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Efficient emulators for scattering using eigenvector continuation

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KVP method

$$Du_{\text{exat}}(r) = \left(-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + \boxed{U(r)} - p^2\right) u_{\text{exat}}(r) = 0$$

Parameter dependent potential

1. Introduce a functional
2. Put into some ansatz as trial
3. Solve the optimization problem

$$\beta\left[u_{\text{t}}\right] = \tau_{\text{trial}} - \int_0^\infty dr u_{\text{t}}(r) D u_{\text{t}}(r) \qquad u = \sum_i c_i \psi_i$$

$$u_t(r) \xrightarrow[r\to\infty]{} \frac{1}{p}\sin\left(pr - \ell\frac{\pi}{2}\right) + \tau_{\text{trial}}\cos\left(pr - \ell\frac{\pi}{2}\right)$$

We choose a set of basis functions, and minimize the functional by selecting the coefficients

How to construct the functional

Boundary condition of scattering wave function (Definition of the K-matrix)

$$u_{\ell,E}(r) \xrightarrow[r\to\infty]{} \frac{1}{p}\sin\left(pr - \ell\frac{\pi}{2}\right) + \frac{\mathcal{K}_\ell(E)}{p}\cos\left(pr - \ell\frac{\pi}{2}\right)$$

$$\mathcal{K}_\ell(E) = \tan(\delta_\ell)$$

Take a variation at the exact scattering wave function

$$\delta\beta = \delta\tau - \int_0^\infty dr u_{\mathrm{exact}}(r) D\delta u(r) + \mathcal{O}\left(\delta u^2\right)$$

Carry out the integration by parts for two times

$$\int_0^\infty dr u_{\mathrm{exact}}(r) D\delta u(r)\,\% = \int_0^\infty dr u_{\mathrm{exact}}(r)\left(-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + U(r) - p^2\right) u_{\mathrm{exat}}\delta u(r)$$

$$= \left(u_{\mathrm{exact}}\delta u' - u'_{\mathrm{exact}}\delta u\right)\Big|_0^\infty + \int dr u D u_{\mathrm{exat}}$$

How to construct the functional

With the boundary condition and some sin/cos algebras

$$\left(u_{\text{exact}}\delta u' - u'_{\text{exact}}\delta u\right)\Big|_0^\infty = \delta\tau$$

So we have proved $\quad \delta\beta[u]\Big|_{u_{\text{exact}}} = \delta\tau - \delta\tau = 0$

Remind that $\quad \beta\left[u_{\text{exact}}\right] = \frac{1}{p}\left[\mathscr{K}_\ell(E)\right]_{\text{exact}} = \frac{1}{p}\left[\tan\delta_\ell(E)\right]_{\text{exact}}$

EC with KVP

EC provides us with a set of basis, and reduce the size of the basis

Snapshots $D(\boldsymbol{\theta}_i)u_i = 0 \qquad i = 1, 2, \ldots, N_b$

Differential equation

↕

Finite difference ⟹ Number of the grid points >> N_b

↕

Linear equation ⟹ Size of the matrix >> N_b

R-matrix: solve the large linear equations "exactly" for 1000 times

EC: solve "exactly" N_b times + emulate other situations $1000 - N_b$ times

Where the efficiency comes from

EC with KVP

Insert the trial solution into the functional

$$\beta\left[u_{\mathrm{t}}\right]=\sum_{j} c_j \tau_j(E)-\sum_{jk} c_j c_k \int_0^{\infty} d r u_j(r ; E)\left[-\frac{d^2}{d r^2}+\frac{l(l+1)}{r^2}+2 \mu V(r ; \boldsymbol{\theta})-p^2\right] u_k(r ; E)$$

$$=\sum_{j} c_j \tau_j-\sum_{jk} c_j c_k \int_0^{\infty} d r u_j(r ; E)(2 \mu)\left[V(r ; \boldsymbol{\theta})-V_k(r)\right] u_k(r ; E)$$

Define the U matrix for convenient

$$\Delta U=\int_0^{\infty} d r u_j(r ; E)(2 \mu)\left[V(r ; \boldsymbol{\theta})-V_k(r)\right] u_k(r ; E)$$

