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Review of the recent applications of the stochastic variational method

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The recent applications of the stochastic variational method is reported. Besides the review of the earlier calculations for atomic, nuclear and subnuclear systems, recent developments on quantum dots, quantum wells and on atoms in strong magnetic field is presented.

1. Introduction

The stochastic variational method (SVM) optimizes the variational trial functions by randomly selecting their nonlinear parameters. This approach has a long history and has been used in different subfields of physics. In quantum chemistry the explicitly correlated gaussian basis functions has often been parametrized by "random tempering" [1] and the basis functions which most significantly contribute to the ground state energy are selected by "sorting" [1]. In nuclear physics the stochastic variational method has been invented to solve few-nucleon problems by successively increasing the variational basis adding randomly selected new states [2]. Condensed matter physicists often face the problem of diagonalization of extremely large matrices and the "stochastic diagonalization" [3] has proved to be a very useful tool. All of these methods are examples of stochastic optimization, a method that has earned its popularity by being able to avoid traps of local minima.

In this work the following variant of the stochastic variational method is used: First we set up a basis by successively increasing the number of states adding randomly selected new elements to the basis. To select a new element we randomly generate several states and compare the energy gain obtained by adding them to the basis. The state which lowers the energy most is added to the basis. This procedure is continued until energy "significantly" decreases. After the energy seems to converge and further increase of the dimension does not really improve the ground state energy, we start to "refine" the basis parameters. In the refining cycle the number of basis states is fixed and the basis states are reoptimized replacing the previous states by a new better random set. This procedure is cyclically repeated until there is no improvement in the energy. Further details can be found in Ref. [4].

We have used correlated Gaussian basis functions in our calculations. The correlated Gaussians offer computational advantages: fast analytical evaluation of the matrix ele-

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Table 1

Energy of Coulombic few-body systems (in atomic units). The mass of the proton is assumed to be infinite in PsH and it is taken as 1836.15 in H₂.

system	SVM	basis size	other method	Reference
HPs	-0.789196553	1200	-0.7891967147	[5]
H ₂	-1.164023731	100	-1.164025023	[6]
Ps ₂	-0.516003778	1200	-0.516001	[7]

ments and good approximation to various wave functions. They also have well-known drawbacks such as their slow convergence (compared to exponential functions) and the fact that they do not satisfy the cusp condition. The correlated gaussians can be written in two equivalent forms:

$$\exp\{-\frac{1}{2}\mathbf{x}^\dagger A\mathbf{x}\} = \exp\{-\frac{1}{2}\sum_{k<l}^N \alpha_{kl}(\mathbf{r}_k - \mathbf{r}_l)^2\}, \quad (1)$$

where

$$\mathbf{x}^\dagger A\mathbf{x} = \sum_{i,j=1}^{(N-1)} A_{ij}\mathbf{x}_i \cdot \mathbf{x}_j, \quad (2)$$

$\mathbf{r}_i$ are the positions of the particles, $\mathbf{x} = \mathbf{x}_1, \dots, \mathbf{x}_{N-1}$ is a set of relative coordinates. The parameters α_{ij} can be expressed by A_{ij} and vice versa. The advantage of latter notation (left side of eq. (1)) is that it explicitly connects the nonlinear parameters α_{ij} to the pair correlation between particle i and j .

2. Atomic physics

To test the method we have calculated many well-known quantum mechanical systems, especially Coulombic systems (small atom and molecules) and compared the results to those of other methods. Our results are in very good agreement with those of other methods for Coulombic few-body systems. Some examples are shown in Table 1.

We have investigated the stability and structure of systems comprising a negative ion and positrons [8] by the stochastic variational method. It is shown that the H⁻ and the Li⁻ ions can bind not only one but two positrons. The binding energies of these double positronic atoms $E(\text{H}^-, e^+, e^+) = 0.57\text{eV}$ and $E(\text{Li}^-, e^+, e^+) = 0.15\text{eV}$ are somewhat smaller than those of their single positronic counterparts ($E(\text{HPs}) = 1.06\text{eV}$ and $E(\text{LiPs}) = 0.32\text{eV}$). We have also found that a system of Ps⁻, Ps⁻ and a proton is bound. (See Table 2.)

