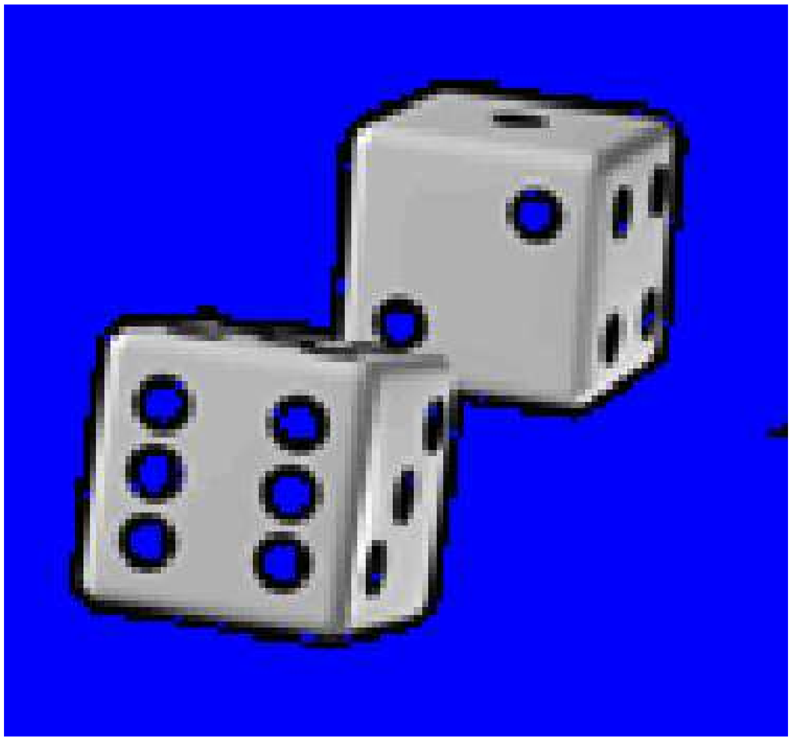
THE STOCHASTIC VARIATIONAL METHOD



Recent Applications

Outline of the talk

- The stochastic variational method
- The trial functions
- Applications:
  - Atomic physics: Coulombic few-body problems
  - Subnuclear physics: Constituent quark models of baryons
  - Solid state physics: Quantum dots, Excitonic Complexes
  - Nuclear physics: Structure of light nuclei

Motivations I.

The solution of the N-particle Schrödinger-equation is complicated.

$$H\Psi = E\Psi \tag{1}$$

The Hamiltonian

$$H = \sum_{i=1}^{N} T_i + \sum_{i=1}^{N} U_i + \sum_{i<j} V_{ij} + \dots. \tag{2}$$

Variational solution (one of the simplest approach):

$$\Psi(\mathbf{r}_1, \dots, \mathbf{r}_N) = \sum_{i=1}^{K} c_i \Phi(\mathbf{a}_i; \mathbf{r}_1, \dots, \mathbf{r}_N) \tag{3}$$

red $\mathbf{a}_i$ set of variational parameters: The variational upper bound crucially depends on these parameters. These nonlinear parameters have to be optimized.

Motivations II.

Problem: if one takes a product form

$$\Phi(\mathbf{a};\mathbf{r}_1,\ldots,\mathbf{r}_N)=\phi(a_1,\mathbf{r}_1)\phi(a_2,\mathbf{r}_2)\ldots\phi(a_N,\mathbf{r}_N) \quad (4)$$

with an expansion for the individual motions

$$\phi(a_i,\mathbf{r}_i)=\sum_{k=1}^{K} b_{ik}\varphi(a_{ik},\mathbf{r}_i) \quad (5)$$

one ends up with a K^N dimensional basis. K is typically 5-10, and that limits to N=3,4 particle problems: 10^4 basis states.

The variational upper bound to the exact energy is given by solving the

$$\sum_{i=1}^{K}(H_{ij}-E_K A_{ij})c_i=0 \qquad (j=1,...,K) \quad (6)$$

generalized eigenvalue problem, where matrix elements:

$$O_{ij}=\langle\Phi(\mathbf{a}_i;\mathbf{r}_1,\ldots,\mathbf{r}_N)|O|\Phi(\mathbf{a}_j;\mathbf{r}_1,\ldots,\mathbf{r}_N)\rangle. \quad (7)$$

Motivations III.

The problems with this direct approach:

(1) leads prohibitively large dimensions (all m.e. are nonzero)

(2) the optimization is computationally expensive: full diagonalization+recalculation of all of the matrix elements

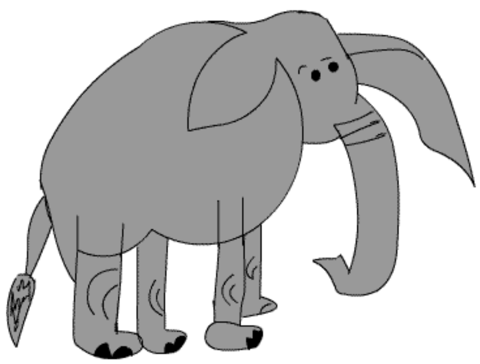
Question: Are all the trial functions equally important? Can we omit some of the trial functions?

