Jastrow相関基底における有効相互作用

——Transcorrelated法の核構造への適用——

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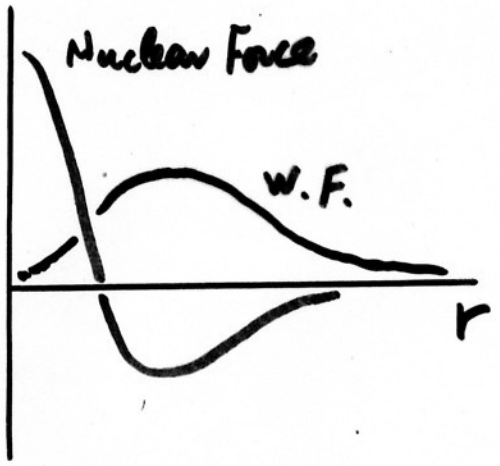
Outline

1. Motivation
2. Transcorrelated Hamiltonian
3. Choice of Jastrow correlation factor
4. Simple examples
5. Solution with non-Hermitean Hamiltonian
6. Summary and problems

Motivation

- Nuclear structure study with realistic interactions
- Short-range (strong repulsion) and long-range (tensor) correlations (⟶binding energy, density, momentum distribution) make a solution difficult
- SVM calculations with correlated Gaussians are successful

$$\exp[-\sum_{i<j} \alpha_{ij}(\boldsymbol{r}_i - \boldsymbol{r}_j)^2]$$



To cope with strong repulsion

1. G-matrix approach
2. Correlation factor

$$\boldsymbol{\Psi} = \mathbf{F}\boldsymbol{\Phi}$$

$$F = \prod_{i<j} f(r_{ij}) : \qquad (\text{Jastrow : state} - \text{independent})$$

$$F = \mathcal{S} \prod_{i<j} \hat{f}_{ij} : \qquad (\text{state} - \text{dependent})$$

$\Phi :$ model wave function (e.g., Slater determinant)

- Calculation with correlated basis functions is performed with VMC methods (Argonne, Pisa, Granada, ...)

$\longrightarrow$ Minimization of the energy

$$E = \frac{\langle F\Phi | H | F\Phi \rangle}{\langle F\Phi | F\Phi \rangle}$$

with respect to the variation of parameters of F and Φ

- Though the quality of VMC performance is acceptable, the VMC calculation is fairly involved.

We ask the following questions in the case of Jastrow basis:

1. Equation of motion for Φ
2. Choice of correlation factor $f(r)$

Transcorrelated Hamiltonian

Equation of motion for Φ:

$$HF\Phi = EF\Phi \quad \longrightarrow \quad H'\Phi = E\Phi$$

with transcorrelated Hamiltonian

$$H' = F^{-1}HF \qquad F = \prod_{i<j} f(r_{ij})$$

For the Hamiltonian containing two-body potentials

$$H = T - T_{\rm c.m.} + V_c + V_t + V_b$$

H' contains operators up to three-body terms and no more

$$H' = T - T_{\rm c.m.} + \sum_{i<j} t_{ij} + T^{(3)} + V_c + V_t + V_b + V_b^{(3)}$$

with ($g' = f'/f$)

$$t_{ij} = -\frac{\hbar^2}{m}\left(g''(r_{ij}) + \frac{2}{r_{ij}}g'(r_{ij}) + g'(r_{ij})^2 + \frac{1}{r_{ij}}g'(r_{ij})\boldsymbol{r}_{ij}\cdot(\nabla_i - \nabla_j)\right)$$

and where

$$T^{(3)} = \sum_{i<j<k}(t_{ijk} + t_{jki} + t_{kij})$$

with

$$t_{ijk} = -\frac{\hbar^2}{m}\frac{1}{r_{ij}}g'(r_{ij})\frac{1}{r_{ik}}g'(r_{ik})\boldsymbol{r}_{ij}\cdot\boldsymbol{r}_{ik}$$

Spin-orbit force:

