Eigenvector Continuation for Two-Body Scattering

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The Ohio State University

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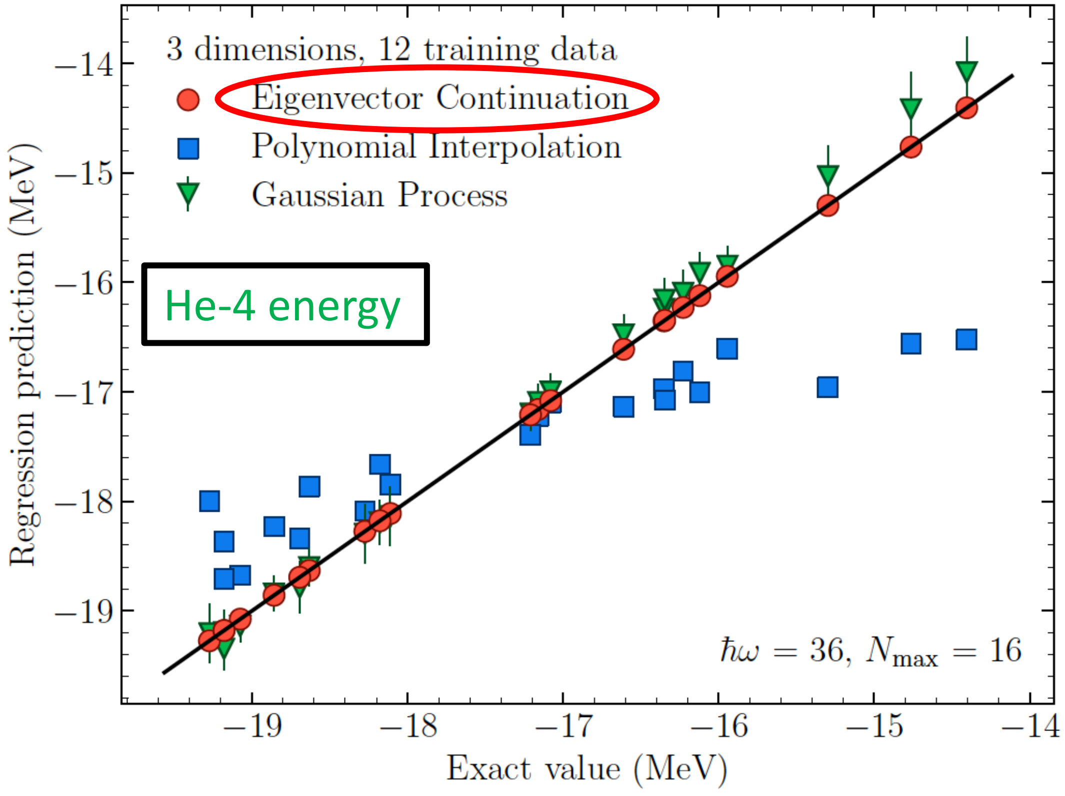
Collaborators: R.J. Furnstahl, P.J. Millican, Xilin Zhang

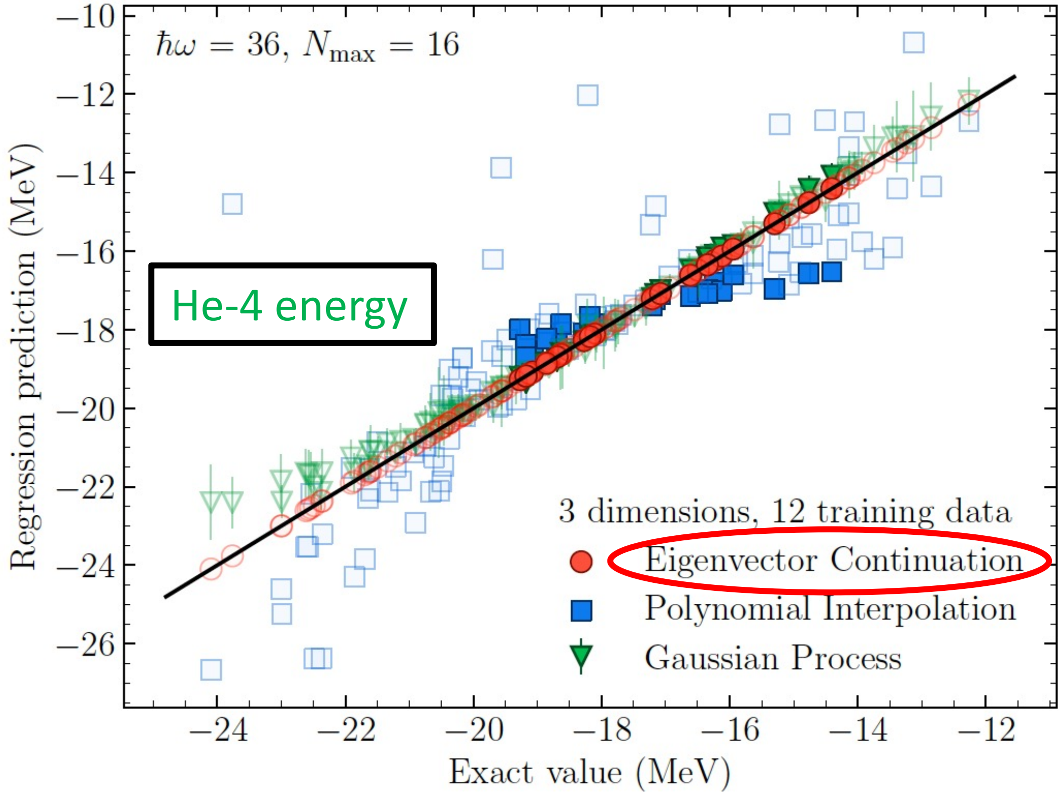
R.J. Furnstahl, ajg, P.J. Millican, and Xilin Zhang,
arXiv: 2007.03635 , Phys. Lett. B 809, 135719 (2020)

The need for emulators for uncertainty quantification (UQ)

- Sampling for UQ can be prohibitively expensive. Alternative: sample from a previously trained computer model.

S. König, et al, "Eigenvector Continuation as an Efficient and Accurate Emulator for Uncertainty Quantification", *Phys. Lett. B 810, 135814 (2020)*





Eigenvector continuation (EC) for bound states

- A variational calculation with a very effective trial wave function

Hamiltonian: Sets of parameters: Ground-state eigenvectors:

$$\hat{H}(\boldsymbol{\theta}) = \hat{T} + \hat{V}(\boldsymbol{\theta}) \rightarrow \{(\boldsymbol{\theta})_i\} \rightarrow |\psi_{gs}(\boldsymbol{\theta}_i)\rangle$$

$$|\psi_{trial}\rangle = \sum_{i=1}^{N_b} c_i |\psi_{gs}(\boldsymbol{\theta}_i)\rangle$$

