Pseudopotentials for cold atoms

Pascal Bugnion, Gareth Conduit and Richard Needs

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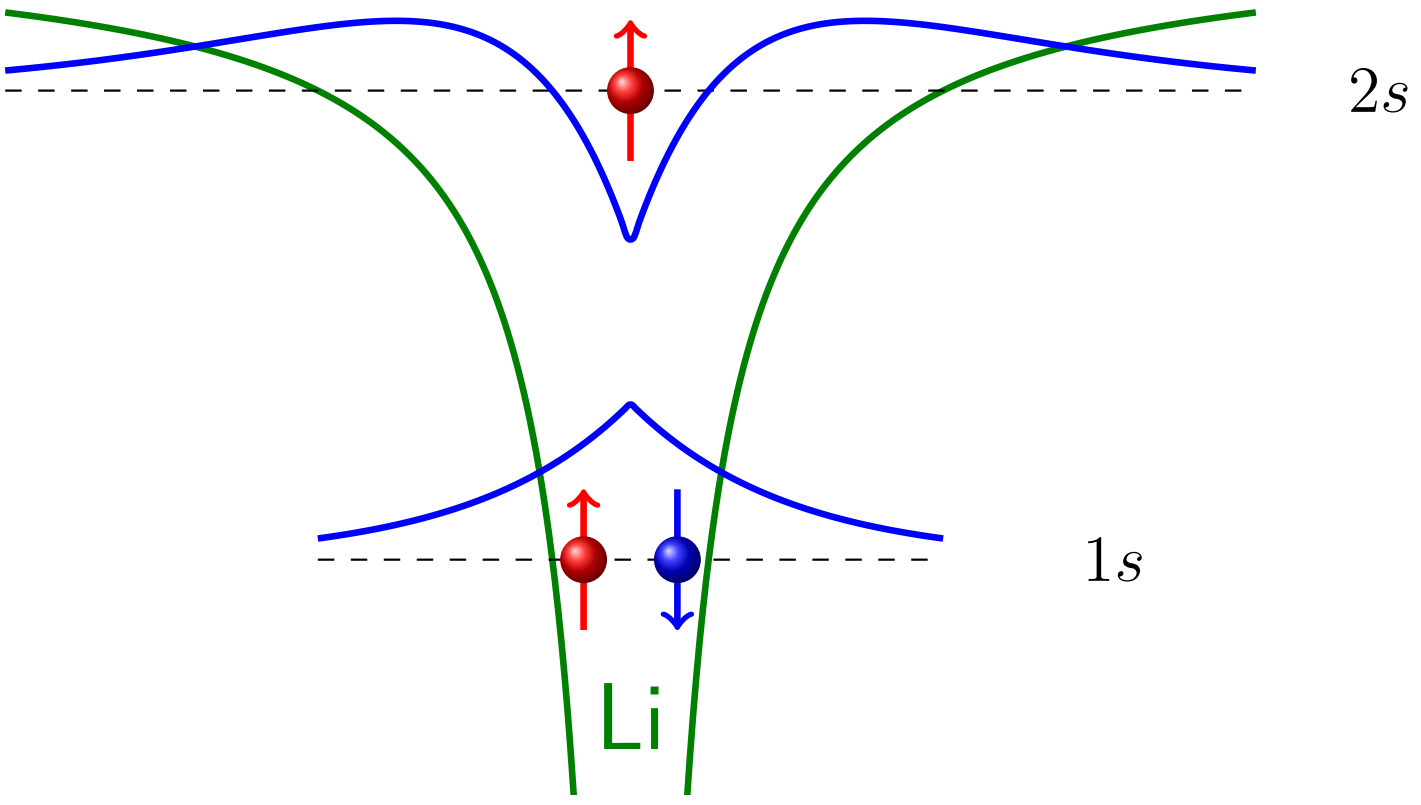
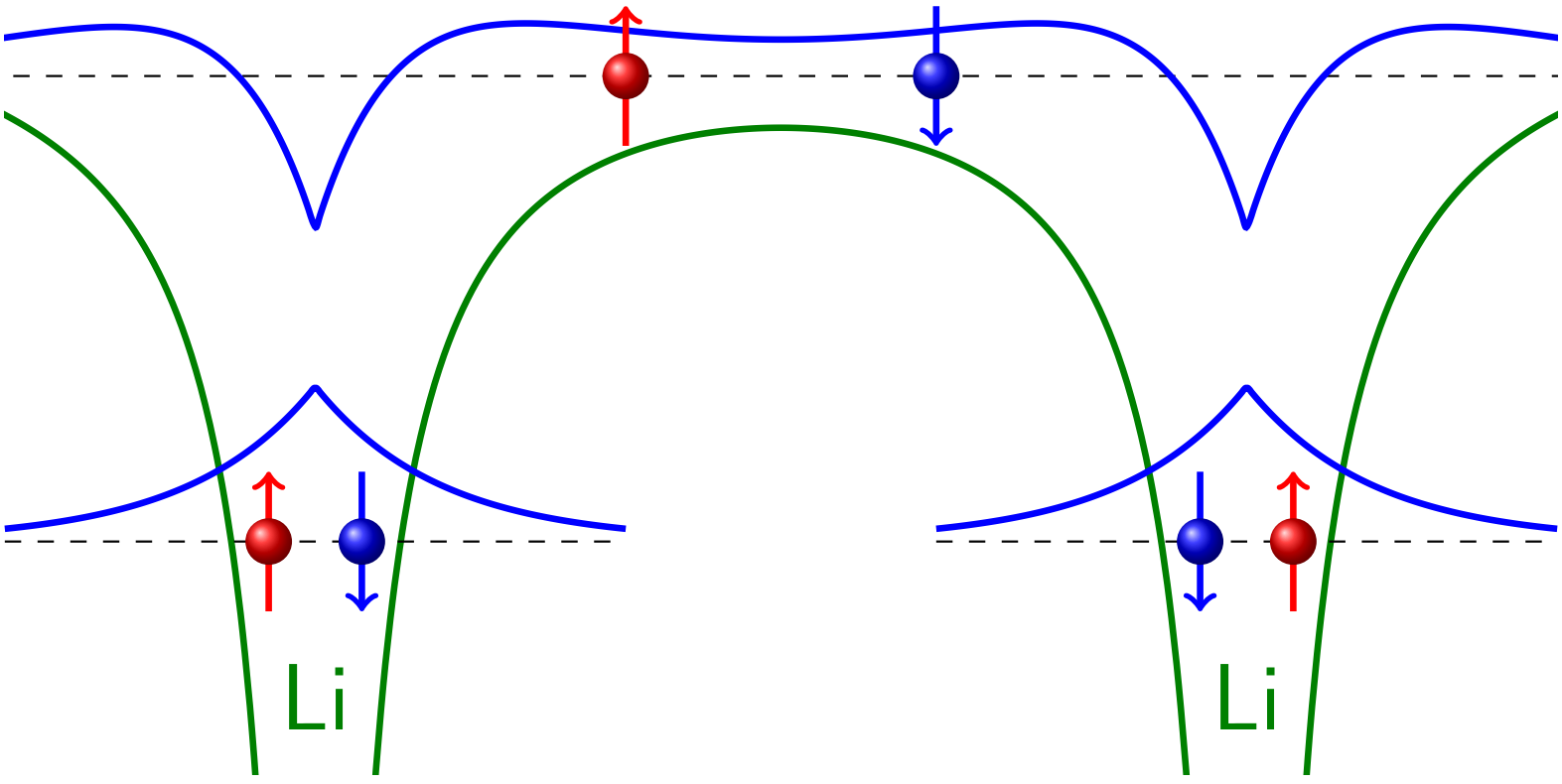
Pseudopotentials 101