For $V_b = \Sigma_{i<j} V_{b_{ij}}$ with

$$V_{b_{ij}} = v_b(r_{ij})\boldsymbol{r}_{ij} \times \frac{1}{2}(\boldsymbol{p}_i - \boldsymbol{p}_j)\cdot(\boldsymbol{s}_i + \boldsymbol{s}_j)$$

$$V_b^{(3)} = \sum_{i<j<k} (v_{ijk}^b + v_{jki}^b + v_{kij}^b)$$

with

$$v_{ijk}^b = -\frac{1}{2} i\hbar v_b(r_{ij})\boldsymbol{r}_{ij} \times \left(\frac{1}{r_{ik}} g'(r_{ik})\boldsymbol{r}_{ik} - \frac{1}{r_{jk}} g'(r_{jk})\boldsymbol{r}_{jk}\right) \cdot (\boldsymbol{s}_i + \boldsymbol{s}_j)$$

Properties of H':

- H' contains operators of up to three-body terms
- Eigenvalues of H and H' are identical
- H' is not Hermitean

Choice of Jastrow correlation factor

Suppose that the central potential is split to two parts:

$$V_c = W_c + U_c$$

where W_c is short-range repulsive potential

f or g' can be chosen to eliminate W_c from H'

$$-\frac{\hbar^2}{m}\left(g''(r) + \frac{2}{r}g'(r) + g'(r)^2\right) + W_c(r) = 0$$

or equivalently

$$-\frac{\hbar^2}{m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) f(r) + W_c(r)f(r) = 0$$

with the boundary condition

$$f(r) \to 1 \qquad \text{for} \;\; r \to \infty$$

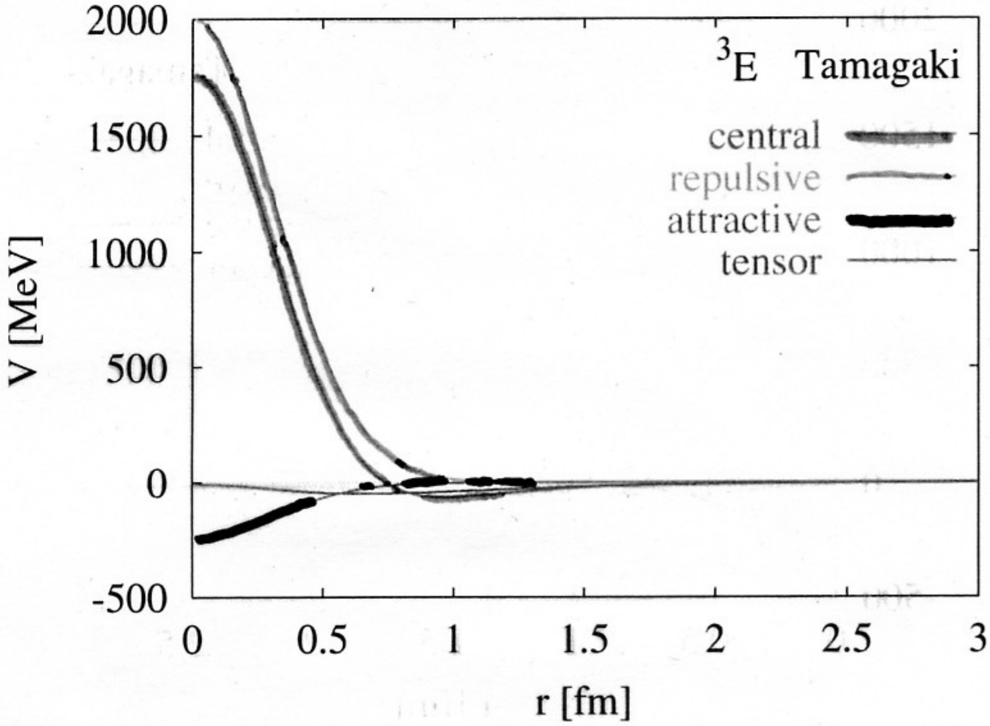
That is, f is a solution of two-nucleon relative motion with S-wave and with zero energy.