The stochastic variational method

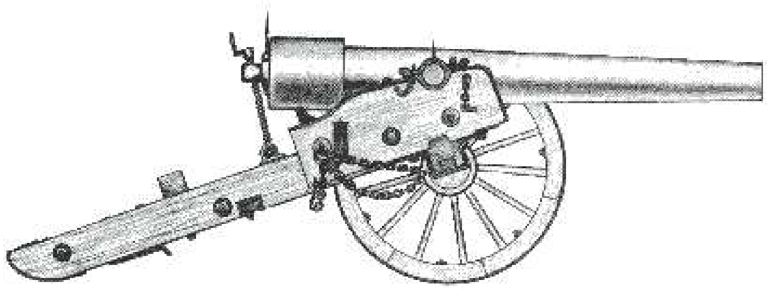
Assume that you got a new job: You are the coach of the national soccer team of Kuwait. You do not know the players in Kuwait, so what can you do? Try to choose players randomly to set up a team. Let them play a game against some other team and select the best players. Replace the rest of the players with other randomly chosen ones. Play a new game.
This is exactly the same problem as the one we face in physics in many cases. This trial and error strategy may sound very simple minded and inefficient but what else can be done if we have no information on the possible candidate/trial functions?

The stochastic variational method

This simple example already nicely illustrates the basic advantage and disadvantage of the method:
(1) Advantage: The more trial you make the better result you get. You can refine your selection until the best choice is reached (provided that the available trial functions are good enough to represent the full Hilbert space).
(2) Disadvantage: This strategy might not work if you are the coach of China. If there are too many players and you are not able to make sufficient number of tests, you will not find adequate solution.



History



- Nuclear physics: Kukulin, Stochastic variational method, 1976
- Quantum chemistry: Random tempering, sorting, 1970's
- Solid state physics: H. De Raedt, Stochastic diagonalization, 1990's, Hubbard model, CI

The trial functions

The suitable trial functions meet the following requirements:

1. They can be easily generalized for an N-body system.
2. Their matrix elements are analytically available.
3. They are easily adaptable to the permutational symmetry of the system.
4. They are flexible enough to approximate even rapidly changing functions.

Correlated Gaussians

$$G_A(\mathbf{x}) = \exp\Big(-\frac{1}{2}\tilde{\mathbf{x}}A\mathbf{x}\Big) \equiv \exp\Big(-\frac{1}{2}\sum_{i=1}^{N-1}\sum_{j=1}^{N-1} A_{ij}\mathbf{x}_i \cdot \mathbf{x}_j\Big) \tag{8}$$

$$= \exp\Big\{-\frac{1}{2}\sum_{j>i=1}^{N} \alpha_{ij}(\mathbf{r}_i - \mathbf{r}_j)^2\Big\}. \tag{9}$$

The matrix elements A_{ij} or, equivalently, α_{ij} are nonlinear parameters of the basis.

Matrix elements

The matrix elements are very simple and the formula is general for N-particles.

$$\langle G_{A'}|G_A\rangle = \left(\frac{(2\pi)^{N-1}}{\det(A+A')}\right)^{\frac{3}{2}}. \tag{10}$$

$$\langle F_{A'}|\sum_{i=1}^{N}\frac{\mathbf{p}_i^2}{2m_i}-T_{\rm cm}|F_A\rangle = \frac{3}{2}\hbar^2{\rm Tr}\Big(A(A+A')^{-1}A'\Lambda\Big)\langle F_{A'}|F_A\rangle. \tag{11}$$

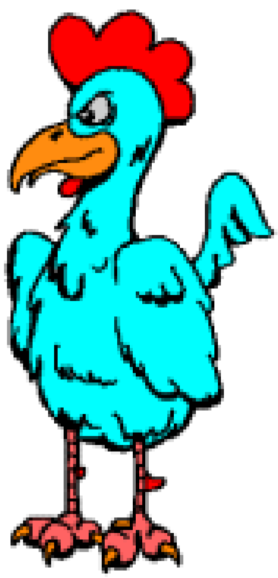
$$\langle F_{A'}|V(\mathbf{r}_i-\mathbf{r}_j)|F_A\rangle = \langle F_{A'}|F_A\rangle\left(\frac{c_{ij}}{2\pi}\right)^{\frac{3}{2}}\int V(\mathbf{r}){\rm e}^{-\frac{1}{2}c_{ij}r^2}d\mathbf{r}, \tag{12}$$

where

$$\frac{1}{c_{ij}} = \widetilde{w^{(ij)}}(A+A')^{-1}w^{(ij)} \tag{13}$$

Properties

1. Symmerization is simple:
$$\mathcal{P}G_A(\mathbf{x}) = G_{PAP}(\mathbf{x}) \tag{14}$$
($\mathcal{P}$ is a permutation operator.
2. The matrix elements for noncentral (spin-orbit, tensor, etc.) forces, for three-body forces are easily available.
3. Nonlocal potentials can be also handled.
4. Works in momentum space as well.



