TALENT School@MITP 2022
Stochastic Variational Method exercise

3/8/2022 and 4/8/2022

Analytical calculation of correlated Gaussian matrix elements :

1. Calculate overlap correlated Gaussian matrix element and matrix elements of the Gaussian potential $V(r) = V_0 e^{-\frac{1}{2}ar^2}$, and Coulomb potential $V_c = 1.440\frac{1}{r}$. Details on correlated Gaussian basis and the corresponding matrix element calculation are given in the Talent notes of prof. Nir Barnea, Section 7.4.

2. Implement calculated matrix elements into the python script. More specifically, it is required to complete `overlap_elem(detB15)` function (overlap), `gauss_pot_elem(vpot,apot,p,detB15)` function (Gaussian potential), and `coulomb_elem(p,detB15)` function (Coulomb potential). Here

$$B = A' + A, \qquad \texttt{detB15} = \left(\frac{1}{\det(B)}\right)^{3/2} \tag{1}$$

and `p` is defined in the Talent notes Eq. (7.40). Notice that `gauss_pot_elem(vpot,apot,p,detB15)` function takes as an input two parameters of the Gaussian potential V_0(`vpot`) and a(`apot`). All matrix elements contain $(2\pi)^{3(N-1)/2}$ factor, where N stands for number of particles. This factor is effectively neglected since it does not contribute to the solution of generalized eigenvalue problem.

Numerical calculation of ^{2}H, ^{3}H, and ^{3}He bound state energies using the SVM python script :

3. Run the python SVM script and use it to obtain ^{2}H, ^{3}H, and ^{3}He bound state energies for the Minnesota NN potential. For ^{3}He system include Coulomb potential setting logical `Coulomb_pp` value to `True`. Use results for Volkov potential given in Tab. 1 as a benchmark.

Advice : For start set SVM optimization loop parameters to `mm0=2` and `kk0=10`. In this specific case very accurate bound state energies can be obtained for a maximum number of basis states `mnb=20` (^{2}H) or `mnb=100` (^{3}H, ^{3}He). Note that SVM solution for two-body bound state energies can be benchmarked using Numerov python script.

Potential	$E_b(^2\mathrm{H})$	$E_b(^3\mathrm{H})$	$E_b(^3\mathrm{He})$
Volkov + Coulomb	-0.5459	-8.4648	-7.7593

Table 1: Bound state energies in MeV.

Numerical calculation of elastic $NN(^3S_1)$ and $nd(^4S_{3/2})$ low-energy scattering via Busch formula :

Setting `HO_trap = True` introduces Harmonic oscillator (HO) trapping potential

$$V_{\mathrm{HO}}(\mathbf{r}) = \frac{m}{2A}\omega^2 \sum_{i<j}(\mathbf{r}_i - \mathbf{r}_j)^2 \,, \tag{2}$$

into the SVM calculation. Here A stands for number of particles and ω is the oscillator frequency.

Consider now the s-wave elastic scattering of two bound subclusters B and C, here $BC \in \{NN, nd\}$, inside the HO trap. Using the trap with length $b_{\mathrm{HO}} = \sqrt{2/(m\omega)}$ much larger than both range of the nuclear interaction and the subclusters size, the subclusters can be considered as point-like particles. As a result one can match the asymptotic $B - C$ part of the trapped A-body wave function to the free solution of an effective two-body BC system. The BC phase shifts δ_{BC} at relative momentum k then can be extracted using Bush formula

$$-\sqrt{4\mu\omega}\frac{\Gamma\left(3/4 - \epsilon^n_\omega/2\omega\right)}{\Gamma\left(1/4 - \epsilon^n_\omega/2\omega\right)} = k\cot\delta_{BC} \,, \tag{3}$$

where $\mu = m_B m_C/(m_B + m_C)$ is the BC reduced mass, $\Gamma(x)$ is the Gamma function, $k = \sqrt{2\mu\epsilon^n_\omega}$, and $\epsilon^n_\omega = E^n_\omega(A) - E_\omega(B) - E_\omega(C)$ is the energy of the A-body n-th excited state in a trap with respect to the $B+C$ threshold. Here, bound-state energies $E_\omega(B)$, $E_\omega(C)$, and $E^n_\omega(A)$ should be calculated using the SVM.

4. Calculate $NN(^3S_1)$ phaseshifts using Minnesota potential. In practice turn on the HO trap setting `HO_trap = True` and use the SVM to calculate bound state energy of the first excited state of $NN(S = 1, I = 0)$ system. Try to use multiple HO trap lengths $b_{\mathrm{HO}} \in [10; 30]$ fm. To set the size of the trap in fm use `HO_trap_length =` b_{HO} variable. From trapped SVM bound state energies calculate scattering phaseshifts using Eq. (3). Use calculated scattering phasehifts, in terms of $k\cot[\delta(k)]$, to fit effective range expansion parameters

- scattering length a and effective range $r_{\rm eff}$. What are their values ? (fitted values of effective range parameters can be compared to results of the Numerov python script) Note that the ground state of the $NN(S=1, I=0)$ system inside the trap corresponds to the trapped deuteron bound state. Consequently, we use an energy of the first excited state which corresponds to the trapped NN scattering scattering state. SVM optimization with respect to the first excited state is selected setting `opt_ener_level = 1`.

5. Repeat the same procedure for the $nd(S=3/2, I=0)$ s-wave elastic scattering. Note that due to the Pauli repuslion this system does not support any bound state outside the trap. As a result we can use directly ground state trapped energies. For SVM optimization with respect to the ground state energy set `opt_ener_level = 0`. Remember that ϵ^n_ω energies in Eq. 3 are defined with respec to the $n+d$ scattering threshold, consequently, $\epsilon^n_\omega = E^n_\omega(nd) - E_\omega(d)$ and you need to calculate as well deuteron bound state energies inside the HO trap using the same $b_{\rm HO}$.

Advice : Use results for Volkov potential given in Tab. and Tab. 2 as a benchmark.

Volkov potential				
$NN(^3S1)$				
$b_{\rm HO}$ [fm]	$E_b(^2{\rm H})$ [MeV]	E_b(1st exct.) [MeV]	k^2 [fm^{-1}]	$k\ \cot(\delta)$ [fm^{-1}]
10	-0.38889933	1.97454712	0.04761387	-0.04179817
15	-0.50817880	0.80558075	0.01942563	-0.07598665
20	-0.53313960	0.42559782	0.01026279	-0.08696486
25	-0.54055077	0.25980082	0.00626479	-0.0917346
30	-0.54330376	0.17399644	0.00419572	-0.09419832
$nd(^4S_{3/2})$				
$b_{\rm HO}$ [fm]	E_b(g.s.) [MeV]		k^2 [fm^{-1}]	$k\ \cot(\delta)$ [fm^{-1}]
10	1.73461113		0.06827459	0.02504229
15	0.35924390		0.02788916	-0.03962709
20	-0.07618957		0.01469175	-0.06157149
25	-0.26275963		0.00893147	-0.07109322
30	-0.35750889		0.00597363	-0.07448689

Scattering	a	r_{eff}
$NN(^3S_1)$	10.067(5)	2.415(5)
$nd(^4S_{3/2})$	11.779(6)	3.22(2)

Table 2: Calculated effective range expansion parameters scattering length a and effective range r_{eff} given in fm.