J. Mitroy and his collaborators have extensively used the SVM and its "fixed core" variant [9–11] to study the binding of positrons and positroniums to atoms. They have proved, for the first time, that a positron can cling itself to a neutral Lithium [9]. Later they have shown that many atoms (Na, Cu, Ag, Be, Mg, Zn) is capable to bind a positron. These electronically stable states do decay by the process of electron-positron annihilation. It is also shown that besides the H atom the Lithium, Sodium and Potassium atoms also form bound state with a positronium (HPs, LiPs, NaPs and KPs).

Table 2
Binding energies of exotic molecules (in a. u.)

system	Basis size	E_{total}	$E_{binding}$
(p,Ps ₂)	400	-0.810152	0.02096
(Li ⁺ ,Ps ₂)	800	-7.80510	0.00918
(p ⁺ ,2e ⁺ ,4e ⁻)	800	-1.05542	0.00423

Table 3

Energy (in MeV) of the alpha particle with the AV6 part of the AV14 [14] interaction calculated by different methods. VMC: [12], GFMC [13].

	SVM	VMC	GFMC
$\langle T \rangle$	101.89	101.19(0.28)	100.61(0.21)
$-\langle V \rangle$	127.42	125.32(0.27)	126.14(0.20)
$-\langle H \rangle$	25.52	24.14(0.02)	25.53(0.01)

3. Nuclear physics

Our primary goal is to use the SVM to calculate the energies and other properties of light nuclei by using realistic interactions. This is an obviously challenging application due to the noncentral forces and strong repulsive core of the nuclear interaction. We have calculated the energies of the triton and the alpha particle by different realistic interactions [16]. The energies obtained were in good agreement with other methods. In particular we agreed with the results of the Green Function Monte Carlo (GFMC) calculations [15] within the statistical error ($\pm 0.2\text{MeV}$) of the GFMC. The GFMC calculations have been greatly improved in the last few years and the statistical error for the alpha particle is about 0.01MeV . We have repeated our calculation for the alpha particle improving our approach in two respects. We have used the full "A" matrix, combined with a global vector representation for the orbital part. In the previous calculation the matrix of the nonlinear parameters were chosen to be diagonal, and a (truncated) partial wave expansion was used. In these calculations not only the nonlinear parameters but the spin-isospin components and the orbital quantum numbers are also randomly chosen. Our results are improved by about 150 keV (see Table 3. and 4.). There is a nice agreement between SVM and the Faddeev-Yakubovskii calculation for the expectation values of the different components of the interactions (the GFMC is only exact for the energies, the expectation values are based on an approximation). Other methods [18] give similar results.

Calculations for $A=6$ nuclei are under way. The convergence of the energy requires considerable larger basis for these systems. At present the energy of the ${}^6\text{Li}$ is below the alpha particle threshold but it is not bound with respect to the alpha-deuteron level. The ${}^6\text{He}$ is likely to be unbound without three-body interaction.

4. Atoms in strong magnetic fields

The theoretical interest in the studies of atomic and molecular systems in magnetic field is motivated by a number of experimental observations. One of these is the discovery of

Table 4

Energy (in MeV) of the alpha particle with the AV8' part of the AV18 interaction calculated by different methods. VMC: [12], GFMC [13], FY:[17]

	VMC	GFMC	FY	SVM
$\langle K \rangle$	92.9	97.12	99.23	99.21
$\langle V_4 \rangle$	-41.41	-42.55	-42.55	-42.55
$\langle T \rangle$	-73.78	-78.61	-79.45	-79.40
$\langle LS \rangle$	-2.92	-2.76	-2.96	-2.95
E	-25.06	-25.70	-25.71	-25.67

the strong magnetic field on (magnetic) white dwarfs [19] ($\approx 10^7$ G) and on the surface of neutron stars [20] ($\approx 10^{12}$ G). (The strongest available laboratory magnetic field strength is about 10^6 G.) On the other hand there are a lot's of experiments on excitons, excitonic complexes and quantum dots in semiconductors. The small effective masses and large dielectric constant results in very large effective field strength in these systems.