The functional now turns into a matrix form

$$\beta=\sum_{j} c_j \tau_j-\sum_{jk} c_j c_k \Delta U_{jk}$$

EC with KVP

Take the partial derivatives and add an Lagrange multiplier

$$\frac{\partial}{\partial c_i}\left[\sum_j c_j\tau_j - \sum_{jk} c_j c_k \Delta U_{jk} - \lambda\left(\sum_j c_j - 1\right)\right] = 0$$

$$\frac{\partial}{\partial \lambda}\left[\sum_j c_j\tau_j - \sum_{jk} c_j c_k \Delta U_{jk} - \lambda\left(\sum_j c_j - 1\right)\right] = 0.$$

Finally we have the expression for the coefficients and multiplier

$$c_j = \sum_i (\Delta \widetilde{U})^{-1}_{ji}\left(\tau_i - \lambda\right) \qquad \lambda = \frac{\sum_{ij} (\Delta \widetilde{U})^{-1}_{ji}\tau_i}{\sum_{ij} (\Delta \widetilde{U})^{-1}_{ji}}$$

Kohn anomalous issues

The matrix to be inverted may be expected to be increasingly ill-conditioned as the basis size increases.

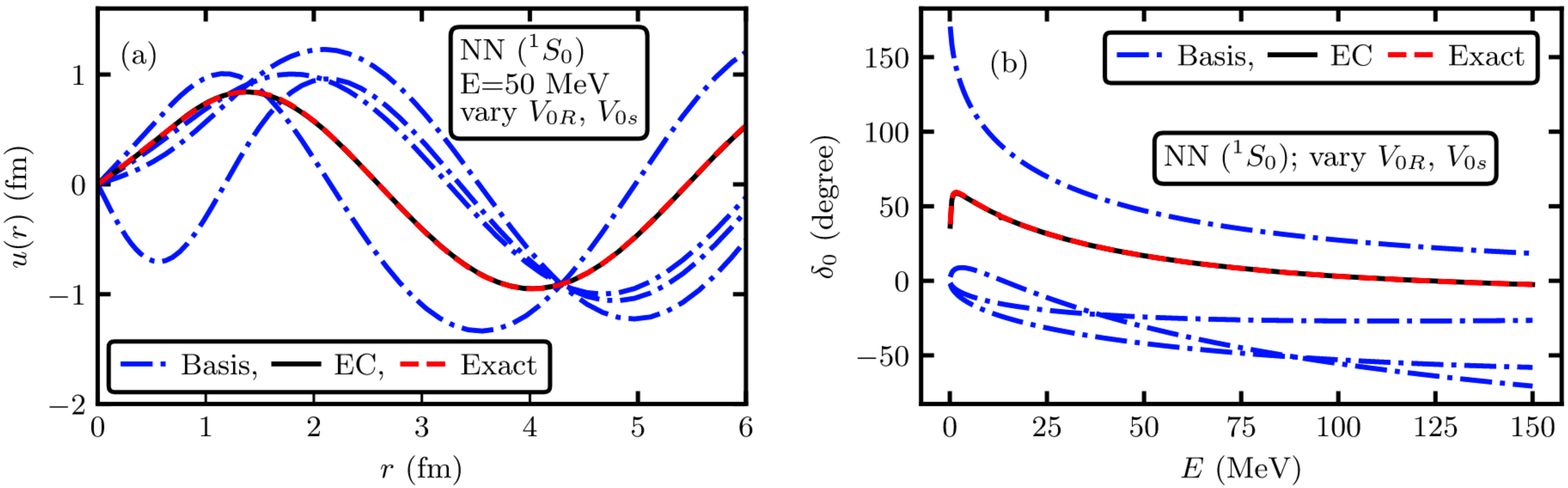
1. Complex formulation of S- matrix
2. Pseudo inverse method
3. Regularization: adding a small value to the diagonal