Pseudopotentials 101



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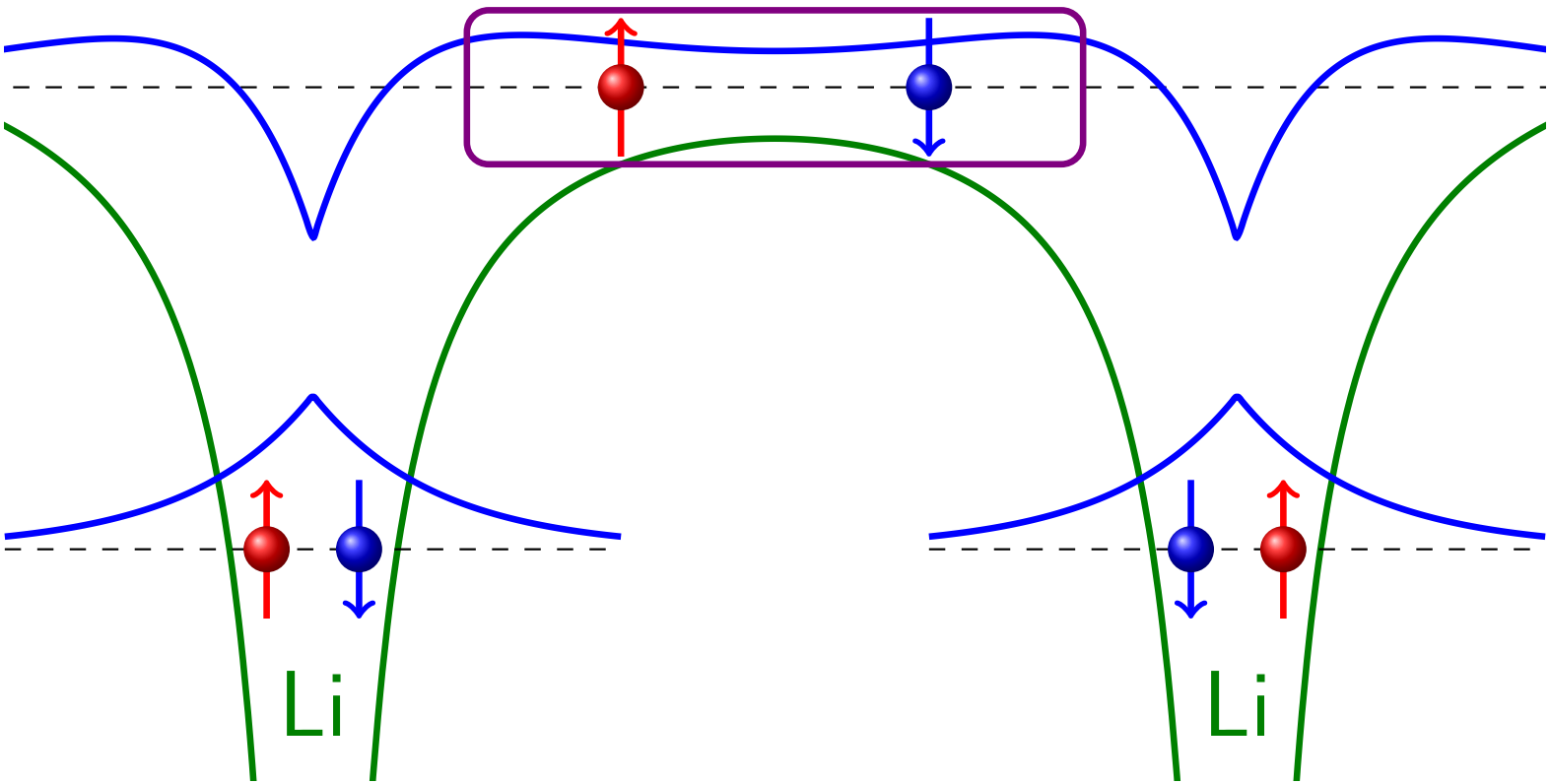

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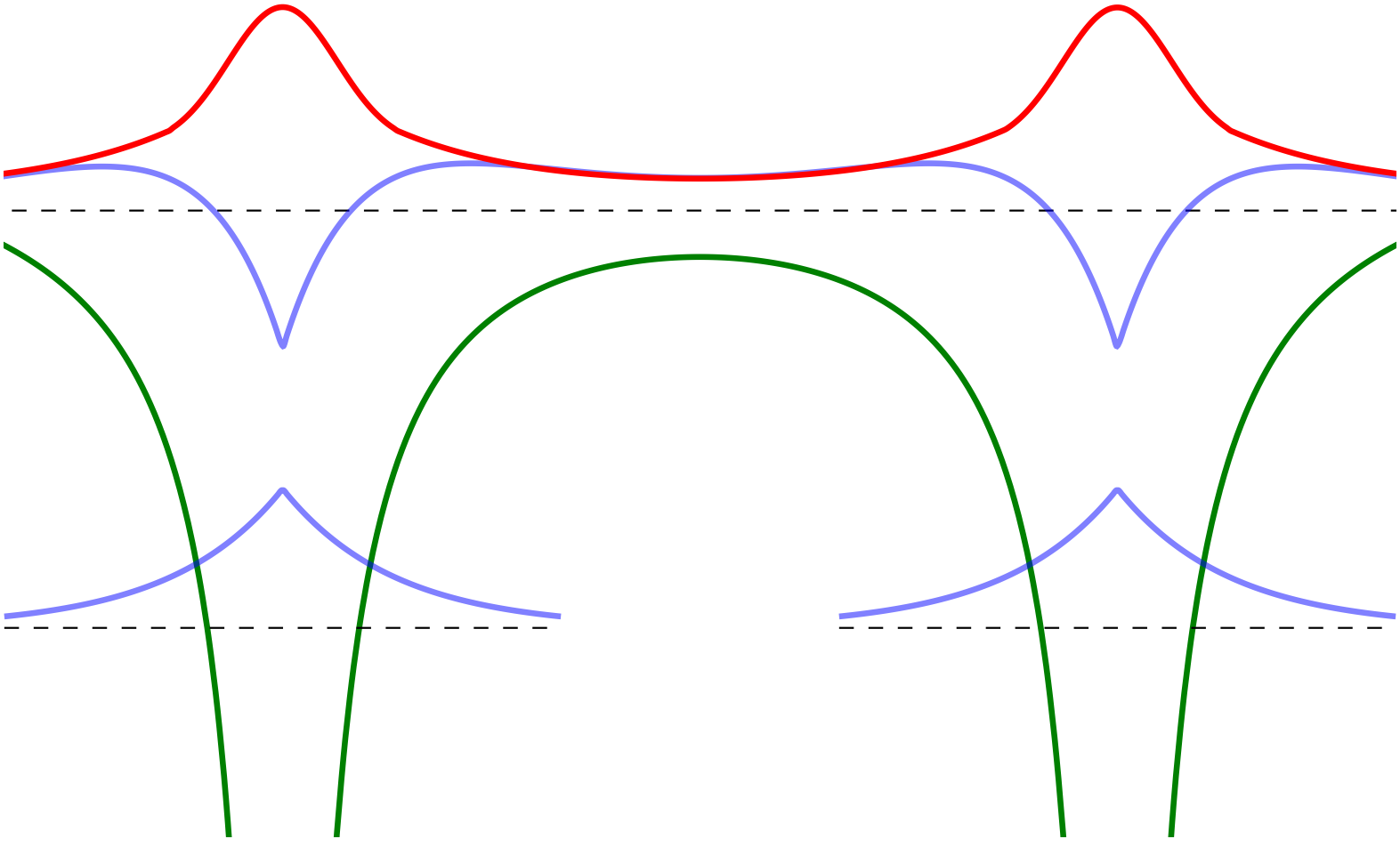