Random basis vs. optimization

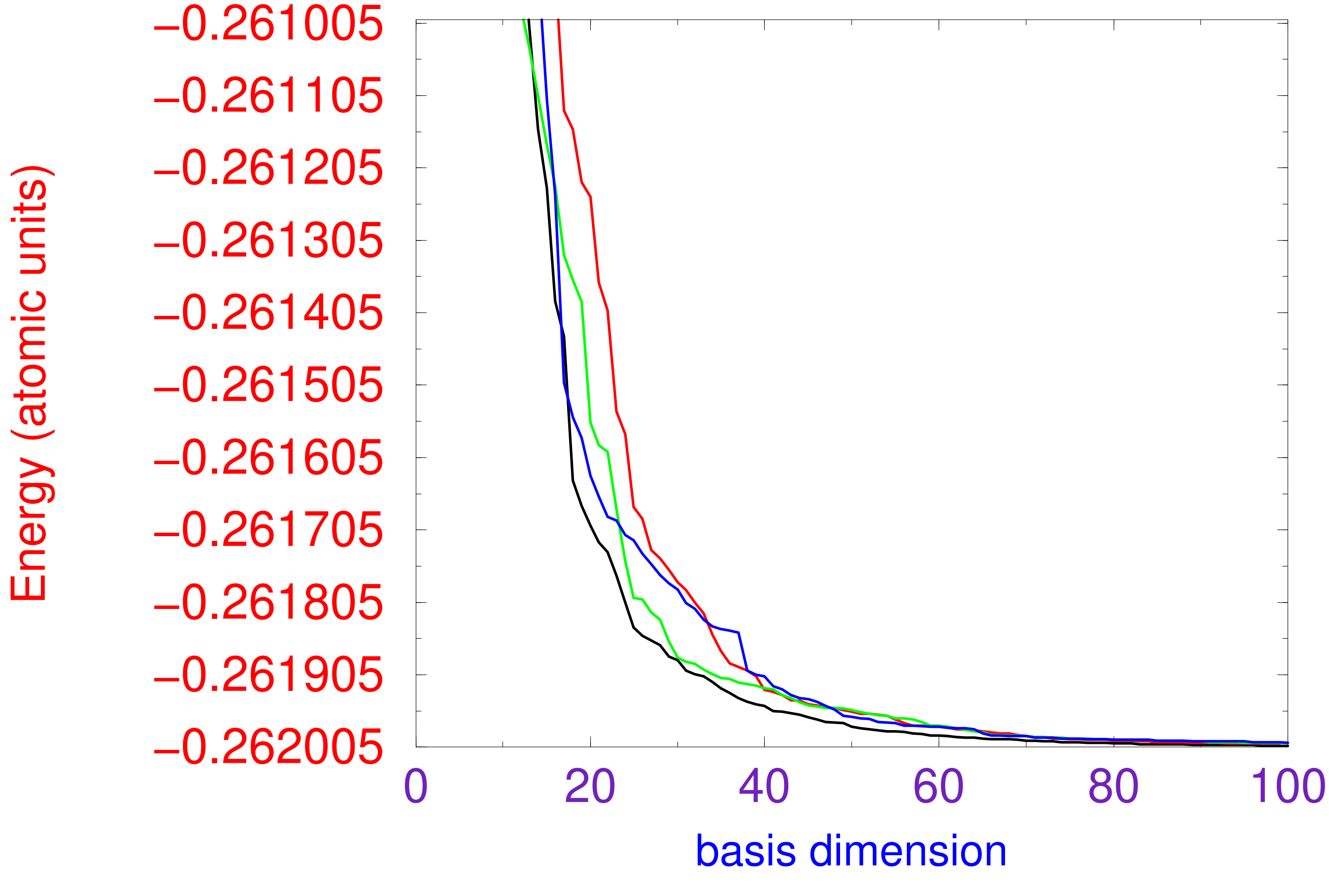
	$K = 100$	$K = 400$	Best 100
E1	-0.2617619	-0.2620032	-0.2619995
E2	-0.2617281	-0.2620026	-0.2619978
E3	-0.2617918	-0.2620016	-0.2619956
$N_{\rm eval}$	5050	80200	80200

Method	Powell	SVM($n = 10$)	Refining ($n = 10$)
E1	-0.26200016	-0.26199427	-0.26200231
E2	-0.26199947	-0.26199382	-0.26200351
E3	-0.26200164	-0.26199733	-0.26200312
$N_{\rm eval}$	35466150	86150	805050
time	7200	43	195

Basis dimension: 100. Exact energy: -0.262005

SVM: Convergence of the energy

Calculation of the energy of the Ps^-=(e^-,e^-,e^+) ion starting from different random parameters (RGB curves). The black curve obtained by increasing the number of trials.

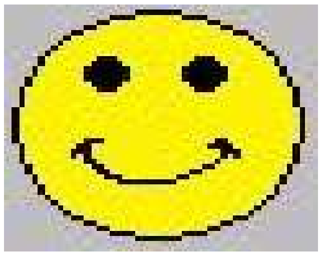


Test of SVM

Comparison to other methods

	SVM (K=200)	SVM (K=600)	Hylleraas
E	-0.2620050648	-0.262005070226	$-0.262005070232 8$
$\langle r_{+-} \rangle$	5.48962	5.489633252	5.489633252
$\langle r_{--} \rangle$	8.54856	8.548580655	8.548580655
$\langle r_{+-} \rangle^{\frac{1}{2}}$	6.95832	6.95837	6.95837
$\langle r_{+-} \rangle^{\frac{1}{2}}$	9.65284	9.65291	9.65291
η	0.34×10^{-6}	0.54×10^{-10}	0.23×10^{-10}

$\eta = |1 + \langle V \rangle / (2\langle T \rangle)|$; Hylleraas-type calculation: Y. K. Ho, PRA48, 4780 (1993).