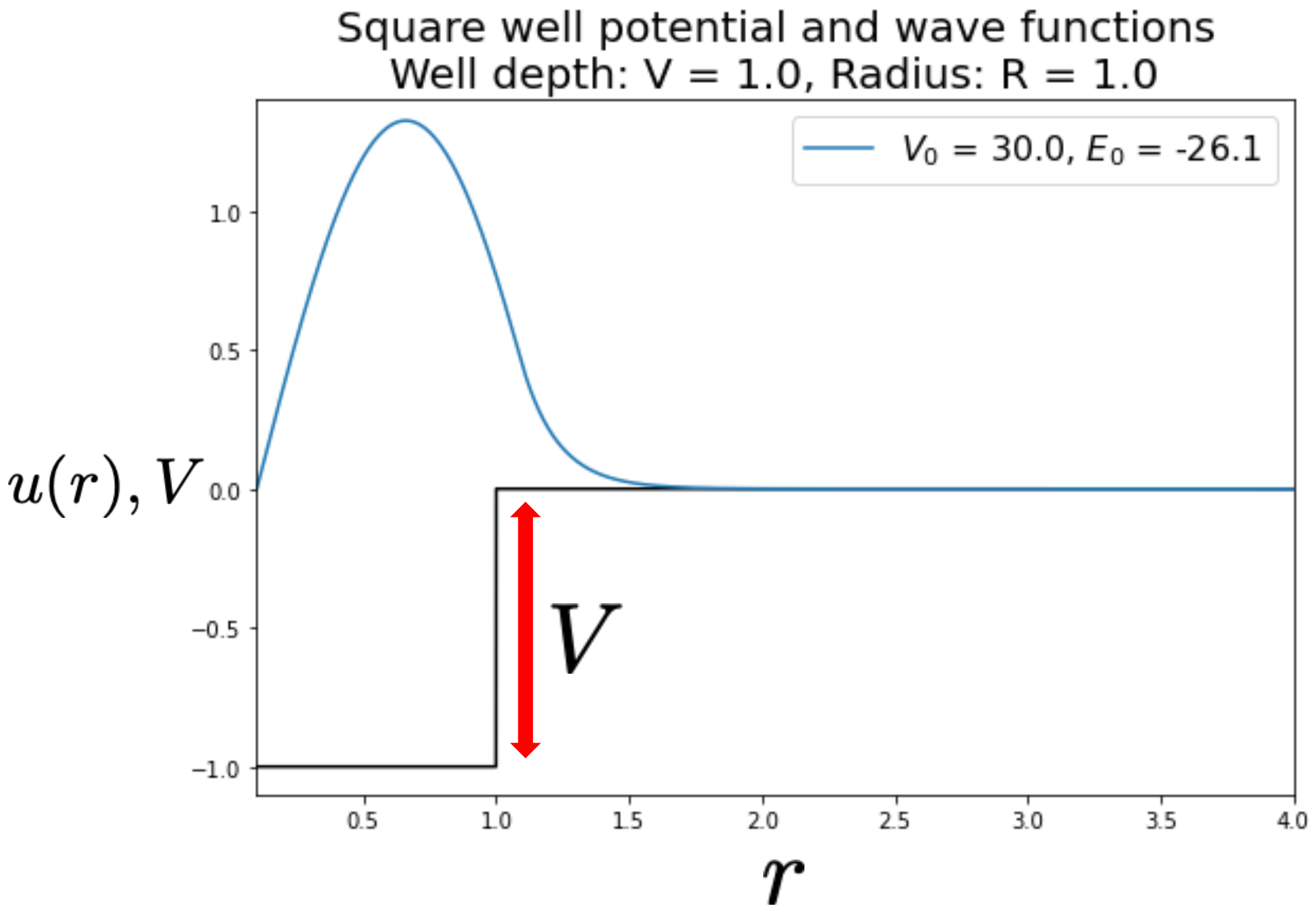
D. Frame, et al, "Eigenvector continuation with subspace learning", Phys. Rev. Lett. 121, 032501 (2018)

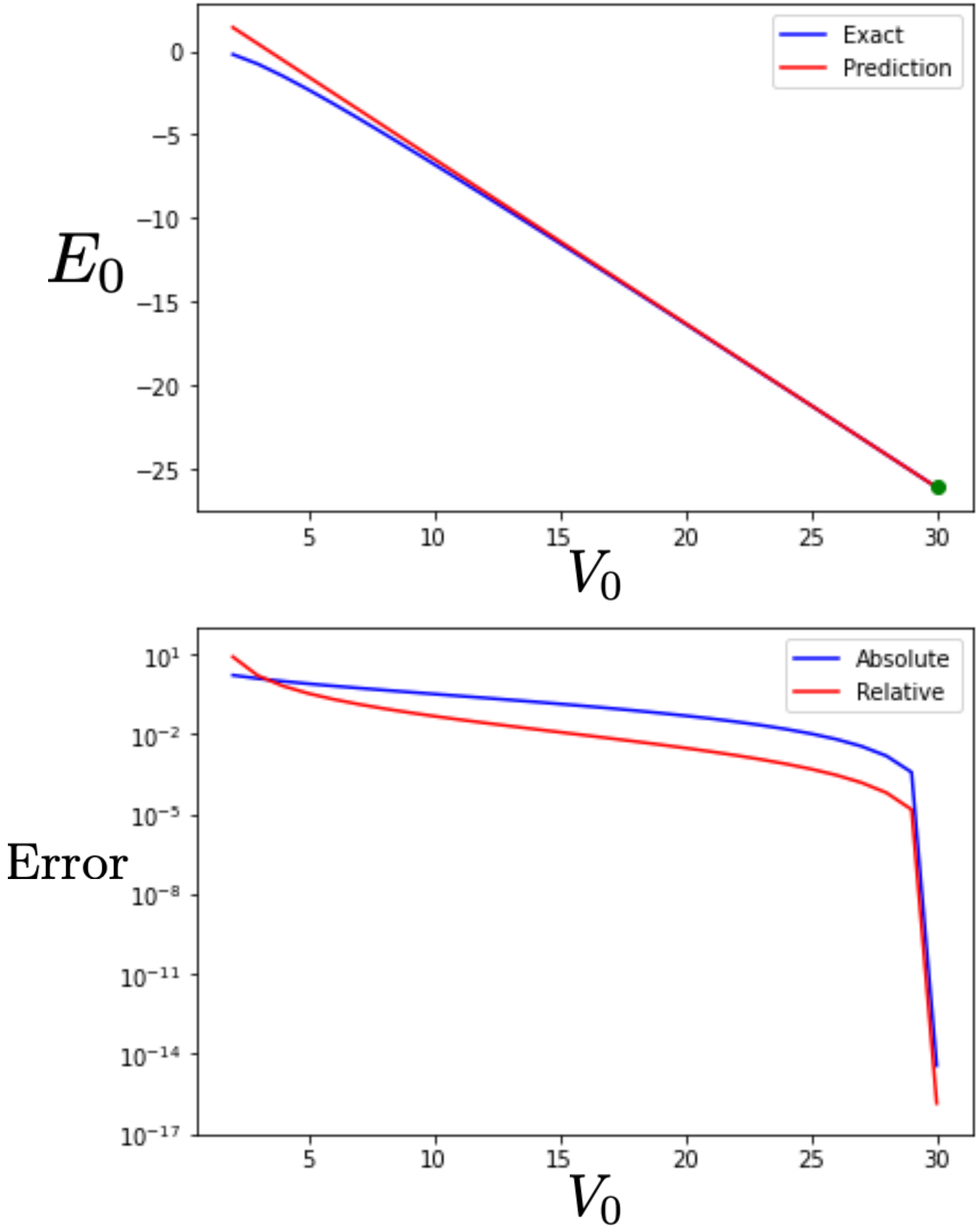
$$\delta\Big[\langle\psi_{trial}|\hat{H}(\boldsymbol{\theta})|\psi_{trial}\rangle - \lambda\big(\langle\psi_{trial}|\psi_{trial}\rangle - 1\big)\Big] = 0$$

$$\sum_k (H_{jk} - \lambda N_{jk}) c_k = 0 \rightarrow \begin{array}{l} H_{ij}(\boldsymbol{\theta}) \equiv \langle\psi_{gs}(\boldsymbol{\theta}_i)|\hat{H}(\boldsymbol{\theta})|\psi_{gs}(\boldsymbol{\theta}_j)\rangle \\ N_{ij}(\boldsymbol{\theta}) \equiv \langle\psi_{gs}(\boldsymbol{\theta}_i)|\psi_{gs}(\boldsymbol{\theta}_j)\rangle \end{array}$$