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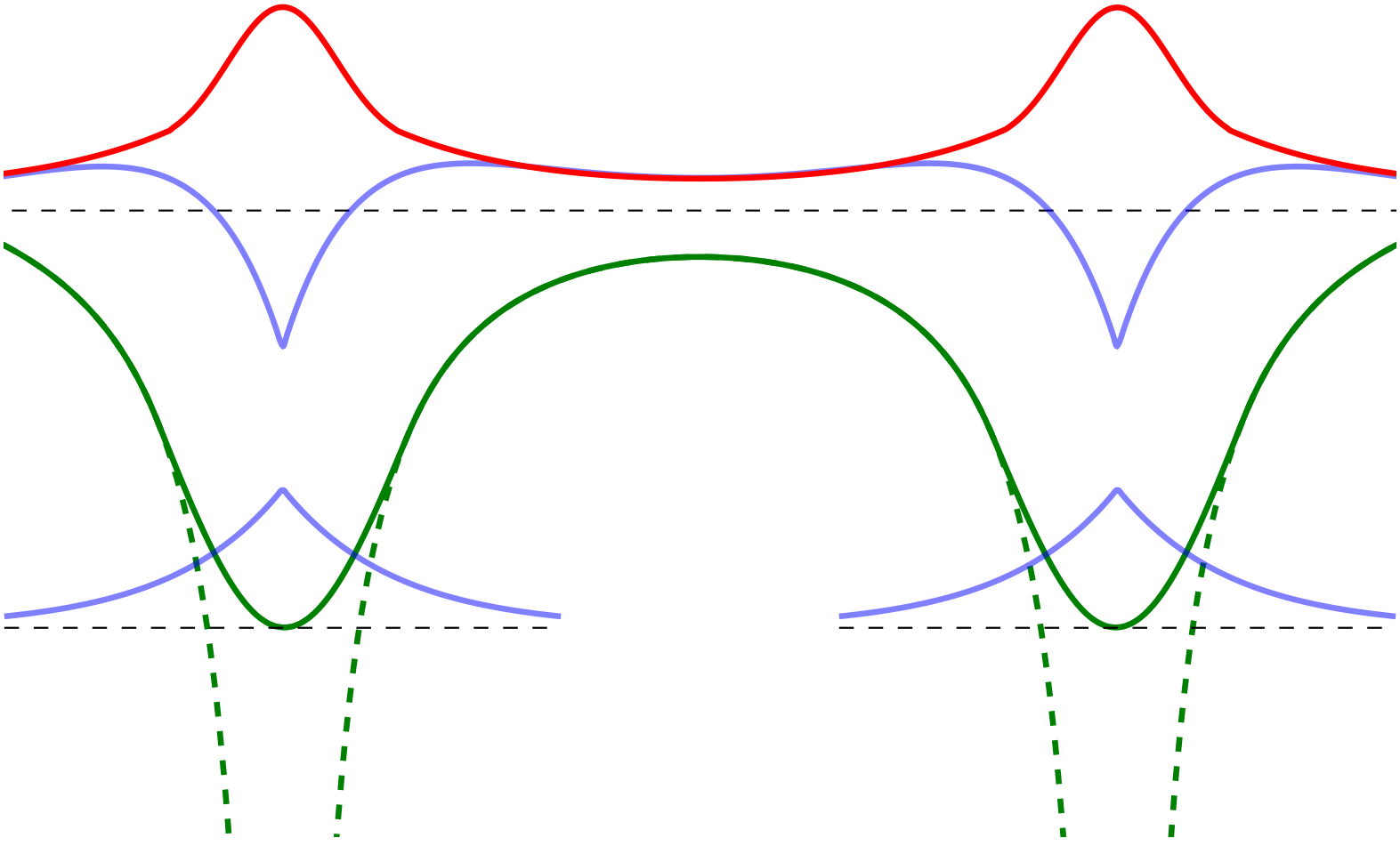
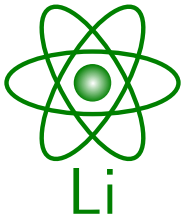