With this choice H' reduces to

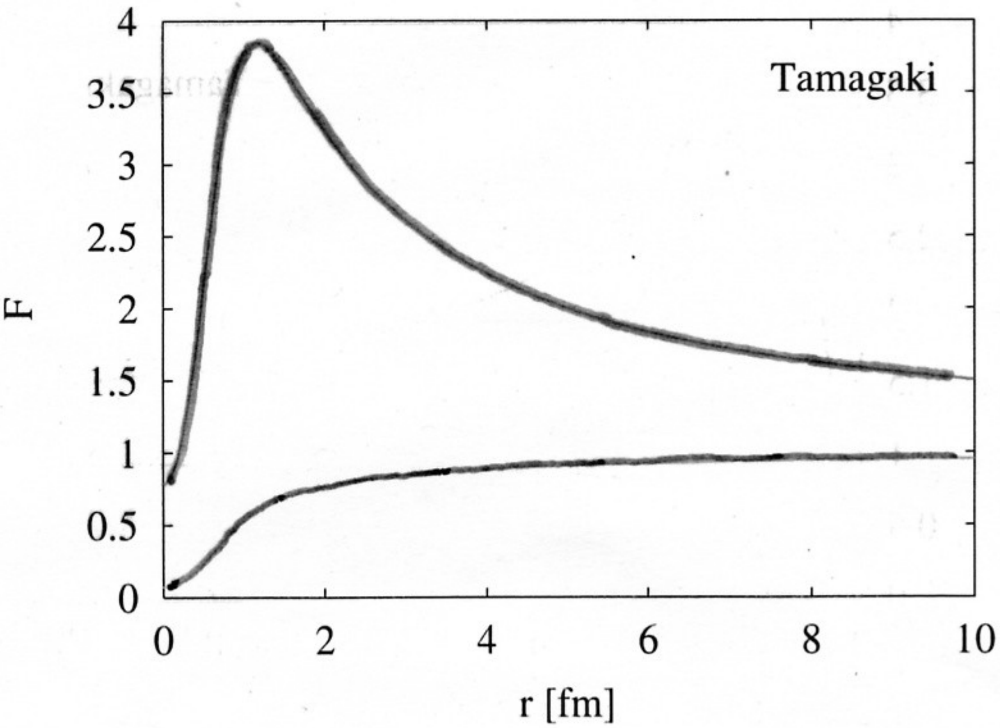
$$H' = T - T_{\text{c.m.}} + T^{(2)} + T^{(3)} + U_c + V_t + V_b + V_b^{(3)}$$

with

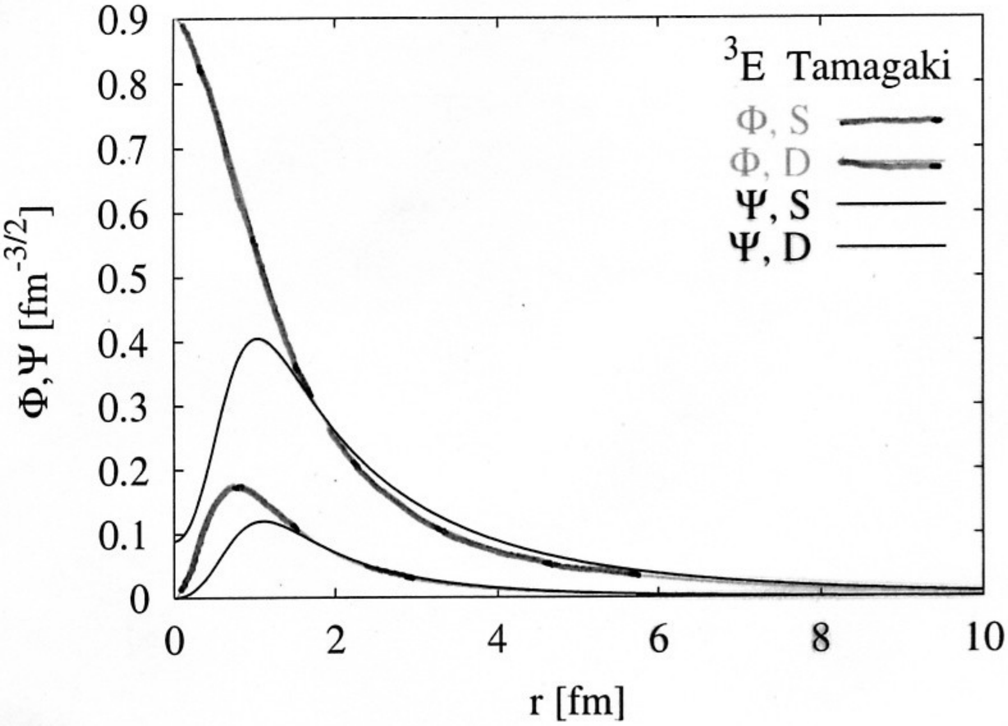
$$T^{(2)} = -\frac{\hbar^2}{m}\sum_{i<j}\frac{1}{r_{ij}}g'(r_{ij})\boldsymbol{r}_{ij}\cdot(\nabla_i - \nabla_j)$$



