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USING AN EVOLUTIONARY ALGORITHM BASED ON CELL DIVISION OPERATION TO CALCULATE GROUND-STATE ENERGIES OF DOUBLE-ELECTRON SYSTEMS IN MAGNETIC FIELDS*

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In this paper we adopt a new approach—the evolutionary algorithm based on cell division operation—to deal with ground-state energies of double-electron systems. This algorithm is based on the evolution of sets and can incorporate other search algorithms. Firstly, we make a search for several good subsets of solution space at the same time. Then, we make a fine search in the neighbourhood of some better points obtained in the first step to determine the final optimal results. In addition, the cell division enables the solution subspaces to become smaller and smaller, and thus increase the convergence speed. We have tested this approach on double-electron systems in magnetic fields, and the results obtained have shown that it can improve not only the efficiency but also the accuracy of the calculations compared with other methods.

Keywords: double-electron system, ground-state energy, subspace of solution space, evolutionary algorithm based on cell division operation

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I. INTRODUCTION

The evolutionary algorithm (EA)[1,2] is a newly developed method that has been successfully applied in many fields.[3−6] We once tried to use this kind of algorithm for studying atomic structures and obtained better results than with traditional algorithms.[7] But in the computing processes we found that, for traditional EAs, the basic element of evolution is a point in the whole solution space. Though the solution space of a practical problem is very large or even infinite, we want to search through only a finite number of objects. Also, genetic operators are random operations, which will result in many useless regions being examined frequently and cause much waste of calculating time, especially in the multi-parameter problems. In order to improve the traditional EAs, we propose a new approach—evolutionary algorithm based on cell division operation (EACDO)—in which the basic elements of evolution will be sets. That is, the individual is no longer a point but a set, called a cell. Evolutionary results are one or more regions which may contain the optimal solution. Then for different problems we can select different local search methods to gain the ultimate result. We have applied this algorithm to solve the problem of atomic ground-state energy. The results obtained have shown that it yields better results than the traditional EA.

This paper is organized as follows. Section II briefly describes the physical theory on atomic structure, and section III explains in detail the EACDO. The relevant experimental results are listed in section IV. Section V presents the conclusion.

II. THE PROBLEM UNDER STUDY

The ground-state energies of a double-electron system in a uniform magnetic field can often be converted to a complex nonlinear functional optimization problem, in which we will obtain the minimum of energies.

Ignoring relativity effects and taking $B \leq 10^5$T, we have the Hamiltonian of a double-electron system (adopting a geocentric coordinate system, and atomic units)

$$\hat{H} = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} + \frac{1}{2}\beta^2(\rho_1^2 + \rho_2^2) + \beta(M_L + 2M_s). \quad (1)$$

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In the ground state, $M_L = 0, M_s = 0$; $r_{12} = |\boldsymbol{r}_1 - \boldsymbol{r}_2|$ is the repulsion potential between electrons; and $\beta \equiv (2.12715 \times 10^{-10}\text{a.u./T})B(T)$; $\rho_1 = r_1 \sin\theta_1 = \sqrt{x_1^2 + y_1^2}$, $\rho_2 = r_2 \sin\theta_2 = \sqrt{x_2^2 + y_2^2}$.

In this problem we neglect the electronic spin-orbit interaction, the electronic spin-spin interaction, nuclear mass and volume effects, nuclear electromagnetic multi-dipole moments and other super-fine interactions. In the ground state, the parity $\hat{P}$ and the orbital angular Z momentum $\hat{L}_z$ are conserved quantities. Hence, according to formula (1), the corresponding stable-state Schrödinger equation is

$$\hat{H}\,\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2) = E\,\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2), \tag{2}$$

where E is the energy of the double-electron system, and $\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2)$ is the stable-state wavefunction of the system. It is very difficult to accurately solve Eq.(2). Because of the different symmetries of the Coulomb and the anti-magnetic terms, we could not separate the variables in Eq.(2). Also, we could not use the stationary perturbation theory to solve Eq.(2). But, by using the Ritz variation method,[8] we can convert the ground-state problem from solving Eq.(2) to solving an optimization problem of the function

$$\overline{H} = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle}. \tag{3}$$