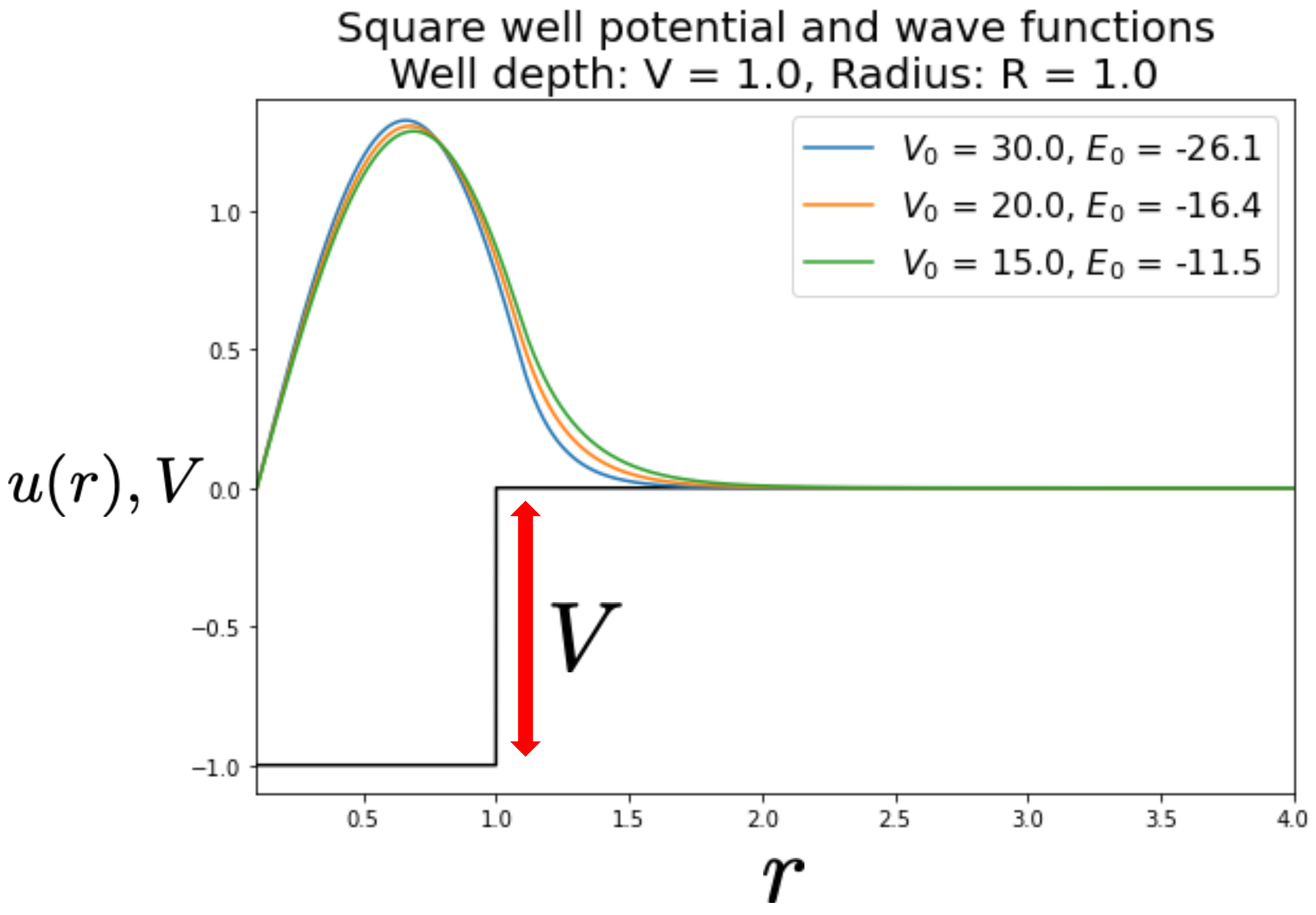
- Eigenvalue problem in a small space → inexpensive (also can precalculate)
- Can interpolate and extrapolate solutions of the Hamiltonian