Test of SVM

Method	Ps_2 $(L=0)$	Ps_2 $(L=1)$
SVM $(K=100)$	-0.516000069	-0.334376975
SVM $(K=200)$	-0.516003119	-0.334405047
SVM $(K=400)$	-0.516003666	-0.334407561
SVM $(K=800)$	-0.516003778	-0.334408177
SVM $(K=1200)$	-0.5160037869	-0.334408234
SVM $(K=1600)$	-0.516003789058	-0.3344082658
CG	-0.5160024	
QMC	-0.51601 ± 0.00001	
$\langle\delta(r_{12})\rangle$	0.0221151	0.0112091
$\langle\delta(r_{13})\rangle$	0.0006259	0.00014591
$\lvert 1+\langle V\rangle/(2\langle T\rangle)\rvert$	0.3×10^{-9}	0.36×10^{-6}

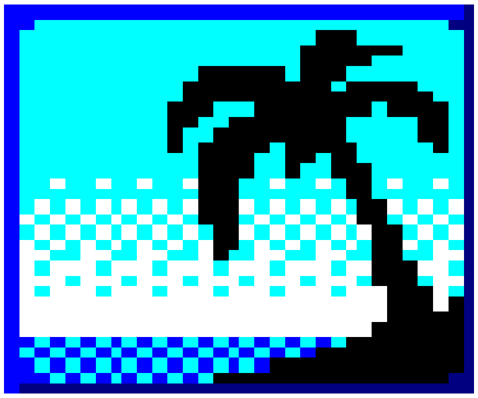
CG: by Frolov PRA55, 2662 (1997), QMC: D. Bressanini, PRA55, 200 (1997).

Excited states

Energy of the ground state and the first four ^1S excited states of the Helium atom (in a.u.).

State	SVM	"Exact"
E_1	-2.9037243769	-2.90372437698
E_2	-2.1459740452	-2.14597404605
E_3	-2.0612719880	-2.06127198974
E_4	-2.0335866779	-2.03358671702
E_5	-2.0211768312	-2.02117685157

Exotic atoms



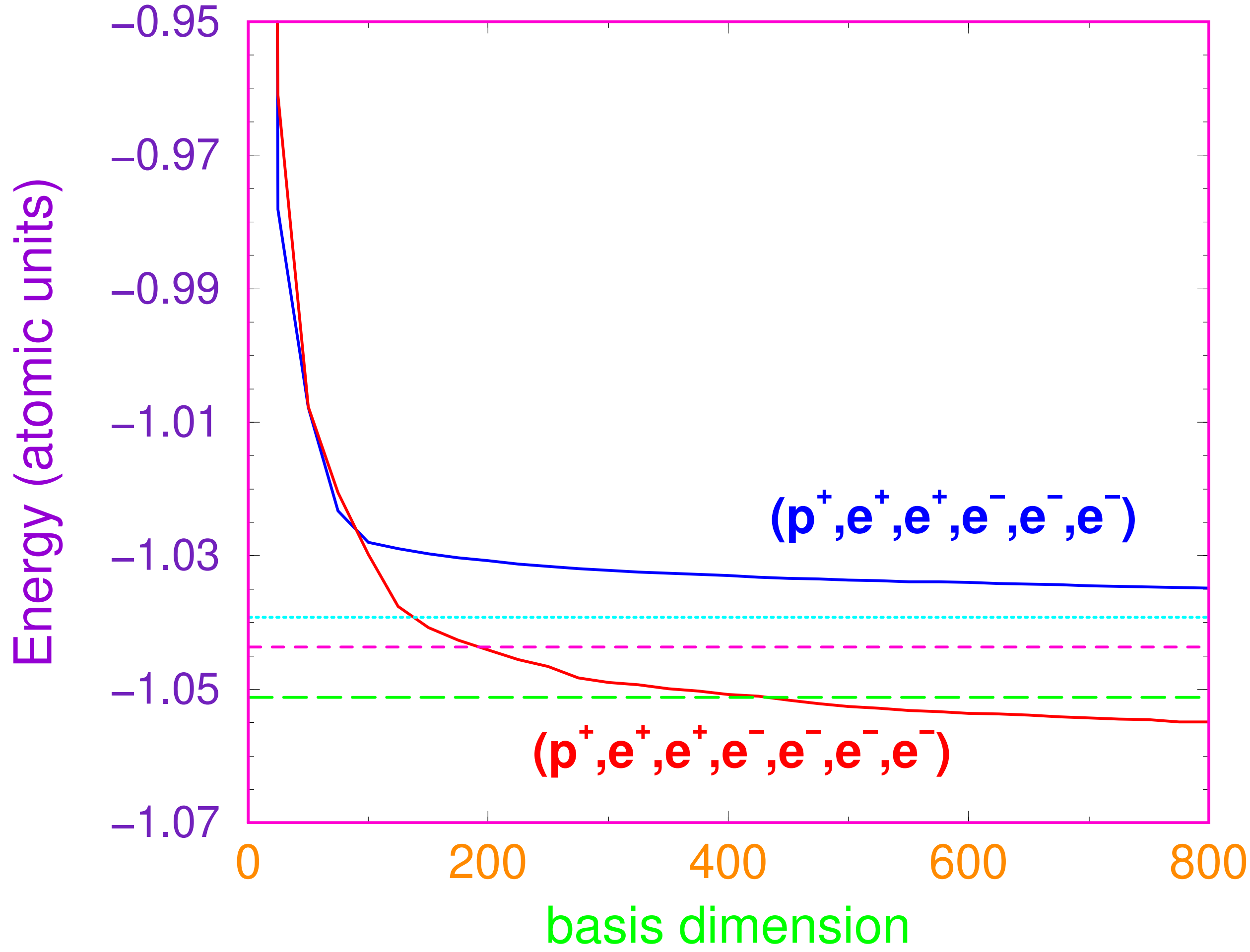
- The system of a neutral atom and a positron (e. g. Li+e^+) is predicted to be unbound by several methods: The calculation requires extreme accuracy.
- The **SVM** has proved, for the first time, that the Lie^+ is bound (Ryzikh & Mitroy).
- Many systems predicted to be stable by the **SVM**:
  - Microscopical calculation: Bee^+, Hee^+
  - Fixed Core SVM (Ryzikh & Mitroy): Nae^+,NaPs, Cue^+, KPs, etc.