Then, in Eq.(3), we adopt the variational principle

$$\delta \overline{H} = 0. \tag{4}$$

Finally, we obtain the approximate ground-state energy of a complex system. Thus we can apply the modified configuration interaction (MCI) method introduced by Goldman[9] to represent $\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2)$ by the linearly iterated addition of infinitely many infinite configuration wavefunctions

$$\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2) = \sum_{i=1}^{N} a_i \Phi_i(\boldsymbol{r}_1, \boldsymbol{r}_2), \tag{5}$$

where $\{\Phi_i\}$ is a complete orthonormal set, and each Φ_i is an electron-configuration wavefunction, corresponding to the Slater-type determinant. In order to improve the convergence rate and the accuracy of calculations, we let

$$\begin{aligned}\Phi_i(\boldsymbol{r}_>, \boldsymbol{r}_<) =& \mathrm{e}^{-\sigma_i r_< - \tau_i r_>} r_<^{s_i} r_>^{t_i} \\ & \times [\Lambda_{l_{1i} l_{2i}}^{L_i M_i}(\hat{r}_1, \hat{r}_2) \pm \Lambda_{l_{1i} l_{2i}}^{L_i M_i}(\hat{r}_2, \hat{r}_1),\end{aligned} \tag{6}$$

$$r_> = \max(r_1, r_2), r_< = \min(r_1, r_2). \tag{7}$$

Here σ_i and τ_i are variational parameters, and different s_i and t_i are used in different bases. The terms $\Lambda_{l_{1i} l_{2i}}^{L_i M_i}(\hat{r}_1, \hat{r}_2)$ are hyper-spherical harmonics. Equation (5) is a trial wavefunction of this problem, and $1/r_{12}$ (the Coulomb interaction between two electrons) can be expanded by spherical-harmonics functions of a single electron

$$\frac{1}{r_{12}} = \sum_{\lambda=0}^{\infty} \frac{4\pi}{2\lambda + 1} \frac{r_<^{\lambda}}{r_>^{\lambda+1}} \sum_{q=-\lambda}^{\lambda} Y_{\lambda q}^*(\hat{\boldsymbol{r}}_1) Y_{\lambda q}(\hat{\boldsymbol{r}}_2). \tag{8}$$

In the ground state, $l_1 = l_2 = 0$, $L = 0$ and $\dfrac{1}{r_{12}} = \dfrac{1}{r_>}$.

In addition, we should pay attention to the computation

$$\begin{aligned}&\frac{\partial r_>}{\partial r_2} = \xi(r_2 - r_1), \quad \frac{\partial r_<}{\partial r_2} = 1 - \xi(r_2 - r_1), \\ &\frac{\mathrm{d}\xi(x)}{\mathrm{d}x} = \delta(x), \quad \xi(x) = \begin{cases} 1, & x > 0 \\ 0, & x < 0 \end{cases}.\end{aligned} \tag{9}$$

In principle, $\{\Phi_i\}$ is complete and N in Eq.(5) should be infinite, but in practical calculations, N can only take finite values. Substituting Eq.(5) into Eq.(3), we can obtain the energy expectation value of this system, written as $E(\sigma, \tau)$,

$$\begin{aligned}\overline{H} =& \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \cdot \\ =& \frac{\sum\limits_{ij} a_i^* a_j \langle \Phi_i | \hat{H} | \Phi_j \rangle}{\sum\limits_{ij} a_i^* a_j} = E(\sigma, \tau).\end{aligned} \tag{10}$$

Then, applying the variational principle to function $E(\sigma, \tau)$ and regarding σ and τ in Eq.(10) as variational parameters, we have

$$\delta E(\sigma, \tau) = 0. \tag{11}$$

Finally, we can obtain the best variational parameters σ and τ, and then obtain the upper limit of the basic state energy, and the approximate value of the basic state wavefunction of the system.

Hence, the atom structure problem is at last converted to a problem of solving the minimal value of Eq.(10), denoted as

$$\min\{E(x), x_i > 0, \ \ x_i \in R, i = 1, 2, 3, \ldots N.\} \tag{12}$$

In this paper we will adopt EACDO to solve Eq.(12).