$$\text{Nugget: } 10^{-8} \sim 10^{-10}$$

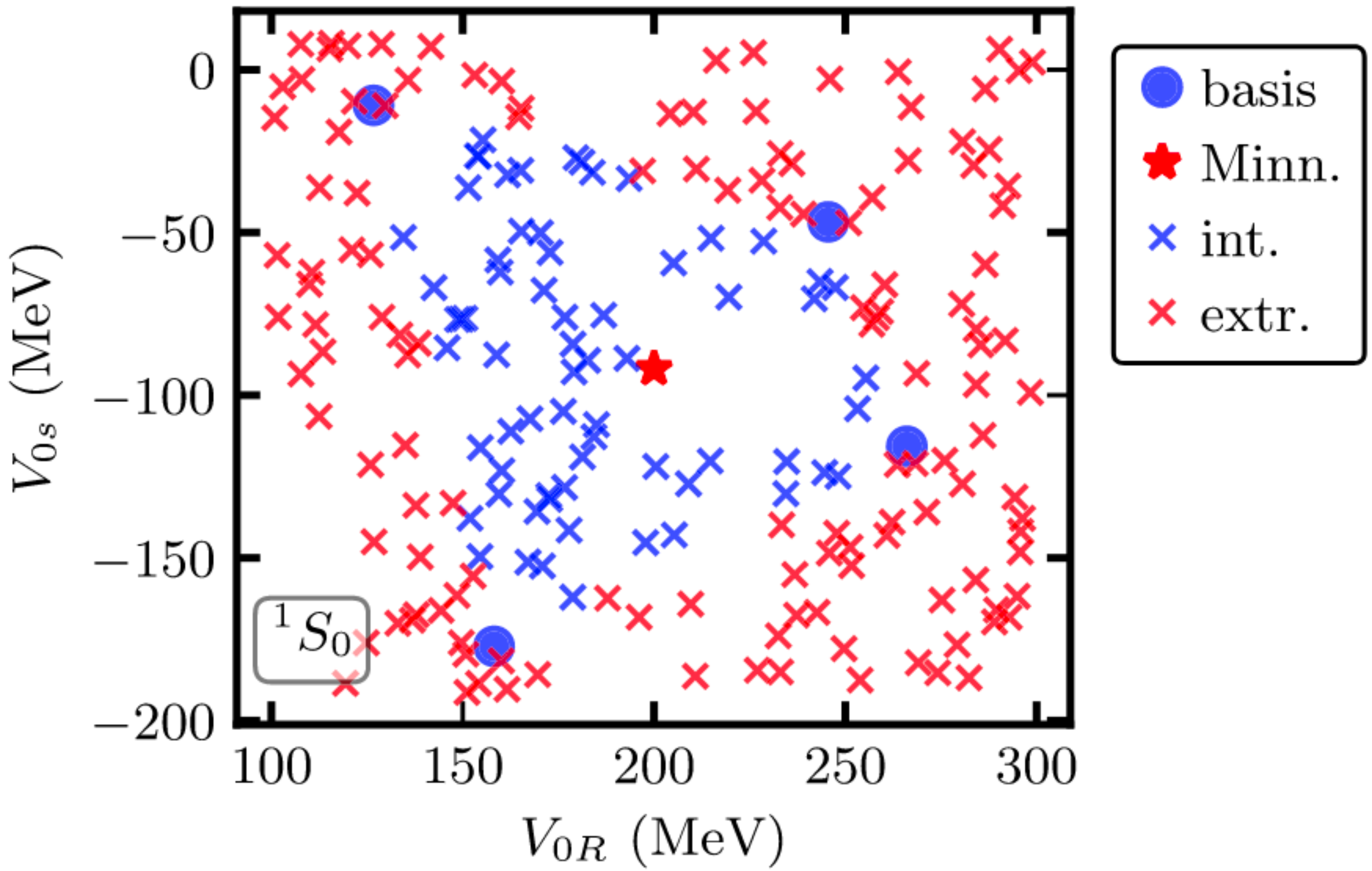
N-N scattering

$$V_{^1S_0}(r) \equiv V_{0R} e^{-\kappa_R r^2} + V_{0s} e^{-\kappa_s r^2}$$

$$V_{^3S_1}(r) \equiv V_{0R} e^{-\kappa_R r^2} + V_{0t} e^{-\kappa_t r^2}$$

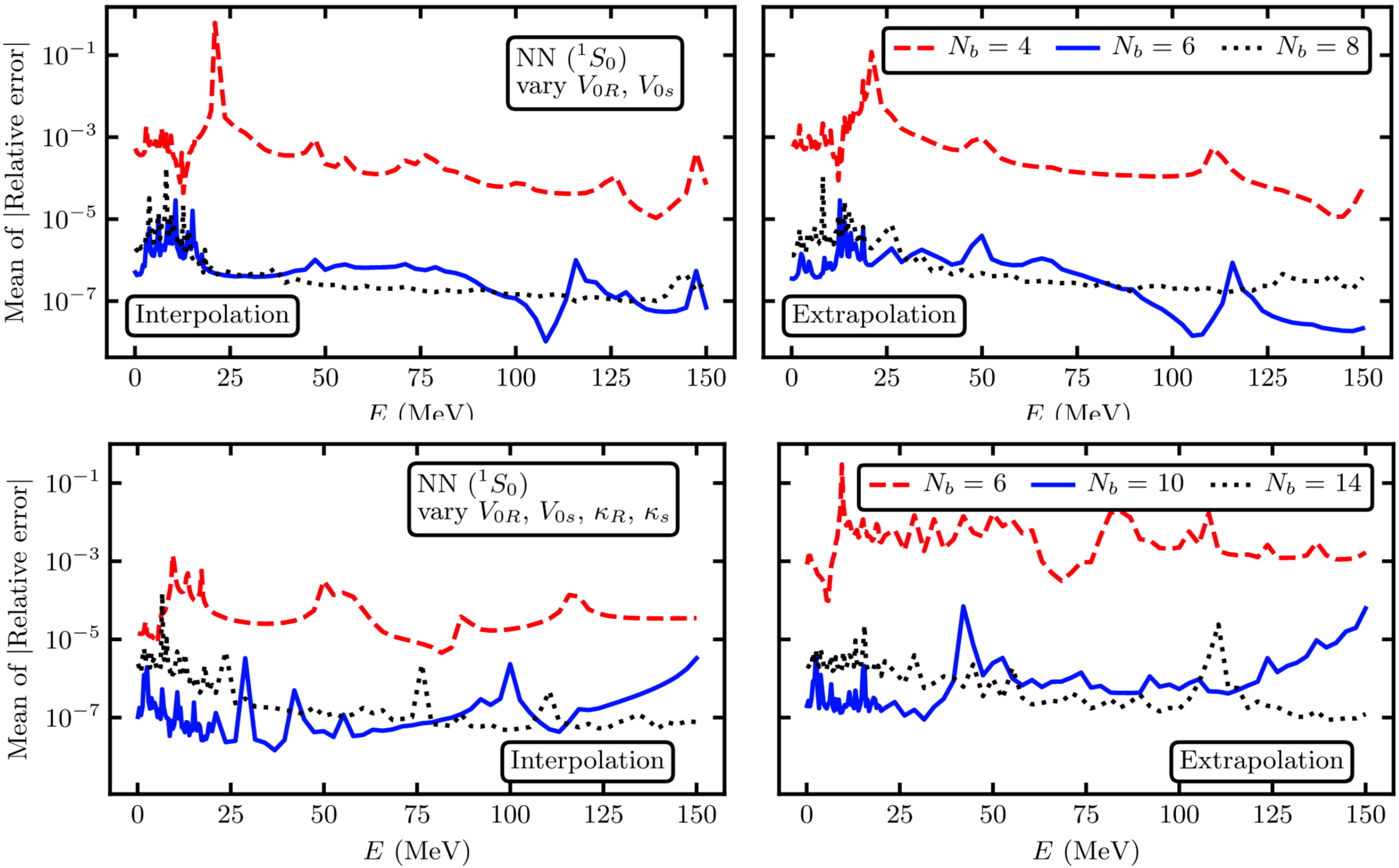


N-N scattering



Latin-hypercube sampling method