Beyond the perturbation regime, the Coulomb interaction is rivaled by the external magnetic field and the calculation of the binding energies of multielectron-systems becomes very complicated. In these systems the spherical symmetry of the Coulomb interaction is strongly broken by the magnetic field. This intricate geometry of the highly anisotropic charge distribution is very challenging for conventional theoretical approaches and only the hydrogen and helium atom has been solved with accuracy required by the spectroscopical needs. Precise calculation of the spectra of light elements in magnetic field would greatly help the interpretation of the optical absorption spectra and therefore the understanding of the composition of the atmosphere of stars.

The conventional form of the CG's are spherically symmetric, so for example for a two-particle system they are assumed in the simple $\exp\{-\alpha_1 r_1^2 - \alpha_2 r_2^2 - \beta \mathbf{r}_1 \mathbf{r}_2\}$ form. In the case of a strong magnetic field the particles are in the field of an isotropic harmonic oscillator in the x-y plane. The spherical CG basis does not provide sufficient flexibility to describe this situation because its parameters in the x-y and z direction are equal. The simplest extension of the CG's to tackle this problem is to choose different nonlinear parameters in the x-y plane and in the z direction: $\exp\{-\alpha_1(x_1^2 + y_1^2) - \alpha_{1z}z_1^2 - \alpha_2(x_2^2 + y_2^2) - \alpha_{2z}z_2^2 - \beta(x_1x_2 + y_1y_2) - \beta_x z_1 z_2\}$. By choosing equal parameters in the x-y plane and z-direction the deformed CG (DCG) basis trivially reduces to the spherical one, but in the case of magnetic field it has the required flexibility to be able to describe of the harmonic oscillator wave function in the x-y plane and motion governed by the Coulomb interaction in the z direction. At the same time, the basis allows for the correlation between the electrons. The Hamiltonian:

$$H = \sum_{i=1}^N \frac{1}{2m_i} (\mathbf{p}_i + \frac{e_i}{c} \mathbf{A}_i)^2 + \sum_{i<j} \frac{e_i e_j}{\epsilon r_{ij}} \quad (3)$$

where $\mathbf{A}_i = \frac{1}{2} \mathbf{r}_i \times \mathbf{B}$ and the magnetic field is $\mathbf{B} = (0, 0, B)$, m_i, e_i are the masses and charges.

Table 5
Energies of singlet states of helium with M=0.

β			
0.0	-2.90372437	-2.90372437	[21]
0.1	-2.89583445	-2.89583	[22]
0.2	-2.87287076	-2.87287	[22]
0.3	-2.83646731	-2.83646	[22]
0.4	-2.78842446	-2.78842	[22]
0.5	-2.73000000	-2.73038	[22]

Table 6
Energies of singlet states of helium with M=-2.

β			
0.0	-2.05561573	-2.05562	[23]
0.1	-2.07937321	-2.07949	[22]
0.2	-2.03241599	-2.03308	[22]
0.3	-1.96555463	-1.96735	[22]
0.4	-1.88652446	-1.89021	[22]
0.5	-1.79908755	-1.80500	[22]

We choose a deformed form of the correlated Gaussians (DCG):

$$\exp\left\{-\frac{1}{2} \sum_{i,j=1}^N A_{ij} \rho_i \cdot \rho_j - \frac{1}{2} \sum_{i,j=1}^N B_{ij} z_i \cdot z_j\right\} \quad (4)$$

where the nonlinear parameters are different (and independent) in the "xy" and "z" directions ($\rho_i = (x_i, y_i)$). This extension brings a great deal of flexibility by allowing a separate description on the "xy" plane and along the "z" axis. The Hamiltonian does not commute with L^2 but it has common eigenfunctions with L_z . The above form of the DCG belongs to $M = 0$. To allow for $M \neq 0$ states we multiply the basis by

$$\prod_{i=1}^N \xi_{m_i}(\rho_i) \quad \text{where} \quad \xi_m(\rho) = (x + iy)^m. \quad (5)$$

where Thus our variational trial function reads as

$$\Phi_M(\mathbf{r}) = \mathcal{A}\left\{\left(\prod_{i=1}^N \xi_{m_i}(\rho_i)\right) - \frac{1}{2} \sum_{i,j=1}^N A_{ij} \rho_i \cdot \rho_j - \frac{1}{2} \sum_{i,j=1}^N B_{ij} z_i \cdot z_j\right\}, \quad (6)$$

where $M = m_1 + m_2 + \dots + m_N$, and m_i are integers.