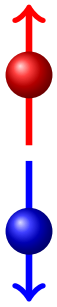
Why cold atoms?

Simulate complex many body systems that are often difficult to observe in the solid state.



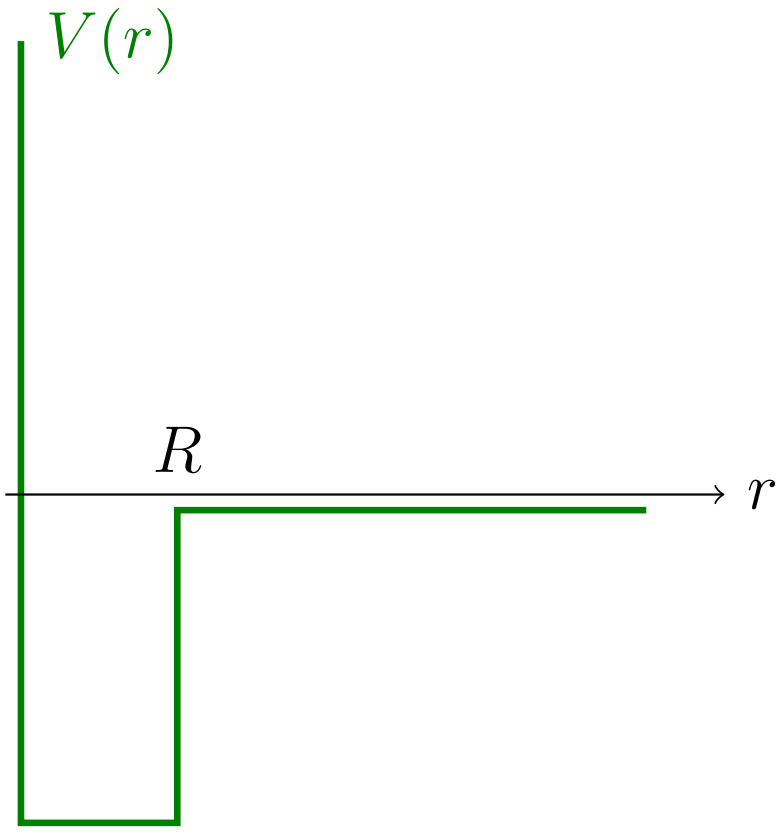
$$|F = 1/2, m_F = 1/2\rangle \longrightarrow$$

$$|F = 1/2, m_F = -1/2\rangle \longrightarrow$$



The inter-atom interactions can be tuned by changing an external magnetic field.