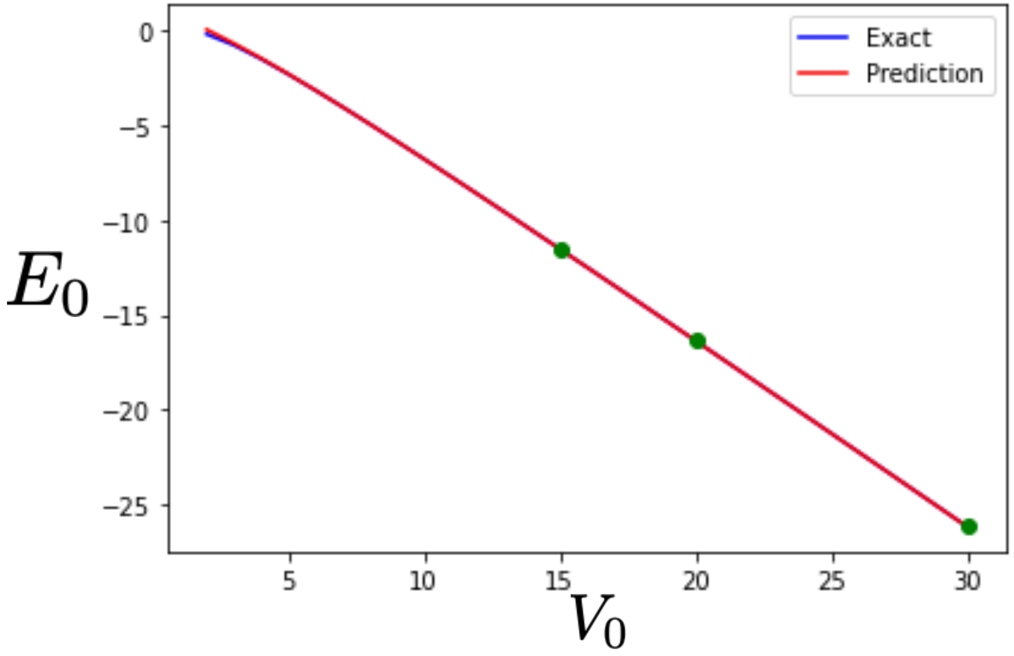
Square-well bound states

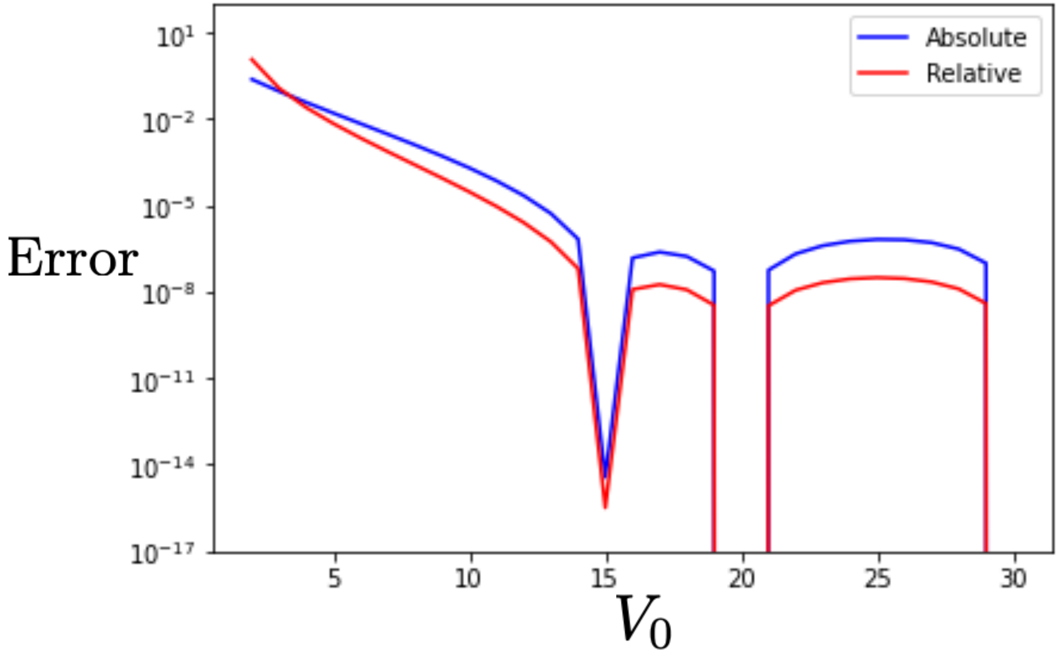




Square-well bound states







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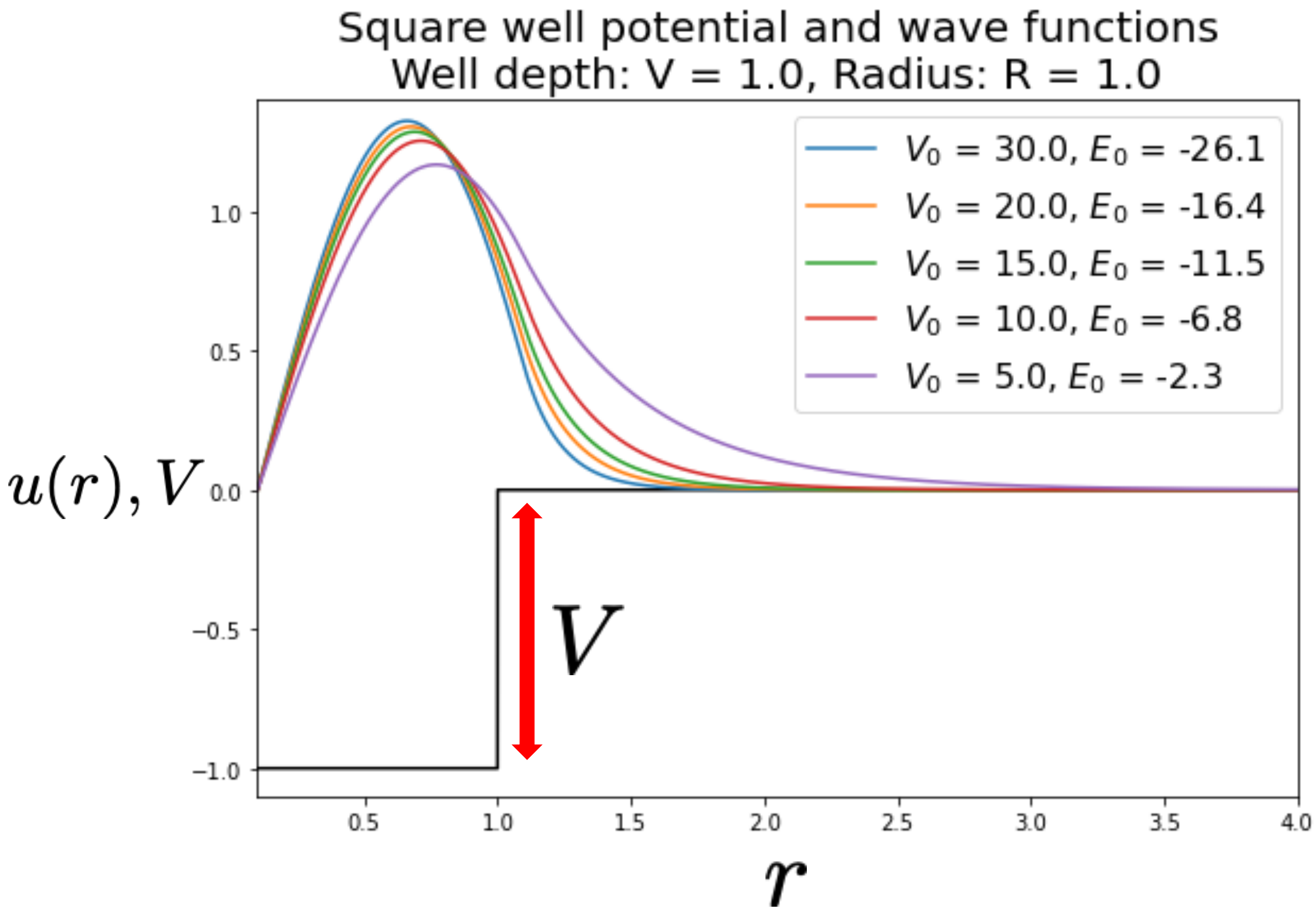
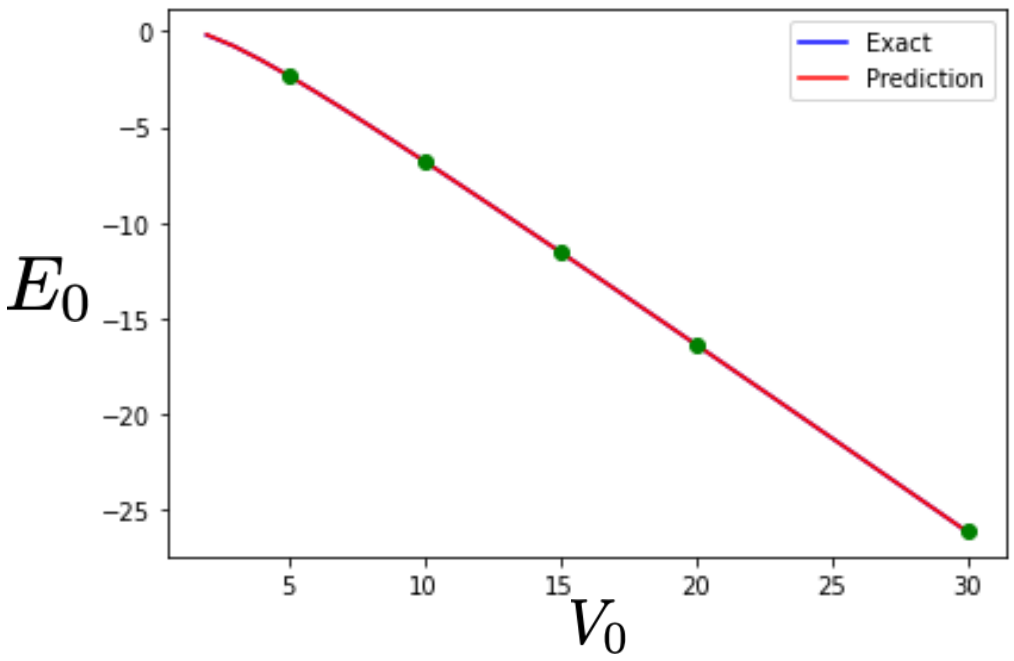
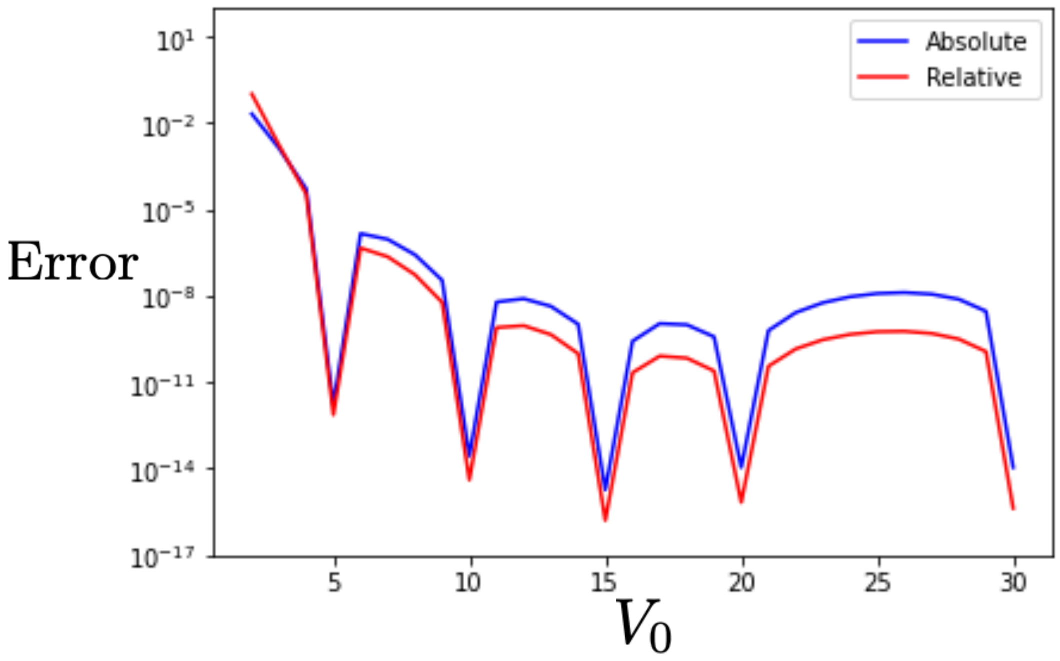