Exotic systems

- The (e^+,e^+,e^-) and (e^+,e^+,e^-,e^-) system is bound but the five or more particle electron-positron systems are not.
- The neutral (e^+,e^+,e^-,e^-) forms bound states with positive charges, the (e^+,e^+,e^-,e^-,x^+) is bound for any m_x provided that x^+ and e^+ are distinguishable.

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

Stability of exotic systems



The (p^+,e^+,e^+,e^-,e^-,e^-,e^-) system is bound but the (p^+,e^+,e^+,e^-,e^-,e^-) system is not. The dotted (cyan) line is the HPs+Ps, the dashed (magenta) line is the H^-+Ps_2, the long dashed (green) line is the HPs+Ps^- threshold.

Quantum dots

N	(L,S,π)	E (SVM)	E (SM)	E (SM-eff)
3	$(1,1/2,-)$	4.013240	4.01324	4.01344
3	$(1,3/2,-)$	4.794580	4.79458	4.79460
4	$(1,1,+)$	6.349245	6.3491	6.3506
4	$(0,0,+)$	6.446165	6.4458	6.4479
5	$(0,3/2,-)$	8.996317		9.0032
5	$(2,1/2,-)$	9.056655		9.0587
5	$(1,1/2,-)$	9.095370		9.0988

Energies of few-electron quantum dots (harmonic confinement, $\omega = 0.5$) calculated by SVM and by the large scale shell-model approach (by P. Navratil) using the Coulomb potential (SM) and the two-body effective interaction derived from the Coulomb potential(SM-eff).

Nuclear systems

The trial function is given as a combination of the correlated Gaussians:

$$\psi_{(LS)JMTM_T}(\mathbf{x}, A) = \mathcal{A}\{\exp\left(-\frac{1}{2}\tilde{\mathbf{x}}A\mathbf{x}\right)[\theta_L(\mathbf{x})\chi_S]_{JM}\,\eta_{TM_T}\}, \tag{15}$$

where

$\mathbf{x} = \{\mathbf{x}_1, ..., \mathbf{x}_{N-1}\}$

is a set of relative (Jacobi) coordinates,

the operator red $\mathcal{A}$ is an antisymmetrizer, χ_{SM_S} is the spin function, and η_{TM_T} is the isospin function.

The matrix A is an $(N-1) \times (N-1)$ symmetric, positive-definite matrix of nonlinear variational parameters.

Nuclear systems

The spin and isospin functions are successively coupled, for example

$\chi_{SM_S} = \chi_{(S_{12}S_{123}\ldots)SM_S} = [[[\chi_{1/2}\chi_{1/2}]_{S_{12}}\chi_{1/2}]_{S_{123}}\ldots]_{SM_S}$

Question: How to represent the orbital part $\theta_{LM_L}(\mathbf{x})$?

(1) Partial wave expansion:

$$\vartheta_L(x) = \left[\left[[Y_{l_1m_1}(\hat{x}_1)Y_{l_2m_2}(\hat{x}_2)]_{l_{12}}\, Y_{l_3m_3}(\hat{x}_3)\right]_{l_{123}} \ldots\right]_{LM}$$

Partial waves in a four-body system

	l_1	l_2	l_3	l_{12}	L		l_1	l_2	l_3	l_{12}	L
1	0	0	0	0	0	21	0	2	2	2	1
2	1	1	0	0	0	22	0	2	2	2	2
3	1	1	0	1	1	23	2	1	1	1	0
4	1	1	0	2	2	24	2	1	1	1	1
5	1	0	1	1	0	25	2	1	1	1	2
6	1	0	1	1	1	26	2	1	1	2	1
7	1	0	1	1	2	27	2	1	1	2	2
8	0	1	1	1	0	28	2	1	1	3	2
9	0	1	1	1	1	29	1	2	1	1	0
10	0	1	1	1	2	30	1	2	1	1	1
11	2	0	0	2	2	31	1	2	1	1	2
12	0	2	0	2	2	32	1	2	1	2	1
13	0	0	2	0	2	33	1	2	1	2	2
14	2	2	0	0	0	34	1	2	1	3	2
15	2	2	0	1	1	35	1	1	2	0	2
16	2	2	0	2	2	36	1	1	2	1	1
17	2	0	2	2	0	37	1	1	2	1	2
18	2	0	2	2	1	38	1	1	2	2	0
19	2	0	2	2	2	39	1	1	2	2	1
20	0	2	2	2	0	40	1	1	2	2	2