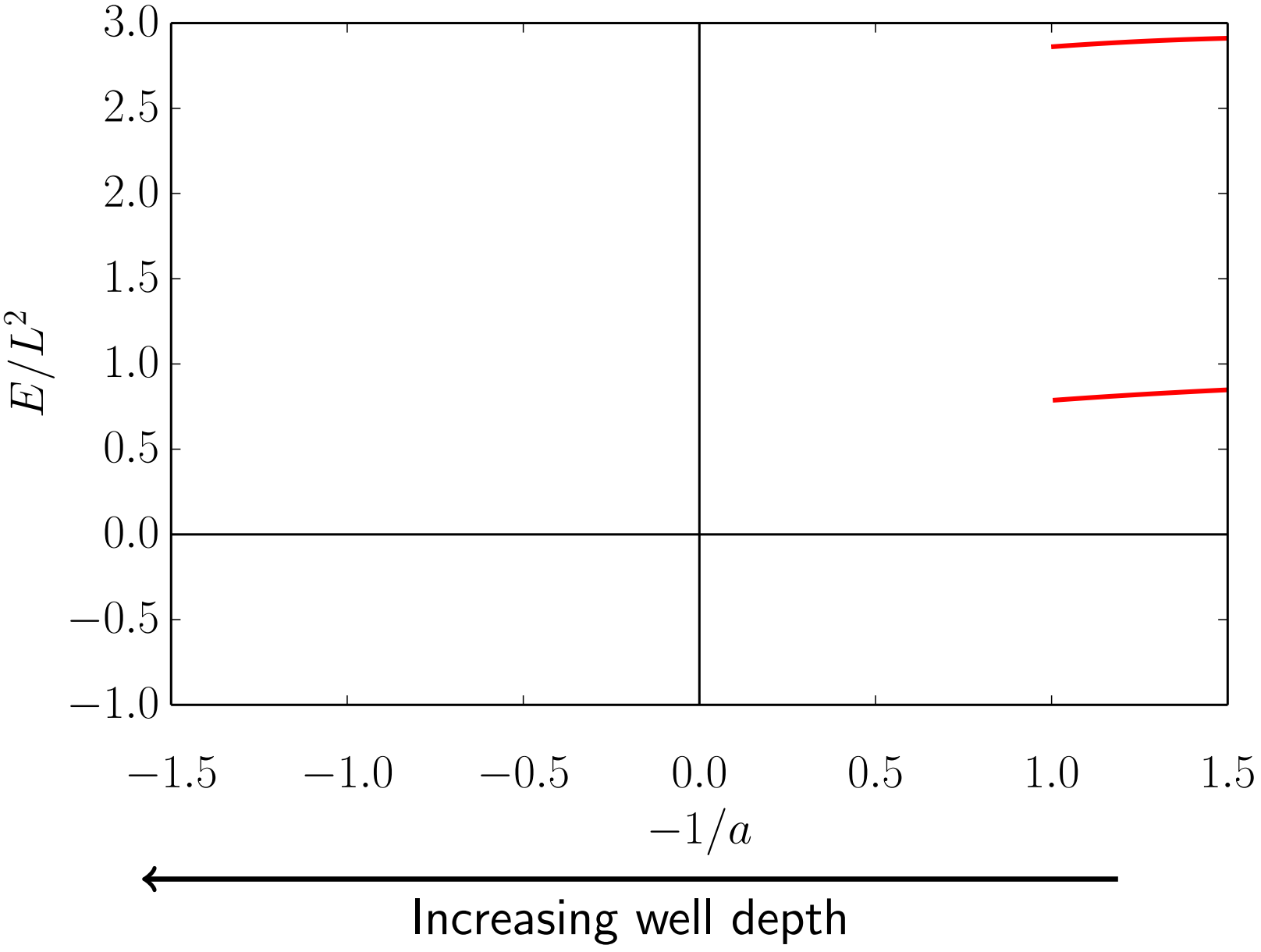
Inter-atomic potential



$$V(r) = \lim_{R \to 0} \begin{cases} -V_0 & r \leqslant R \\ 0 & \text{otherwise} \end{cases}$$