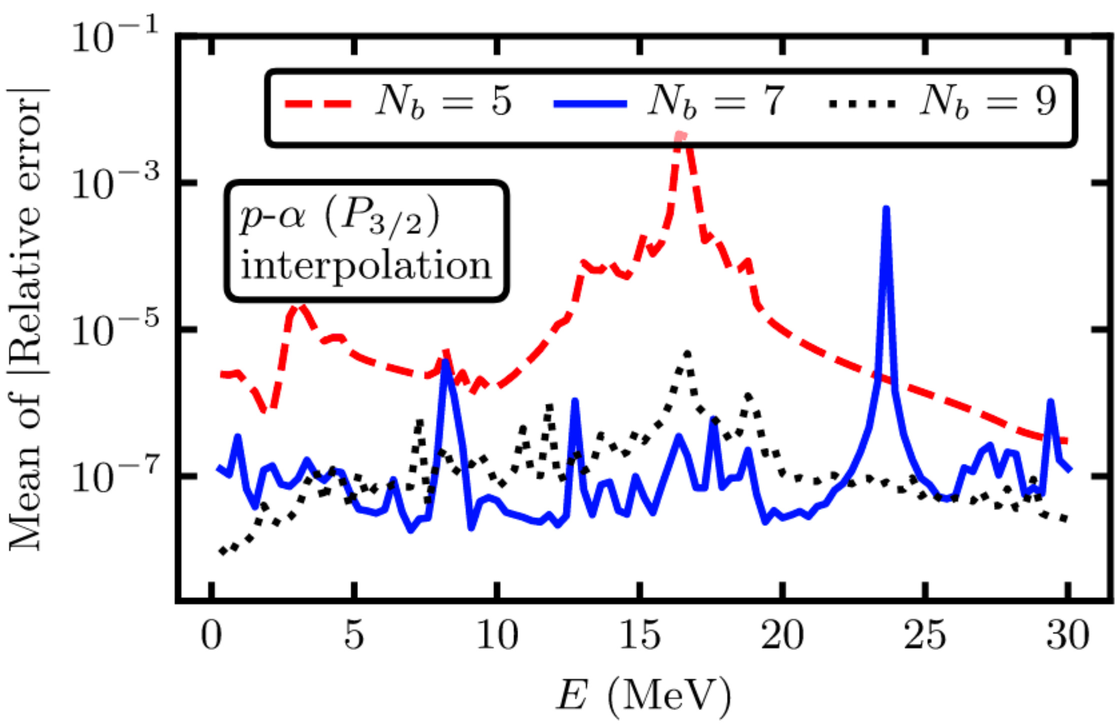
N-N scattering



Other applications

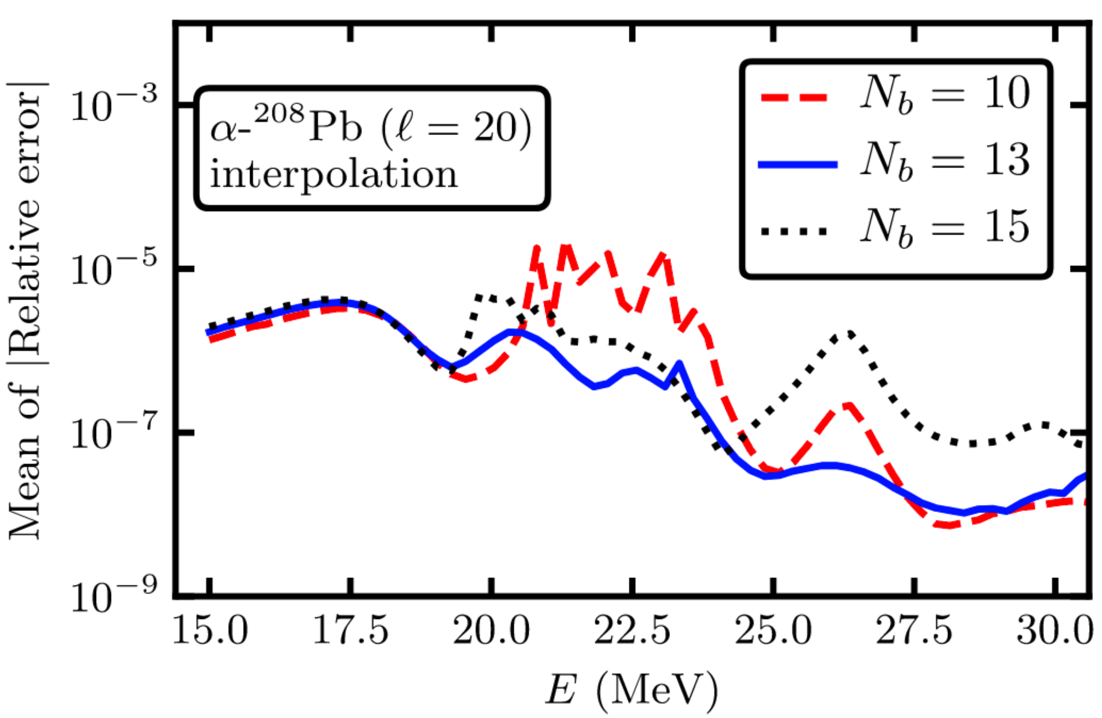
$p-\alpha$ scattering

$$V_\ell(r',r) = V^{(0)}_{p\alpha,\ell}\, r'^{\ell}\, r^{\ell} e^{-\beta_\ell\,(r'+r)}$$



$\alpha -{}^{208}$Pb scattering

Woods-Saxon form



Summary

EC basis for KVP is accurate and efficient:

1. It can produce good results compared with the exact R-matrix method
2. Instead of carrying out the diagonalization, only the inverse operations and some multiplication are need.

But there are some limitations:

1. Can only deal with a specific energy
2. Can only deal with a specific partial wave
3. Cannot emulate the observable