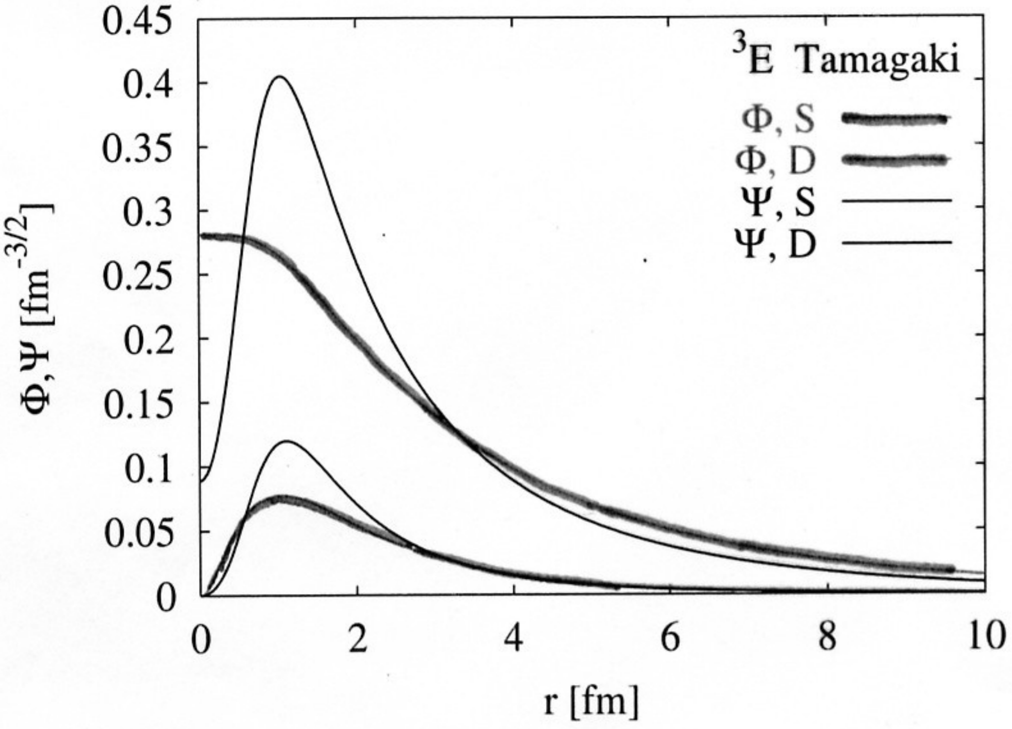
^3E Tamagaki
central
repulsive
attractive
tensor
V [MeV]
r [fm]
2000
1500
1000
500
0
-500
0
0.5
1
1.5
2
2.5
3



Tamagaki
F
r [fm]
4
3.5
3
2.5
2
1.5
1
0.5
0
2
4
6
8
10



^{3}E Tamagaki
Φ, S
Φ, D
Ψ, S
Ψ, D
Φ,Ψ [fm$^{-3/2}$]
r [fm]



^{3}E Tamagaki
Φ, S
Φ, D
Ψ, S
Ψ, D
Φ,Ψ [fm$^{-3/2}$]
r [fm]

Deuteron

$$H = T + V \qquad\qquad H' = T + U + H_1$$

Potential	$\langle T \rangle$ [MeV]	$\langle V \rangle$ [MeV]	$\langle U \rangle$ [MeV]	$\langle H1 \rangle$ [MeV]	$\langle E \rangle$ [MeV]
Minnesota	10.487	−12.689			−2.202
	10.514		−12.747	0.0310	−2.202
	22.340		−43.100	18.557	−2.202
Volkov No.1	4.273	−4.818			−0.545
	4.424		−5.131	0.161	−0.545
	7.233		−12.042	4.263	−0.545
ATS3	12.115	−14.330			−2.215
	13.728		−19.258	3.314	−2.215
	30.370		−81.139	48.552	−2.215