$$V_0 R^3 = \text{const.}$$

Inter-atomic potential



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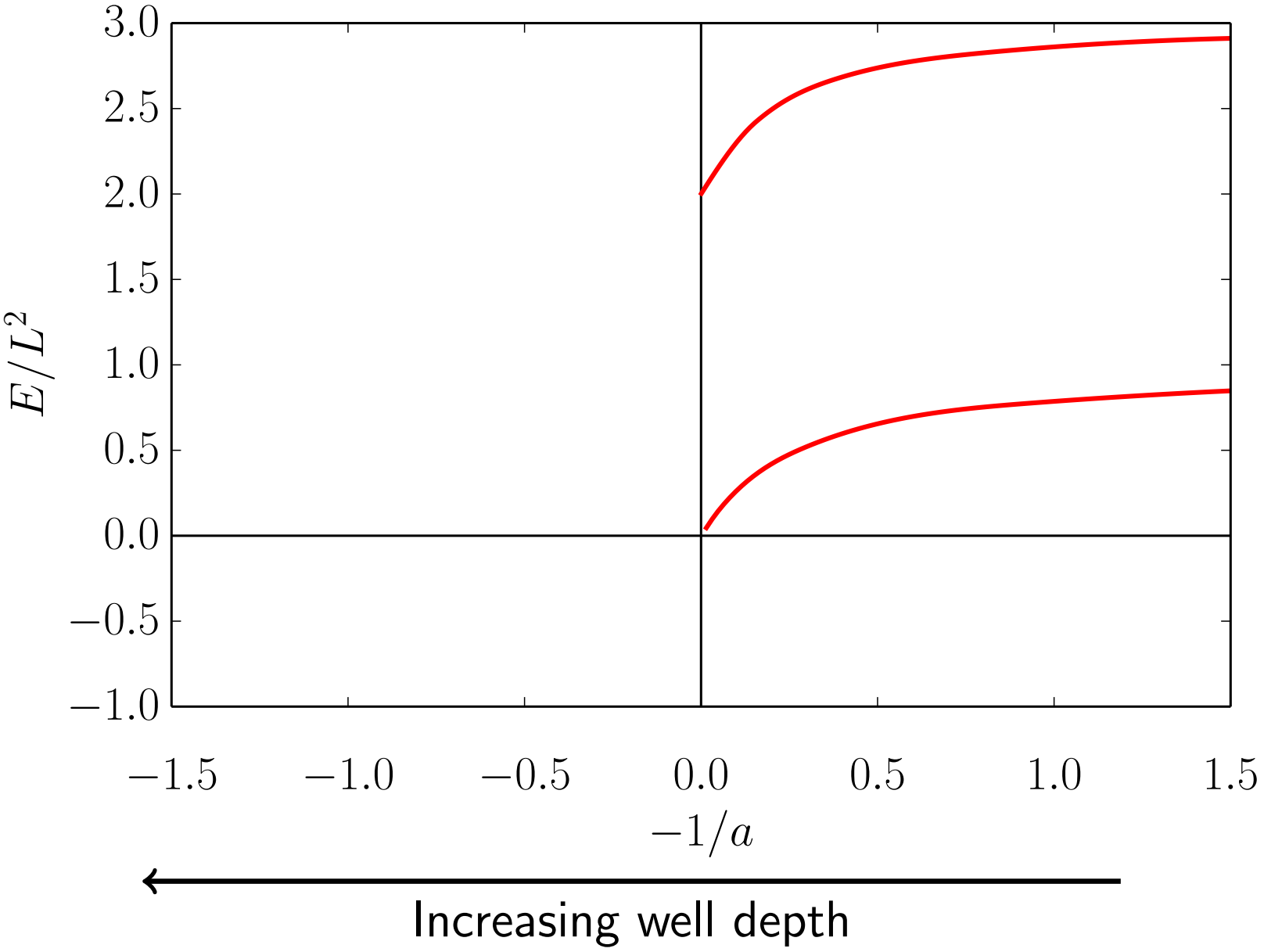