Nuclear systems

(2) Global vector representation:

$$\vartheta_L(x) = [[Y_{l_1 m_1}(\hat{v}_1) Y_{l_2 m_2}(\hat{v}_2)]_{LM}$$

where

$$v_1 = \sum_{i=1}^{N} u_{1i} r_i \qquad v_2 = \sum_{i=1}^{N} u_{2i} r_i$$

Hints

(1)

$$|r_1 + r_2|^L Y_{LM}(\hat{r}_1 + r_2) = \sum C_L^{l_1 l_2} {r_1}^{l_1} {r_2}^{l_2} \left[Y_{l_1}(\hat{r}_1) Y_{l_2}(\hat{r}_2)\right]_{LM}$$

(2)

$$x_1 = r_2 - r_1 \quad x_2 = r_3 - \frac{r_1 + r_2}{2} \quad x_3 = r_4 - \frac{r_1 + r_2 + r_3}{3}$$

Nuclear systems

Results for A=3 and A=4

^{3}H				^{4}He			
K	AV6	AV8	RV8	K	AV6	AV8	RV8
25	-6.63	-7.36	-6.53	100	-24.37	-25.15	-23.35
50	-7.04	-7.69	-7.41	200	-25.05	-25.50	-24.15
75	-7.11	-7.74	-7.54	300	-25.28	-25.60	-24.35
100	-7.15	-7.79	-7.59	400	-25.40	-25.62	-24.49

A=3

	SVM	GFMC	Faddeev	VMC	CHH
AV8					
$\langle T\rangle$	46.3				
$\langle V_6\rangle$	-52.9				
$\langle V_{LS}\rangle$	-1.2				
$\langle r^2\rangle^{\frac{1}{2}}$	1.75				
P_S	91.1				
P_P	< 0.1				
P_D	8.9				
E	-7.79		-7.79		-7.79
RV8					
$\langle T\rangle$	52.2	54.0(0.20)	52.2		
$\langle V\rangle$	-59.8	$-62.0(0.20)$	-59.8		
$\langle r^2\rangle^{\frac{1}{2}}$	1.75	1.68(0.07)	1.76		
P_S	90.3				
P_P	< 0.1				
P_D	9.7				
E	-7.59	$-7.54(0.10)$	-7.59	$-7.44(0.03)$	-7.60

A=4

	SVM	GFMC	FY	VMC	CHH
AV8					
$\langle T \rangle$	98.8				
$\langle V \rangle$	-124.4	$-124.20(1.0)$			
$\langle V_6 \rangle$	-121.5				
$\langle V_{LS} \rangle$	-2.9				
$\langle r^2 \rangle^{\frac{1}{2}}$	1.50	1.51(0.01)			
P_S	85.5				
P_P	0.3				
P_D	14.2				
E	-25.62	$-25.75(0.05)$	-25.31		-25.60
RV8					
$\langle T \rangle$	111.7	109.2(0.20)			
$\langle V_6 \rangle$	-139.1	$-137.5(0.20)$			
$\langle V_{LS} \rangle$	2.1	2.45(0.23)			
$\langle V_{coul} \rangle$	0.75	0.71(0.02)			
$\langle r^2 \rangle^{\frac{1}{2}}$	1.51	1.53(0.02)			
P_S	84.1				
P_P	0.4				
P_D	15.5	15.5(0.20)			
E	-24.49	$-24.55(0.13)$	-23.79	-24.01	-23.9