Ⅲ. EVOLUTIONARY ALGORITHM BASED ON THE CELL DIVISION OPERATION

A. Basic Concepts

We consider the optimization problem $\max\{f(x_1, x_2, \cdots, x_n)|x_i \in [a_i, b_i], i = 1, 2, \cdots, n\}$, where the solution space X is an n-dimensional cube. We now divide the ith interval $[a_i, b_i]$ into $2C_i$ parts, then the length of each part is $e_i = (b_i - a_i)/(2C_i)$, called the ith unit. Thus, the solution space is divided into $A = 2^n \prod_{i=1}^{n} C_i$ parts, and each part is also an n-dimensional cube which is called the cell and is denoted as B_j, j=1,2,$\cdots, A$. The set including all A cells is called the cell space, denoted by $X_A = \{B_j, j = 1, 2, \cdots, A\}$. In the EACDO, the population $P_A(t)$ consists of N cells from the cell space, where t is an evolutionary generation, N is the population size and the cells in $P_A(t)$ are individuals.

B. Cell Encoding

To any point $(x_1, x_2, \cdots, x_n)$ in a solution space X, there is a corresponding unique cell; hence a cell can be expressed by a point in X. This point is called the nucleus. Conversely, there is a unique nucleus corresponding to this cell, that is, a nucleus can also uniquely express a cell. In this algorithm, the encoding of an individual (i.e. a cell) is expressed by its nucleus $(x_1, x_2, \cdots, x_n)$.

C. Selection of Nuclei and Computation of Fitnesses

Firstly, nuclei in the population are randomly generated. Then, in subsequent operations, new nuclei will replace the old step-by-step. As to the replacement, first we let the old nuclei be initial points; next, we independently search for a better point in every single cell. Once a better point is found, we then let this point replace one of the old nuclei to become the new nucleus.

The fitness of an individual is the function value $f(x_1, x_2, \ldots, x_n)$ of its nucleus.

D. Cell Division Operation

In this algorithm, cells are not unchangeable, but are divided continually. This operation enables the search areas to become smaller and smaller. Thus, the convergence speed and solution precision will improve greatly. Its operation is simple in our design, in which every edge of a cell is just divided into two. Hence, after the cell division, there will be 2^n new small cells.

E. Genetic Operator

In EACDO we adopt three kinds of genetic operators: one is the affine genetic operator, another is the circumrotation genetic operator, and the third is the tangent mutation operator.

1. Affine operator. This operator implements the vaulted-linear combination method; however, its combination coefficient is not limited to the range (0,1). Hence, it is called the affine operator. The evolutionary algorithm using the affine operator breaks through the restriction of the traditional evolutionary algorithms in which reproduction, mutation and crossover are three different operations. It combines the three kinds of operation into one and replaces the worst individual in the present generation one-by-one. The affine genetic operator can be described as follows. If the parents are $Q_j(t) = (q_{1j}(t), q_{2j}(t), \cdots, q_{nj}(t))j = 1, 2, \cdots, m$, then the alleles of their offsprings are $q_i(t+1) = [\sum_{j=1}^{m} \alpha_j q_{ij}(t)]$ $i = 1, 2, \cdots, n$, where α_j is a random number in a fixed range and $\sum \alpha_j = 1$.

2. Circumrotation genetic operator. As suggested by the symmetry of the gene space, this operator implements a circumrotation transformation. This can be best described by the following algorithm. Letting the parent operator be $Q_j(t) = (q_{1j}(t), q_{2j}(t), \cdots, q_{nj}(t))$, two genes $q_{rj}(t)$ and $q_{sj}(t)$ are randomly selected from it, where r and s are random numbers and $r, s \leq n$. The alleles of its offspring, $q_{rj}(t+1), q_{sj}(t+1)$ will be changed into

$$\begin{aligned} q_{rj}(t+1) =& [\cos\theta q_{rj}(t) + \sin\theta q_{rj}(t)]q_{sj}(t+1) \\ =& [-\sin\theta q_{sj}(t) + \cos\theta q_{sj}(t)], \end{aligned}$$

where θ is a random number in the range $[0, 2\pi]$. Others are kept unchanged.

3. Tangent genetic operator. As suggested by the symmetry of the gene space, this operator also implements a circumrotation transformation and it can be described as follows. If the parent operator is $Q_j(t) = q_{1j}(t), q_{2j}(t), \cdots, q_{nj}(t))$, we randomly select h genes $q_{h_kj}(t)$ from it, where $h < n, k = (1, 2, \cdots, h)$, then each h_k is a random number and all these numbers are unequal. The alleles of their offspring are $q_{h_kj}(t+1) = q_{h_kj}(t) + [\tan\theta q_{h_kj}(t)]$, where θ is a random number in the range $(-\pi/2, \pi/2)$. Others are kept unchanged.