Eigenvector continuation (EC) for scattering

Hamiltonian:

$$\hat{H}(\boldsymbol{\theta}) = \hat{T} + \hat{V}(\boldsymbol{\theta})$$

→

Sets of parameters:

$$\{(\boldsymbol{\theta})_i\}$$

→

K-matrix formulation:

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

Kohn variational principle (KVP):

S-wave: $\ell = 0$

$p \equiv \sqrt{2\mu E}$

$$|\psi_{trial}\rangle \xrightarrow[r\to\infty]{} \frac{1}{p}\sin(pr) + \frac{[\mathcal{K}_0(E)]_{trial}}{p}\cos(pr)$$

$$\delta\beta[|\psi_{trial}\rangle] = \delta\left[\frac{[\mathcal{K}_0(E)]_{trial}}{p} - \frac{2\mu}{\hbar^2}\langle\psi_{trial}|\hat{H}(\boldsymbol{\theta}) - E|\psi_{trial}\rangle\right] = 0 \rightarrow \beta[|\psi_{exact}\rangle] = \frac{[\mathcal{K}_0(E)]_{exact}}{p}$$

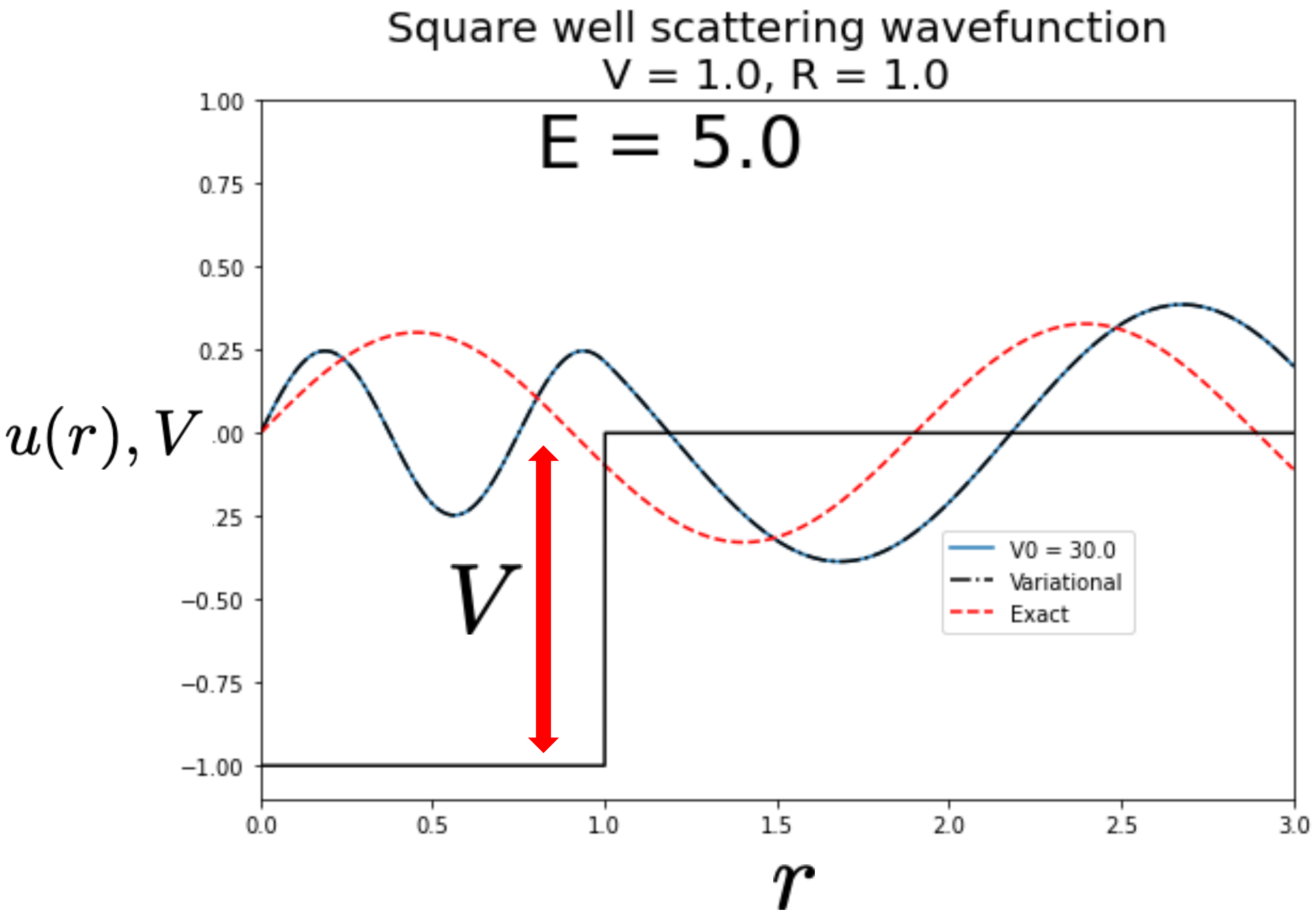
EC implementation:

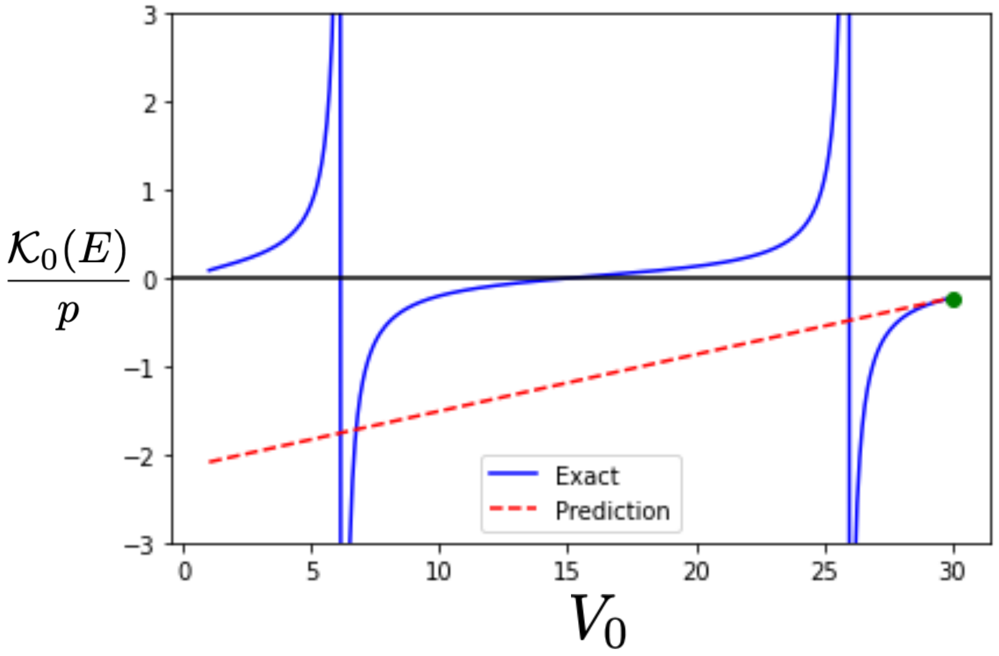
$$|\psi_{trial}\rangle = \sum_{i=1}^{N_b} c_i|\psi_E(\boldsymbol{\theta}_i)\rangle \rightarrow \sum_j \left(\Delta U^T + \Delta U\right)_{ij} c_j = \sum_j \Delta\tilde{U}_{ij} c_j = \frac{\mathcal{K}_0^{(i)}(E)}{p} - \lambda$$

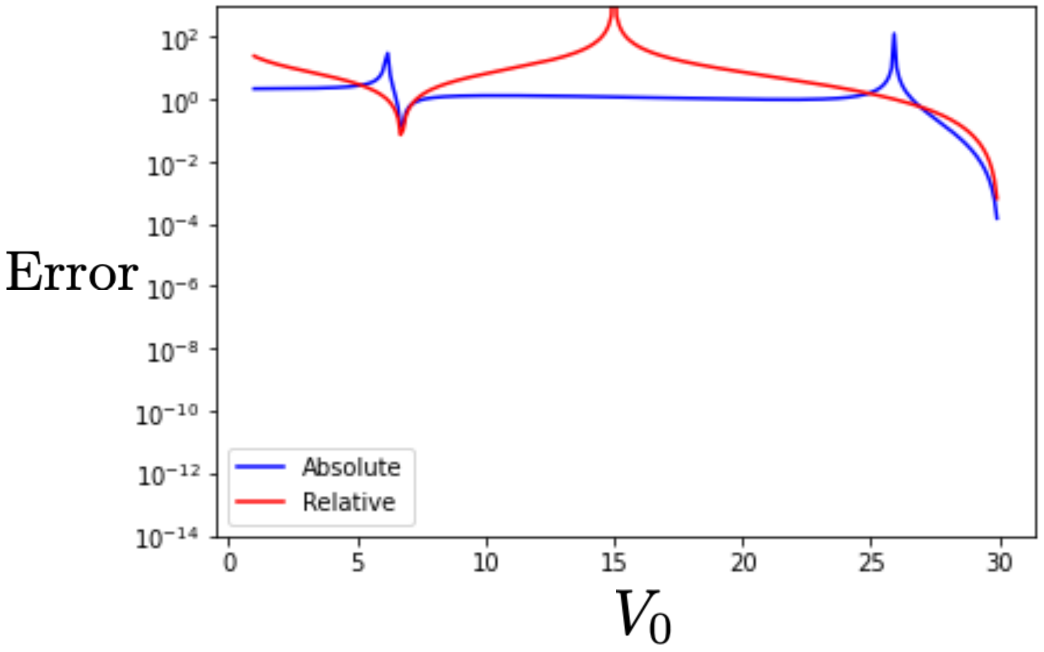
$$\Delta\tilde{U}_{ij} = \frac{2\mu}{\hbar^2}\langle\psi_E(\boldsymbol{\theta}_i)|2\hat{V}(\boldsymbol{\theta}) - \hat{V}(\boldsymbol{\theta}_i) - \hat{V}(\boldsymbol{\theta}_j)|\psi_E(\boldsymbol{\theta}_j)\rangle$$

- Simple matrix inversion + cancellation of Coulomb force!
- Stationary approximation to K-matrix (not an upper/lower bound)