Potential	$\langle T_S \rangle$	$\langle T_D \rangle$	$\langle V_C^S \rangle$	$\langle V_C^D \rangle$	$\langle V_T^{SD} \rangle$	$\langle V_T^D \rangle$			$\langle E \rangle$
Tamagaki	10.842	5.636	−6.644	−0.650	−12.732	1.271			−2.277
	$\langle T_S \rangle$	$\langle T_D \rangle$	$\langle U_C^S \rangle$	$\langle U_C^D \rangle$	$\langle U_T^{SD} \rangle$	$\langle U_T^D \rangle$	$\langle H_1^S \rangle$	$\langle H_1^D \rangle$	$\langle E \rangle$
	17.256	10.175	−30.262	−1.929	−21.567	2.090	21.635	0.324	−2.277
	4.325	2.938	0.0	0.0	−6.576	0.639	−3.237	−0.366	−2.277

Solution with non-Hermitean Hamiltonian

$$H'\Phi = E\Phi$$

- The principle of energy minimization cannot be used to determine E and Φ
- The minimization of the variance of local energy or the norm of the residue vector

  $$(H' - E)\Phi/\sqrt{\langle\Phi|\Phi\rangle}$$

  may be used.

The norm of the residue vector is

$$\begin{aligned}\sigma^2 &= \langle (H' - E)\Phi|(H' - E)\Phi\rangle/\langle\Phi|\Phi\rangle \\ &= \int |\Phi|^2 \left|\frac{1}{\Phi}H'\Phi - E\right|^2 d\tau \Big/ \int |\Phi|^2 d\tau\end{aligned}$$

where the energy E is taken as $(\partial\sigma^2/\partial E = 0)$

$$E = \frac{\langle\Phi|H'\Phi\rangle + \langle H'\Phi|\Phi\rangle}{2\langle\Phi|\Phi\rangle} = \frac{\mathrm{Re}\langle\Phi|H'\Phi\rangle}{\langle\Phi|\Phi\rangle}$$

$$\sigma^2 = \frac{\langle H'\Phi|H'\Phi\rangle}{\langle\Phi|\Phi\rangle} - E^2$$

If Φ is approximated with a single Slater determinant

$$\Phi = \frac{1}{\sqrt{A!}} \begin{vmatrix} \phi_1(1) & \phi_2(1) & \cdots & \phi_A(1) \\ \phi_1(2) & \phi_2(2) & \cdots & \phi_A(2) \\ \vdots & \vdots & \vdots & \vdots \\ \phi_1(A) & \phi_2(A) & \cdots & \phi_A(A) \end{vmatrix}$$

the minimization of σ^2 with the condition $\langle \phi_i | \phi_j \rangle = \delta_{i,j}$ leads to a Hartree-Fock like equation for the single-particle orbits

$$\frac{\delta}{\delta \phi_i^*} \langle \Phi | H' \Phi \rangle = \sum_j \epsilon_{ij} \phi_j$$

$$-\frac{\hbar^2}{2m} \nabla^2 \phi_i(1) + \frac{1}{2} \sum_j \langle \phi_j(2) | v_{12}^{(2)} + v_{21}^{(2)} | \phi_i(1)\phi_j(2) - \phi_j(1)\phi_i(2) \rangle$$

$$+\frac{1}{2} \sum_{j \neq k} \langle \phi_j(2)\phi_k(3) | v_{123}^{(3)} + v_{231}^{(3)} + v_{312}^{(3)} | \begin{vmatrix} \phi_i(1) & \phi_j(1) & \phi_k(1) \\ \phi_i(2) & \phi_j(2) & \phi_k(2) \\ \phi_i(3) & \phi_j(3) & \phi_k(3) \end{vmatrix} \rangle$$

$$= \sum_j \epsilon_{ij} \phi_j(1)$$

Summary

- Transcorrelated Hamiltonian contains only 3-body terms
- Possible to eliminate short-range repulsive potential
- Established a relationship between H' and F

Problems

- Develop a method of solution for $H'\Phi = E\Phi$
- Applications to realistic cases
- Calculation of observables with $F\Phi$

$$\langle F\Phi|\mathcal{O}|F\Phi\rangle / \langle F\Phi|F\Phi\rangle$$