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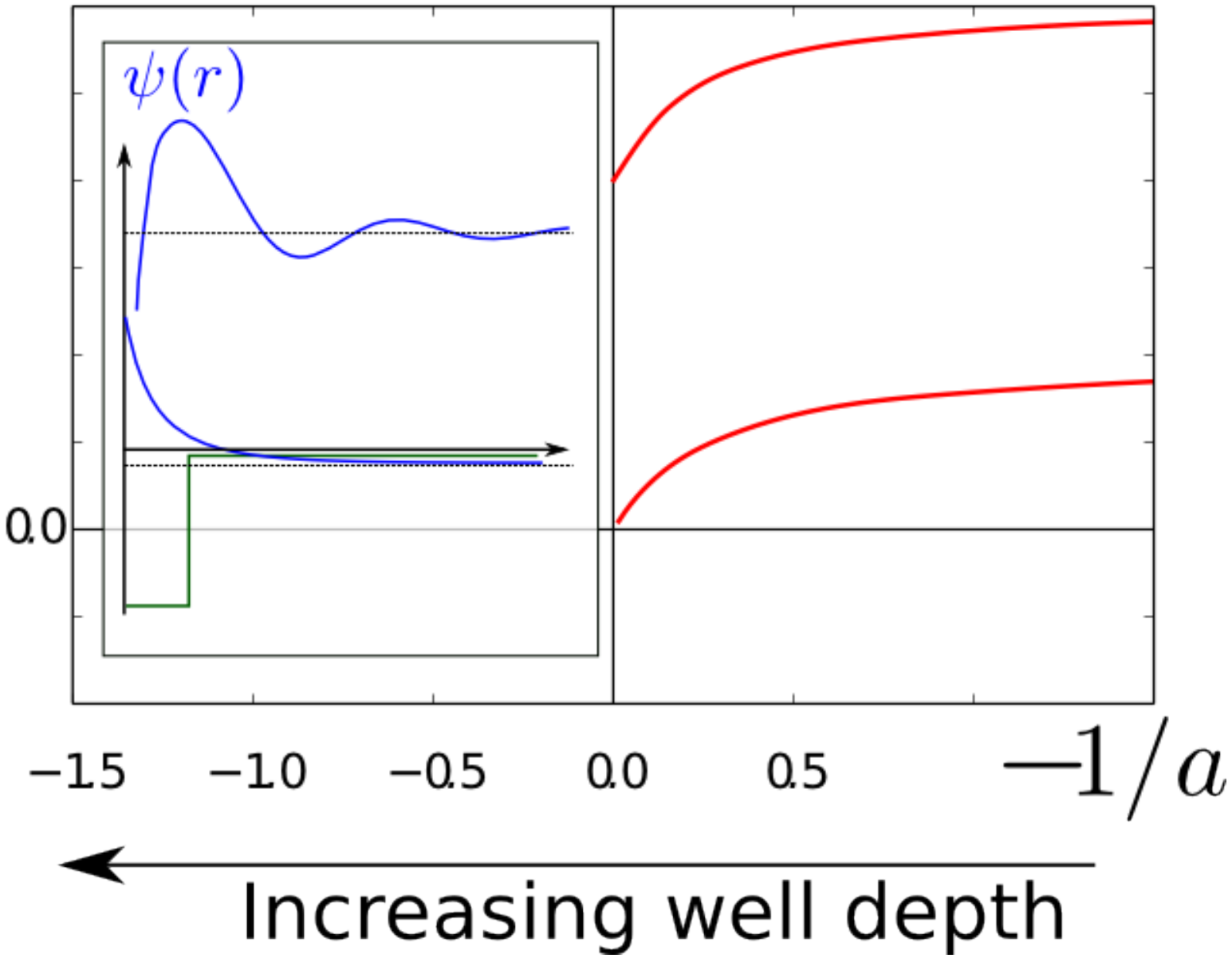