Our results for the M=0 and M=-2 singlet state of the Helium atom are presented in Table 5. and Table 6. The previous results are considerable improved, especially for M=-2. Further calculations for other atoms are under way.

5. Charged excitons in semiconductor quantum wells

Negatively (X^-) and positively (X^+) charged excitons in quantum wells have been the subject of intense studies in the last years, both experimentally and theoretically. These studies revealed that, due to the confinement, the 2 dimensional charged excitons have binding energies which are an order of magnitude larger than the charged excitons in the corresponding bulk materials. Due to the increased binding energy these systems can be studied in room temperature and this also opens the way for various technological applications (e.g. lasers, etc.)

The Hamiltonian of a negatively charged exciton in a quantum well is, in the effective mass approximation, given by

$$\widehat{H} = T_{1e} + T_{2e} + T_h + V_C + V_{1e} + V_{2e} + V_h, \quad (7)$$

where $1e$, $2e$ indicate the electrons and h the hole; V_{ie} , V_h are the quantum well confinement potentials; T_i is the kinetic energy operator for particle i . The confining interaction is modelled by a square well potential:

$$V(z) = 0 \text{ if } |z| < a \text{ and } V(z) = V_0 \text{ otherwise.} \quad (8)$$

Due to this confinement in the z -direction the spherical symmetry is broken and we have to use the trial functions introduced in the previous section. While the Coulomb three-body problem is relatively easily solvable with excellent accuracy in the spherically symmetric case this cylindrical geometry poses considerable difficulties in obtaining accurate results. Our results are compared to the experimental values [26] in Figure 1. This figure shows the dependence of the experimental and theoretical binding energies of the negatively charged exciton on the well widths in a GaAs/AlGaAs quantum well. The theoretical results for the binding energy are represented by a shaded region which gives the accuracy of our calculation for the binding energy. Note that the accuracy obtained for the total energy is better than 1%, however, its error propagates and increases because of the subtractions which have to be made in order to obtain the binding energy, which is one order of magnitude lower than the total energy.

The results are reported in detail in [28]. The investigation of the effect of magnetic field on confined excitonic complexes is under way.

6. Quantum dots

We investigate a system of N_e electrons confined by the potential $V_{\text{con}}(\mathbf{r})$. The Hamiltonian is

$$H = \sum_{i=1}^{N_e} \left(-\frac{\hbar^2}{2m^*} \nabla_i^2 + V_{\text{con}}(\mathbf{r}_i) \right) + \frac{e^2}{\epsilon} \sum_{i < j}^{N_e} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}, \quad (9)$$

where m^* is the electron effective mass, and ϵ is the dielectric constant of the semiconductor. We have studied several $N=2-6$ electron "artificial atoms" with different (harmonic oscillator, spherical square-well and cylindrical square-well) confining interaction in two- and three-dimension. As an example, we compare our results to that of Ref. [29] in Table 7. The agreement with the practically exact results of the Diffusion Monte Carlo calculations is excellent.

Figure 1. The dependence of the experimental and theoretical binding energies of the negatively charged exciton on the well widths in a GaAs/AlGaAs quantum well. The shaded region is our theoretical prediction, the squares are theoretical values from [27]. The open circles are the experimental values [26].

Table 7

Comparison of the energies of 2 dimensional N=5 and N=6 electron systems by different methods ($\omega = 0.28$).

N	HF	LSDA	VMC	DMC	SVM
5	5.8700	5.5735	5.5473	5.5336	5.5325
6	8.0359	7.6349	7.6214	7.5996	7.6020

7. Summary

The SVM is a very simple and powerful approach to solve few-body problems in physics. Flurry of examples in atomic, nuclear and solid state systems shows its effectiveness and usefulness. One of the major limitation of the method is that by increasing the number of particles, the evaluation of the matrix elements gets longer and longer on the computer. That prevents us from trying the necessary number of random candidates and lowers the chance of finding the most appropriate parameters.

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