IV. RESULTS AND DISCUSSION

In this paper, basis vectors Φ_i are separated into three groups. The associated parameters are as follows. In the first set, $\sigma_1(=Z)$ and τ_1 are determined by a variation, s_1=0, t_1=0. In the second set, σ_2 and τ_2 are determined by a variation, s_2=0,1,2,3,0,1,2,3,0,1,2,0, t_2=0,0,0,0,1,1,1,1,2,2,2,3. In the third set, σ_3 and τ_3 are determined by a variation, s_3=2,3,3,4,4,5,5, t_3=–1,–2,–1,–3,–2,–4,–3.

The calculation has two steps: when we consider only the radial convergence and the absence of magnetic fields, using the EACDO, we first calculate τ_1, σ_2, τ_2, σ_3, τ_3 of the double-electron systems with ten kinds of different nuclear charge numbers, then we apply these parameters to determine twenty radial bases. For the angular part, since the system is in the ground state and the parity $\hat{P}$ is even, the total M_z=0 and total L=even reconsidering the triangular principle, taking $l_1 = 0, 1, 2, \ldots, 15, 0, 5, 10, 15$, $l_2 = 0, 1, 2, \ldots, 15, 2, 7, 12, 17$. $L = 0, 0, 0, \ldots, 0, 2, 2, 2, 2$ which includes twenty angular bases, so 20×20=400, which consists of 400 Slater basis sets. Finally, according to those 400 basic functions, we can obtain the ground-state energies of H^-, H_e, L_i^+, B_e^{2+}, B^{3+}, C^{4+} and N^{5+} in the magnetic field with $B \leq 10^5$T. Table 1 lists the final results, which satisfy the experimental expectation.

Table 1. Ground-state energies of H^- etc. Seven kinds of double-electron systems with $B \leq 10^5$T (β is the magnetic field parameter, as in Eq.(1), and the number in the table is the energy E (in atomic units)).

β	H^-	H_e	L_i^+	B_e^{2+}	B^{3+}	C^{4+}	N^{5+}
0	–0.52774	–2.90371	–7.2799	–13.65554	–22.03096	–32.38476	–44.78143
0.00213	–0.52771	–2.90371	–7.2799	–13.65554	–22.03096	–32.38476	–44.78143
0.004	–0.52762	–2.9037	–7.27989	–13.65553	–22.03095	–32.38476	–44.78143
0.0075	–0.52731	–2.90367	–7.27988	–13.65552	–22.03095	–32.38476	–44.78143
0.01064	–0.52687	–2.90362	–7.27986	–13.65551	–22.03094	–32.38475	–44.78143
0.015	–0.52604	–2.90354	–7.27983	–13.65547	–22.03093	–32.38474	–44.78142
0.02127	–0.52442	–2.90335	–7.27977	–13.65544	–22.03091	–32.38473	–44.78141
0.026	–0.52291	–2.90318	–7.2797	–13.65538	–22.03089	–32.38471	–44.7814
0.03191	–0.5207	–2.9029	–7.2796	–13.65534	–22.03086	–32.38469	–44.78138
0.036	–0.51898	–2.90268	–7.27952	–13.65553	–22.03083	–32.38467	–44.78137
0.04	–0.51717	–2.90244	–7.27942	–13.65529	–22.0308	–32.38466	–44.78136
0.045	–0.51472	–2.90211	–7.2793	–13.65523	–22.03076	–32.38463	–44.78134
0.05	–0.51208	–2.90173	–7.27916	–13.65515	–22.03071	–32.3846	–44.78132
0.058	–0.50749	–2.90104	–7.2789	–13.65502	–22.03064	–32.38454	–44.78128
0.064	–0.50377	–2.90947	–7.27868	–13.65491	–22.03057	–32.3845	–44.78124
0.08509	–0.48904	–2.89142	–7.27777	–13.65442	–22.03027	–32.3843	–44.7811
0.1	–0.47727	–2.89581	–7.27693	–13.65399	–22.03001	–32.38412	–44.78097
0.125	–0.45541	–2.89142	–7.27526	–13.65313	–22.02948	–32.38376	–44.78071
0.15	–0.43128	–2.88609	–7.27322	–13.65062	–22.02883	–32.38332	–44.7804
0.2	–0.37751	–2.87273	–7.26804	–13.64936	–22.02717	–32.38221	–44.77959