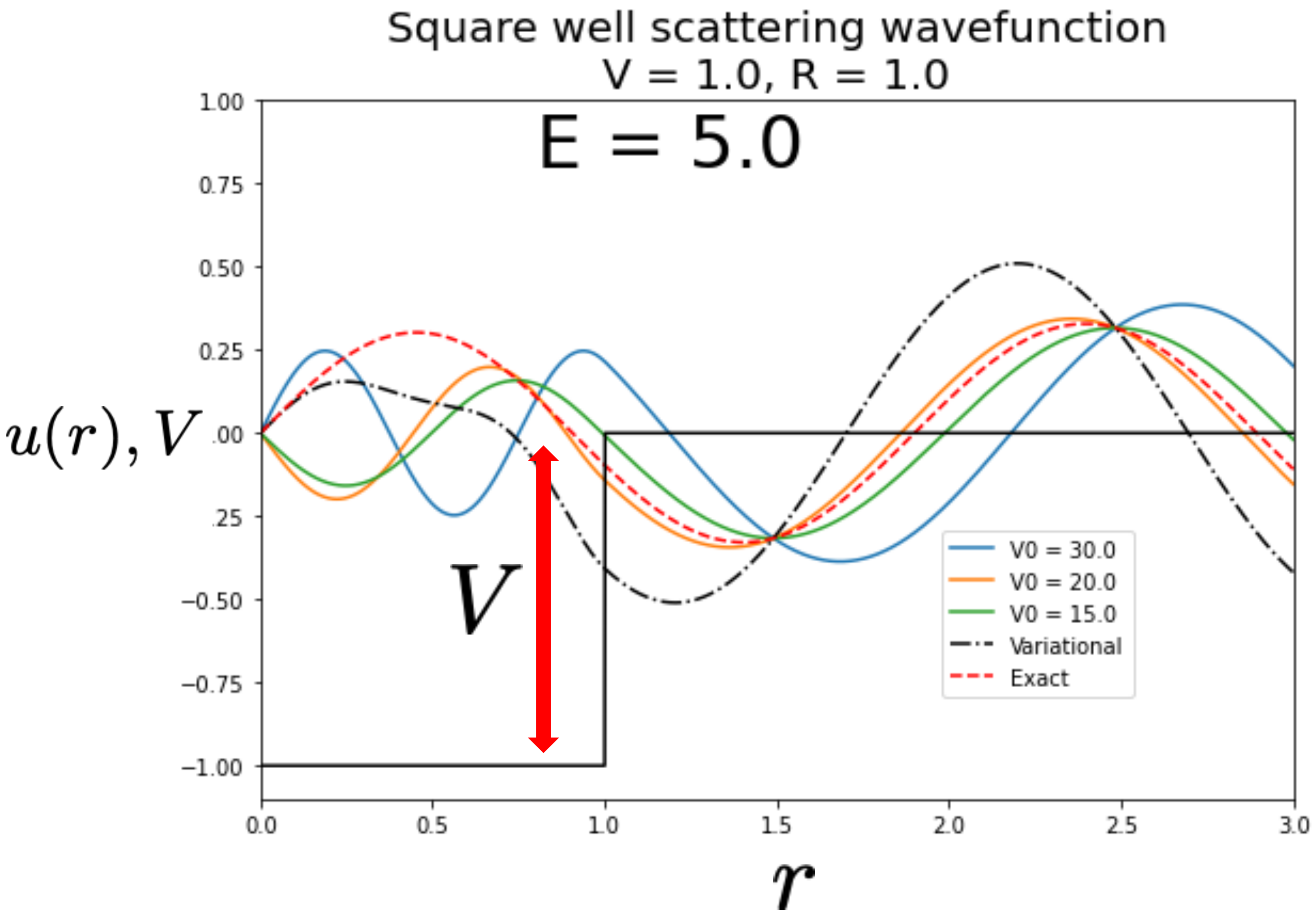
Square-well scattering states

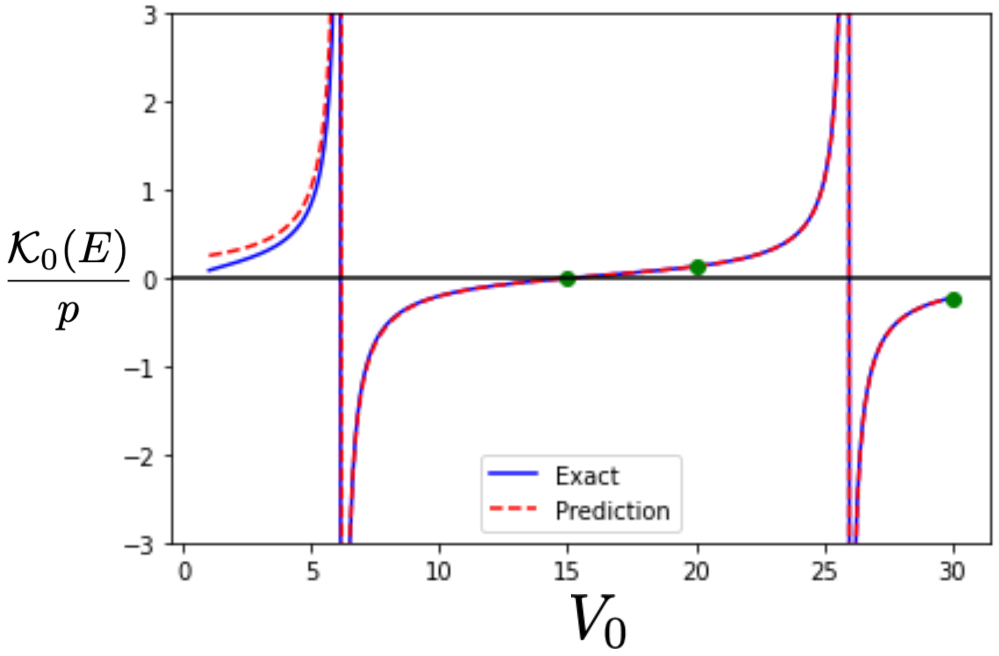


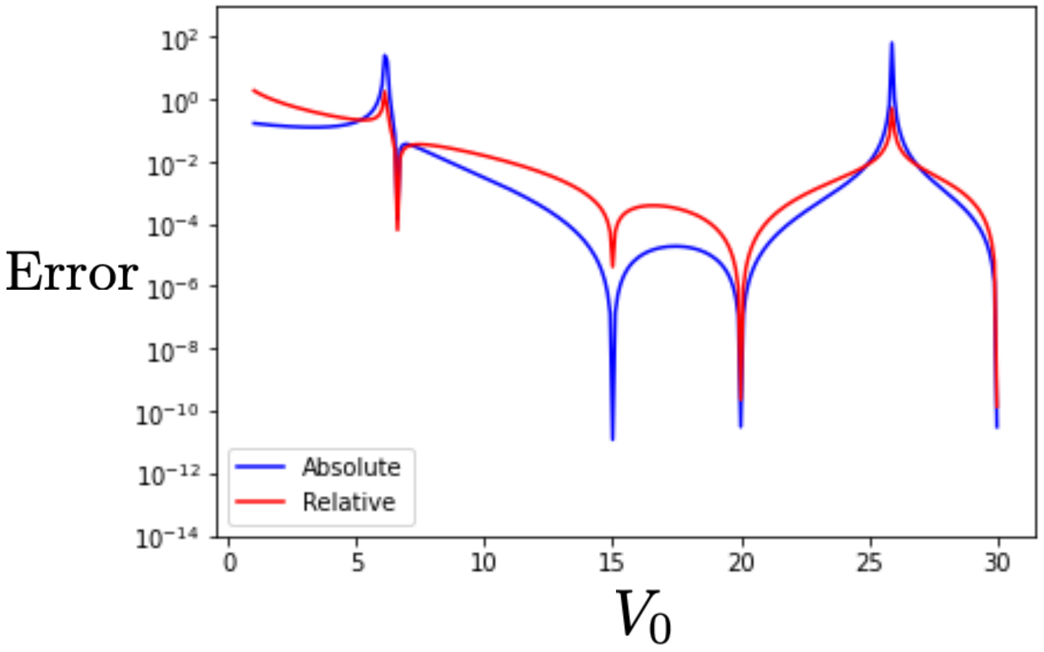




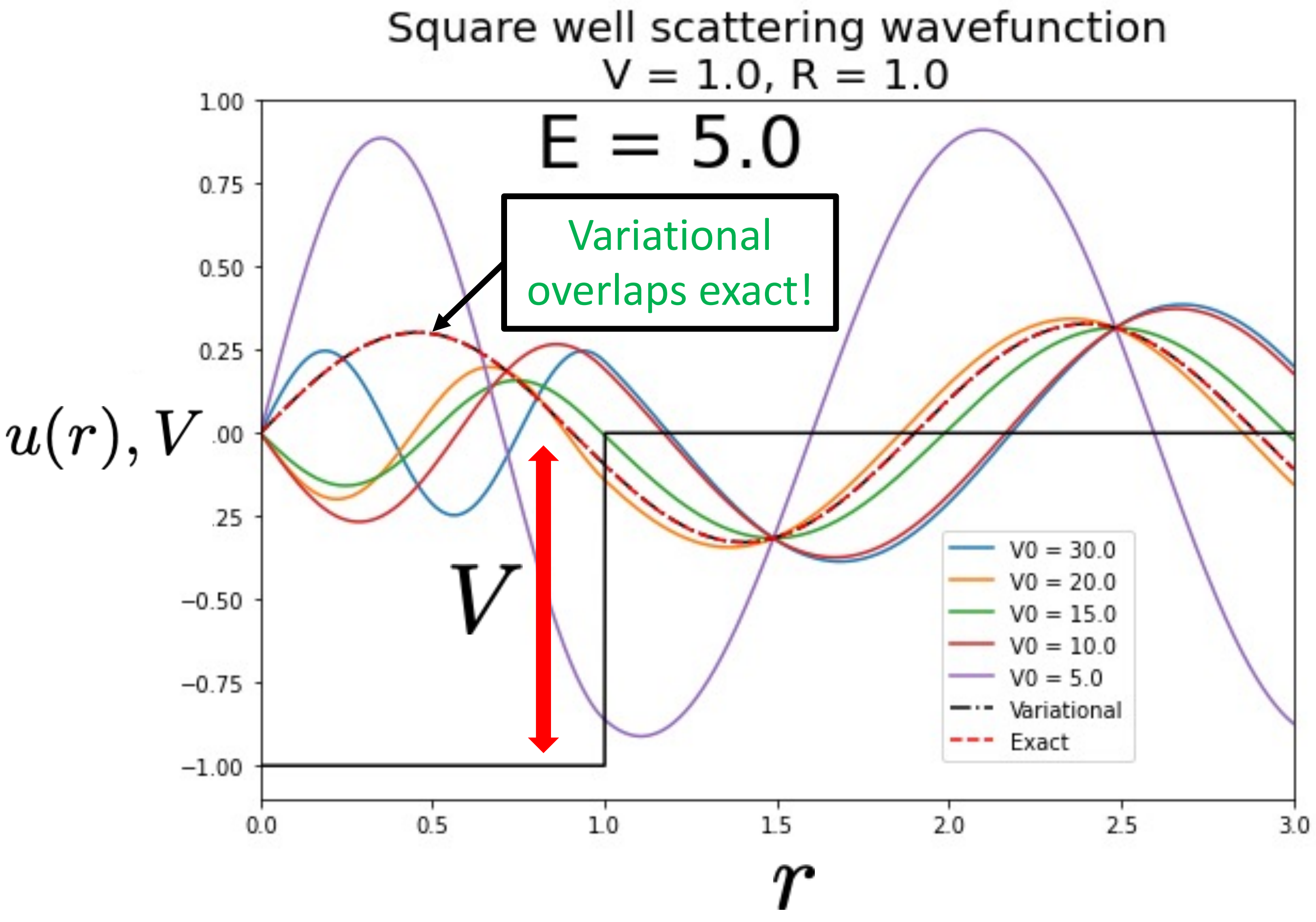
Square-well scattering states

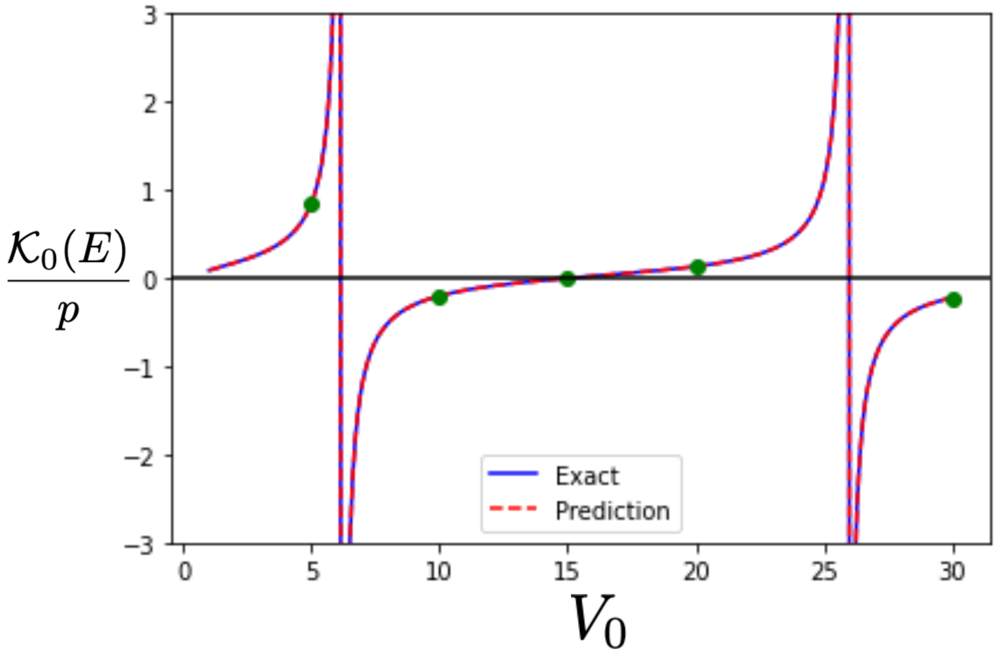


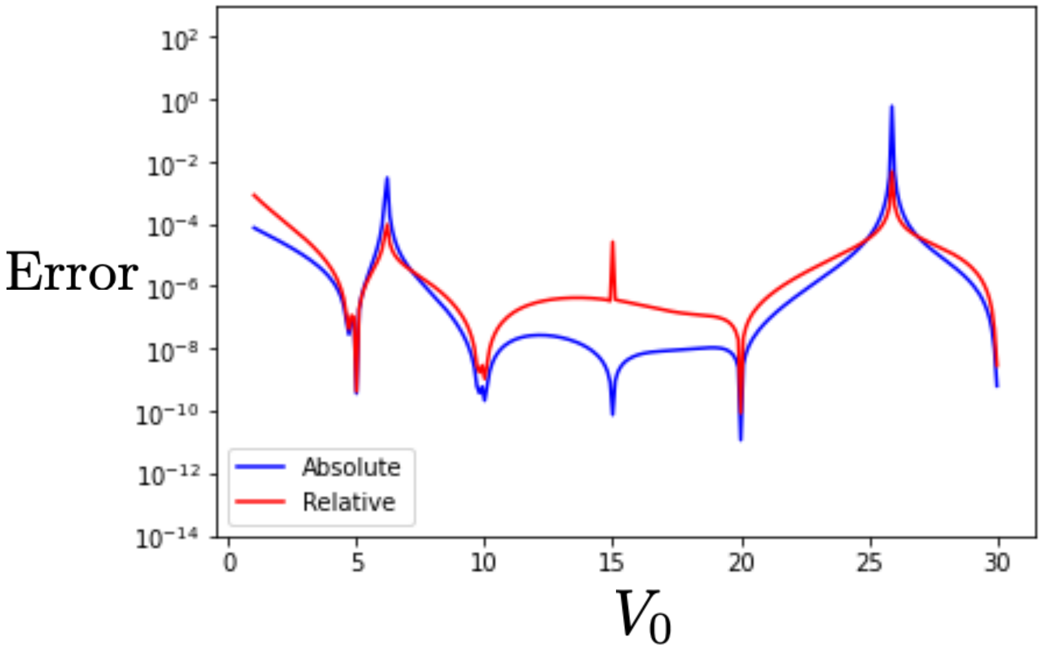




Square-well scattering states







Encountered issues

- The basis gets close to being linearly dependent with increased size causing the condition number to grow
- Leads to the matrix becoming ill-conditioned
  - Option 1: Regularize using a "nugget"

$$\Delta\tilde{U}^{-1} = \left(\Delta\tilde{U} + \lambda \boldsymbol{I}\right)^{-1} \rightarrow \lambda \approx 10^{-9}$$

Empirically chosen

  - Option 2: Use Moore-Penrose pseudo-inverse

- Kohn anomalous singularities:
  - Unphysical singularities
  - Characterized by spikes in graphs at isolated energies
  - Move around with different basis size → easy to mitigate by adding more elements to the basis

Extensions

- Nucleon-nucleon scattering:
  - Minnesota potential
  - No Coulomb interaction or coupled channels

- p-α scattering in $S_{1/2}$ and $P_{3/2}$ channels:
  - Coulomb + non-local potential
  - Different asymptotic behavior of scattering wave function when including Coulomb interaction

$$u_{\ell,E}^{(i)}(r) \xrightarrow[r\to\infty]{} \frac{1}{p} F_\ell(\eta, pr) + \tau G_\ell(\eta, pr)$$

- α- ^{208}Pb low energy scattering:
  - Wood-Saxon optical potential

Results in later talk!

Summary

- EC emulators are numerically efficient and accurate in various two-body scattering problems (more details in later talk)
- Extensions to Nd scattering and NN potential fitting to NN energy energy spectra from Lattice QCD calculations

Ongoing work

- Scattering in momentum space:
  - EC application to chiral EFT
- Coupled channels:
  - Apply EC in coordinate and momentum space
- Three-body systems

Thank you!