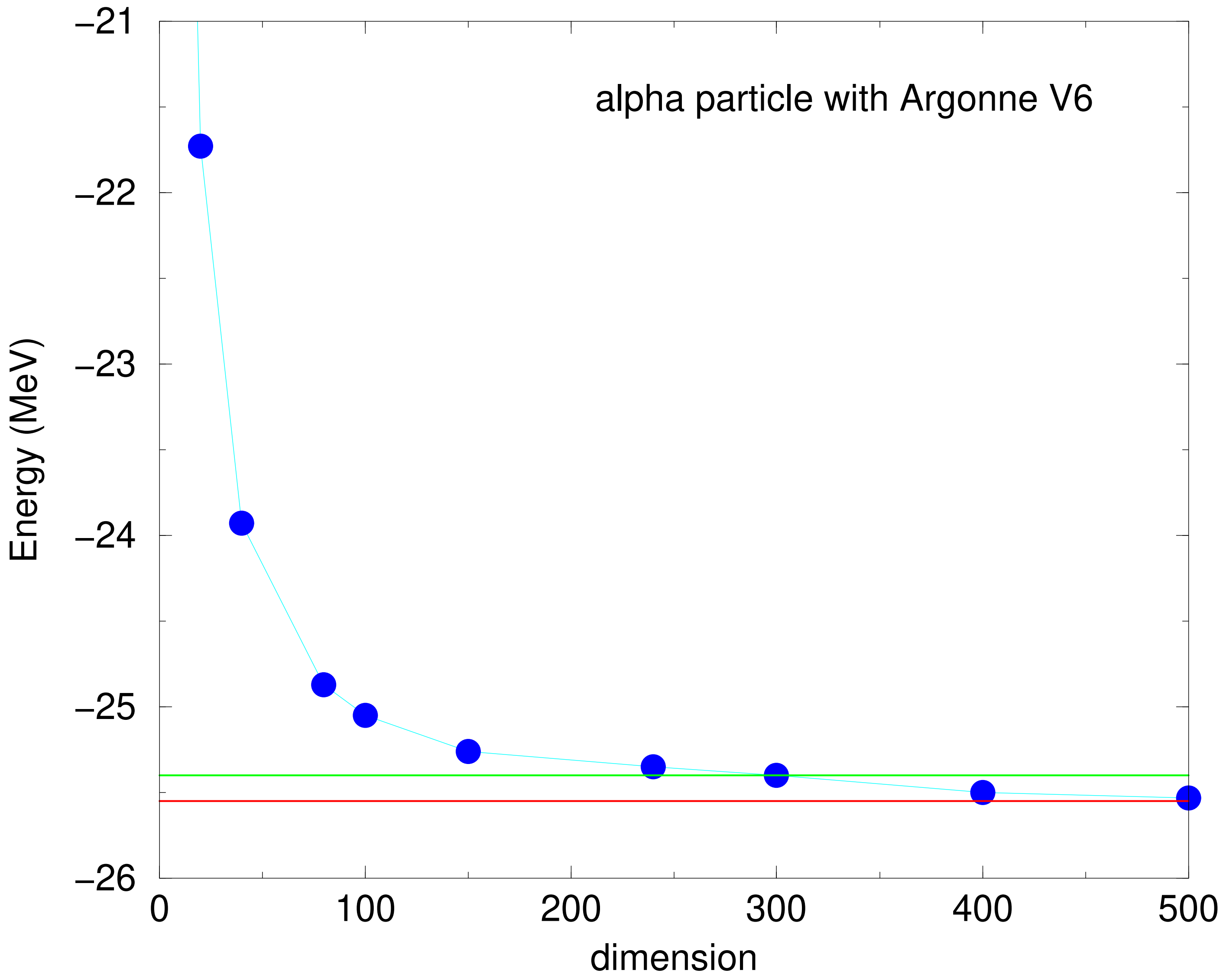
A=4

A few years ago there was a considerable difference between the results by different methods (about 300-500 KeV). We have repeated the calculations recently to try to get more accurate results.

AV6

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

A=4



Convergence of the energy of the alpha particle. Red line: GFMC, green line: our previous SVM.

A=4

AV8' of AV14

	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 results are in a very good agreement. The GFMC exact for the energies (with a very small statistical error $\sim$ 0.01 MeV) but not for the expectation values. The **SVM** and FY gave very similar expectation values.

A=6

Motivation

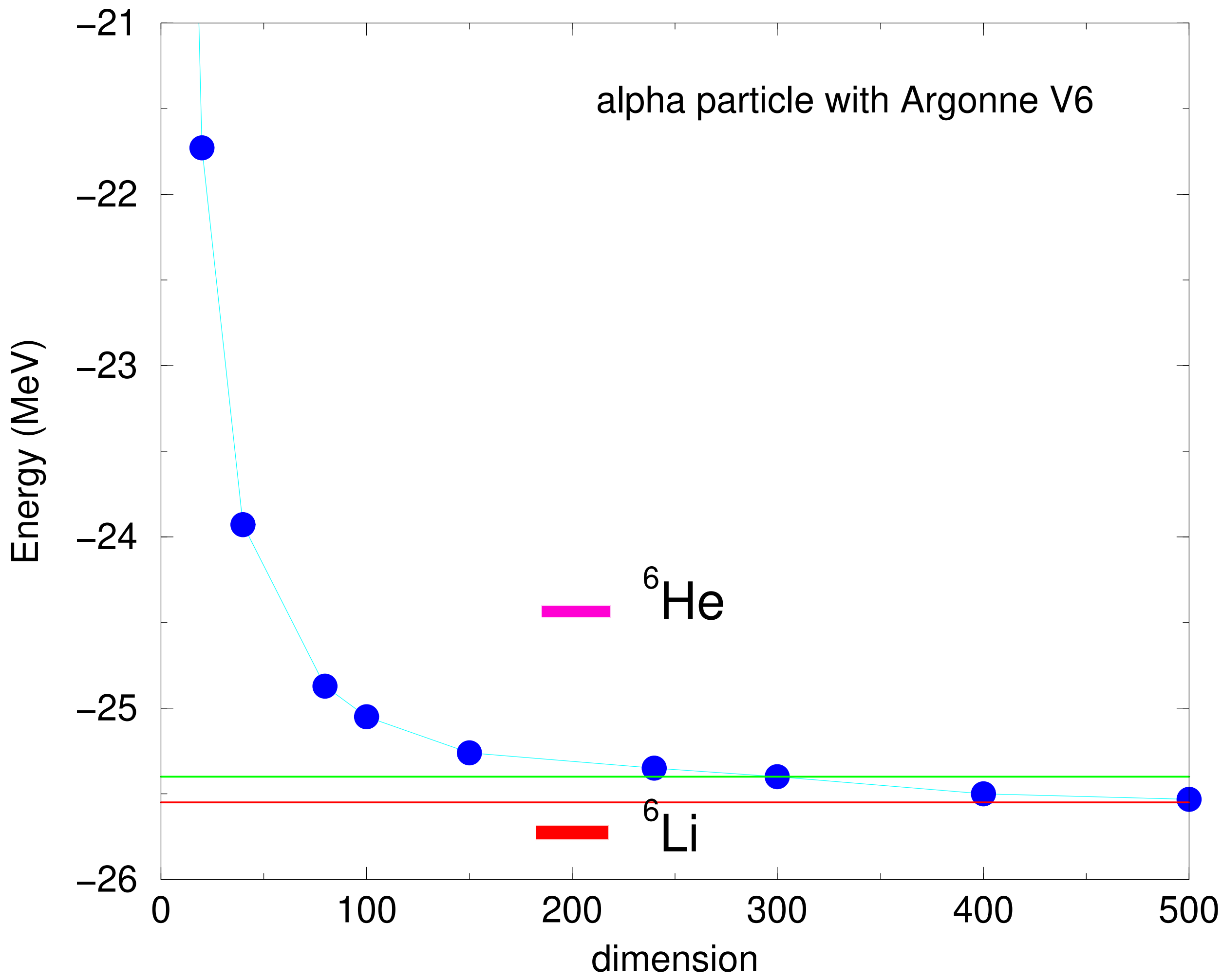
- The GFMC produces a very good energy spectra up to A=8 nuclei but there is no wave function
- The VMC wave function of the A=6 nuclei produces an unbound system with respect to the alpha particle (or alpha+deuteron) threshold.
- Binding mechanism of ^{6}He: Is that a genuine three-body effect (realistic two-body interaction does not bind ^{6}He)?
- "realistic structure" of A=6