Strictly speaking, because optimal parameters are different in different magnetic fields, in order to test EACDO, another method is necessary. We regard superposition coefficients $\{a_i\}$ in Eq.(5) as the evolutionary parameters once again. In the case of 20 bases, the total number of undetermined parameters is 20×20=400. Directly optimizing Eq.(10), we can obtain energy values using only one calculation. Table 2 lists the results obtained by using this method. The results obtained by the two methods are the same. This shows that the EACDO is not only valid but also efficient, especially for multi-dimensional problems.

Table 2. Ground-state energies of H^- etc. Twenty kinds of double-electron systems in the absence of magnetic fields (in atomic units).

Atomic number Z	1	2	3	4	5
Ground-state energy	−0.527745	−2.903716	−7.279901	−13.655554	−22.030958
Atomic number Z	6	7	8	9	10
Ground-state energy	−32.406233	−44.781431	−59.156581	−75.531697	−93.906792
Atomic number Z	11	12	13	14	15
Ground-state energy	−114.281868	−136.656932	−161.031987	−187.407034	−215.782074
Atomic number Z	16	17	18	19	20
Ground-state energy	−246.157110	−278.532142	−312.907170	−349,282195	−387.657217

Table 3 shows the comparisons of calculating speed and calculating accuracy between EACDO and a traditional EA. They show that the EACDO greatly decreases the evolutionary generations and can obtain better solutions at the same time. Especially, when we deal with the optimization problem of more than twenty parameters, the difference between the two methods is more evident.

Table 3. The comparisons between EACDO and traditional evolutionary algorithm in the absence of magnetic fields (in atomic units).

Atomic number Z	EACDO		Traditional EA		Experimental
	Evolutionary generation	Energy (a.u.)	Evolutionary generation	Energy (a.u.)	Energy (a.u.)[12]
1	23	−0.52774599	1000	−0.52217689	−0.5278
2	16	−2.90371667	1000	−2.89756705	−2.9037
3	12	−7.27990125	1000	−7.23962061	−7.2799
4	5	−13.65555438	1000	−13.35365861	−13.6556
5	4	−22.03095883	748	−21.99661189	−22.0310
6	3	−32.40623356	702	−32.37371691	
7	5	−44.78143105	1000	−44.75082357	
8	5	−59.15658156	610	−59.12570399	

V. CONCLUSIONS

The computing results show that the EACDO is superior to the traditional EAs in the calculation of electron ground-state energies in a number of ways.

(1) EACDO is a two-level algorithm. In this paper, both levels of EACDO are evolutionary algorithms. The upper level EACDO is an evolutionary algorithm and the lower level EACDO is also an evolutionary algorithm. The upper algorithm avoids the premature convergence and the lower algorithm enhances the convergence speed. In particular, the cell division operation further enhances the convergence speed.

(2) EACDO is especially well suited for multi-dimensional problems (see Tables 1 and 2). In our calculations, the number of parameters of object functions is up to 400. It is impossible for traditional methods to deal with such huge numbers.

(3) EACDO has a rapid convergence speed compared with traditional EAs. Its evolutionary generation decreases by two orders of magnitude (see Table 3) because it avoids the repeated calculations of fitnesses and complex orders in selections.

(4) EACDO has a better parallelism. Although, in our work, the inherent parallelism of the EACDO did not have full play, its advantage is shown in solving the eigenvalue problem of multi-dimensional functions (such as 400 dimensions). As long as we choose a suitable evolutionary structure and operators for different physical problems, it will be easier and more efficient to solve multi-parameter problems in parallel.

(5) EACDO shows better results in common use. We can obtain the results for all kinds of nuclear charges and magnetic strengths without changing any parameter in the algorithm, and they can accurately satisfy the experimental results and the theoretical explanation (see Table 1). Unlike the simplex method,[11] EACDO does not depend on the selection of initial points and also does not have many restrictions on the objective function.

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