still, our dipole strengths are quite accurate, considering the constraints of our Ansatz in comparison to a full CI method.

TABLE XII. Same as in Table XI but for the transition from (0,0)(1,0) to (0,0)(1,1).

β	E		d	
	2DHFR	Ref. [17]	2DHFR	Ref. [17]
0.25	0.439	0.425 002	1.763	1.888 33
0.4	0.558	0.553 23	1.408	1.432 57
0.5	0.630	0.629 066	1.242	1.248 11
0.8	0.822	0.825 168	0.936	0.926 76
1	0.932	0.937 218	0.815	0.803 19
2.5	1.539	1.547 22	0.458	0.444 60
5	2.193	2.203 976	0.295	0.282 80
10	3.064	3.076 902	0.187	0.178 45
25	4.627	4.650 028	0.101	0.095 48
50	6.195	6.230 862	0.062	0.058 68

TABLE XIII. Transition energies in eV and oscillator strengths $\times 10^{-3}$ (in brackets) of $\Delta M = 0$ bound-bound transitions from electrons $(-m, v = 0)$ of the ground state of neutral carbon to $(-m, v = 1)$ at three different magnetic-field strengths β compared to results from Mori and Hailey [12].

m	$\beta = 200$			$\beta = 500$			$\beta = 1000$		
	HFFER	2DHFR	Ref. [12]	HFFER	2DHFR	Ref. [12]	HFFER	2DHFR	Ref. [12]
0	1024 (42.0)	1051 (45.4)	(41.0)	1370 (12.0)	1394 (12.5)	(13.0)	1696 (6.2)	1718 (6.3)	(5.81)
1	481 (68.4)	485 (70.4)	(59.8)	671 (27.1)	675 (27.4)	(22.5)	854 (15.5)	858 (15.7)	(12.8)
2	314 (99.9)	315 (101.2)	(79.7)	447 (45.7)	448 (46.0)	(39.2)	576 (27.7)	577 (27.8)	(24.7)
3	233 (135.8)	233 (136.6)	(114)	335 (67.9)	335 (68.1)	(61.1)	435 (42.4)	436 (42.5)	(37.7)
4	180 (173.2)	180 (173.7)	(156)	262 (93.0)	262 (93.1)	(86.3)	343 (59.9)	344 (59.9)	(57.2)
5	132 (205.5)	132 (205.8)	(197)	195 (119.9)	196 (120.0)	(116)	259 (80.5)	259 (80.5)	(78.3)

For heavier elements, the amount of accurate data in the literature is still small. Thus, in Table XIII, we compare our oscillator strengths with those from Mori and Hailey [12]. The new results are in good agreement with those obtained with our previous version of the Hartree-Fock-Roothaan method (HFFER): The largest differences in oscillator strength and energy (about 7% and 2.6%, respectively) can be found at the transition of the innermost electron $m = 0$ at the lowest magnetic-field strength $\beta = 200$. Here, the initial single-particle (0,0) state is significantly improved by our new 2D expansion, whereas, the final (0,1) state has a node at $z = 0$ and, thus, can be described adequately well by both expansions (2) and (3). When the error of both the initial and the final single-electron states is of the same order, even expansion (2) proves to be useful and predicts transition energies and oscillator strengths properly as can be seen by looking at the transitions of $m = 5$.

Comparing our oscillator strengths to the results of Ref. [12], one can see quite big differences for all transitions with a maximum difference of 27%. The authors of Ref. [12] mention lacking orthogonality of the initial and final states and only calculated the dipole matrix element for the electron that undergoes a transition. This may explain the large discrepancies. Since we evaluate formula (26) exactly and work with perfectly orthogonal states, our results should be the more accurate ones.

V. SUMMARY AND OUTLOOK

In this paper, we have presented an approach for the very accurate calculation of ground-state energy levels of atoms in strong and intermediate magnetic fields of $\beta_Z \geq 0.1$, combining 2D-Hartree-Fock-Roothaan and fixed-phase diffusion Monte Carlo methods. The results shown for helium states at different magnetic-field strengths and all element ground states from helium up to iron show the efficiency and accuracy of our approach. Including the spin-flipped (0,0, $\uparrow$)

single-electron state into possible ground-state configurations, we found new ground states for sodium to silicon at $B = 10^7$ T and titanium to iron at $B = 5 \times 10^7$ T.

The applied 2DHFR method was optimized to reduce the calculation effort originating from electron-electron interaction integrals, whereas, at the same time, the single-particle Landau expansion was boosted, thus, increasing the overall precision. We demonstrated that the induced additional errors stay very small, resulting in good convergence behavior of this method. In addition, it allows for the calculation of excited states and electronic wave functions, which were directly applied to obtain oscillator strengths for atomic bound-bound transitions and were used as guiding wave functions for even more precise FPDQMC calculations.

The comparison with results in the literature for elements $Z \leq 10$ shows that the accuracy of our Monte Carlo approach can very well compete with other precise methods, whereas, also allowing for the treatment of elements with $Z = 11$ –26. This makes the FPDQMC method, especially in the combination with our 2DHFR approach, a tool well suited for the study of symmetry subspace ground states of mid- Z elements in strong magnetic fields.

We note that the self-healing diffusion quantum Monte Carlo algorithms, proposed recently by Reboredo *et al.* [35] and Reboredo [36], and a method for the calculation of excited states from full configuration-interaction Monte Carlo method, presented by Booth and Chan [42], may be worthwhile avenues to pursue in future papers on atoms in strong magnetic fields.

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