$A{=}6$

Problems

- Huge model space
  - five relative motions
  - lot's of partial wave combinations
  - large spin-isospin space
  - antisymmetrization: $6!{=}720$ terms
- The number of parameters to be optimized and the number of channels to be tested is enormously high.

A=6



Present stage of the A=6 calculation. The ^{6}He is expected to be unbound without three-body interaction, so the energy slowly converges toward the threshold. The basis should be increased for ^{6}Li to get bound state with respect to the alpha+deuteron threshold.

Nuclear systems

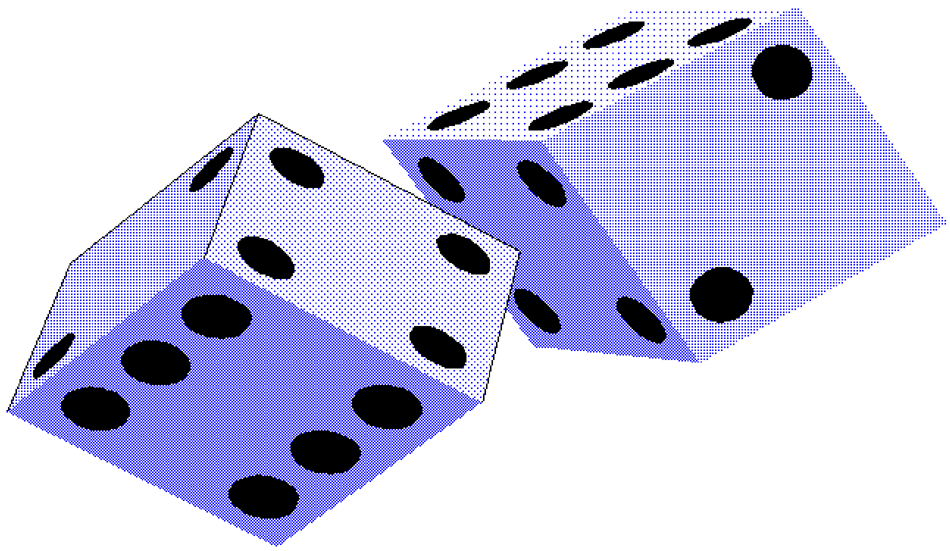
General problem:

- The energy converges very quickly in the beginning, but it is very difficult to get the last 0.5 MeV. For example, 10 basis states gives -20 MeV for the alpha particle, and the energy on 100 basis states is -25.1 MeV. To reach the converged result (-25.52 MeV) one needs 400-500 states.
- The reason of this is the strong repulsion in the central interaction.
- Jastrow-type correlation factors can easily help to cure this problem
- Example: We take a small basis, N=20 basis states. The best optimized SVM wave functions gives -22.5 MeV. Now we multiply this wave function with a product of two-body correlations of the form

$$f(r) = 1 - a\exp\{-br^2\} \tag{16}$$

and that gives -24.7 MeV.

Summary



- The SVM is a very powerful method which can be easily used to solve few-body problems of different fields of physics.
- Very accurate solutions, especially for Coulombic systems.
- The extension to larger systems is possible, but one has to use different bases and settle for less accurate results. Work in this direction is under way.