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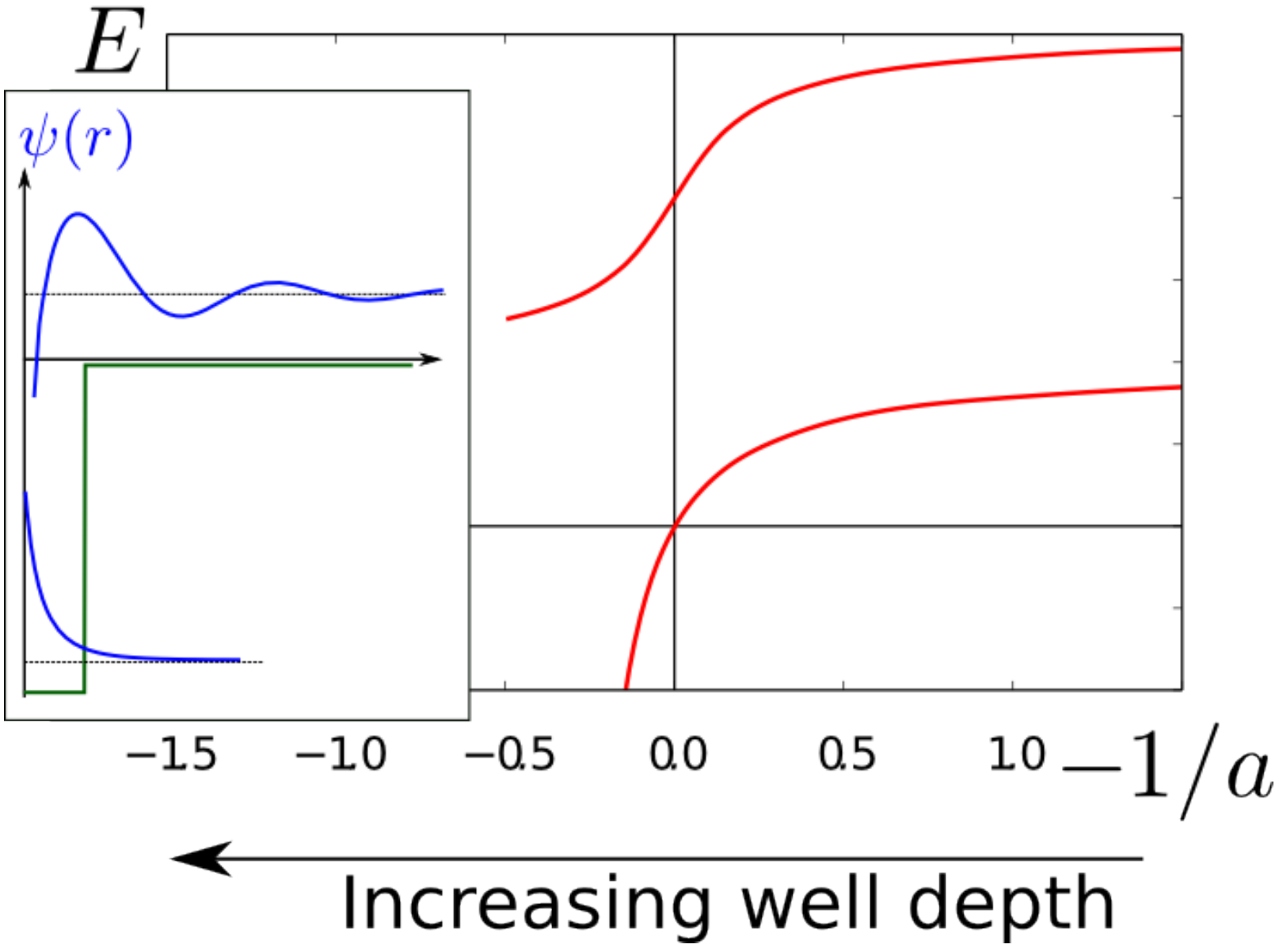

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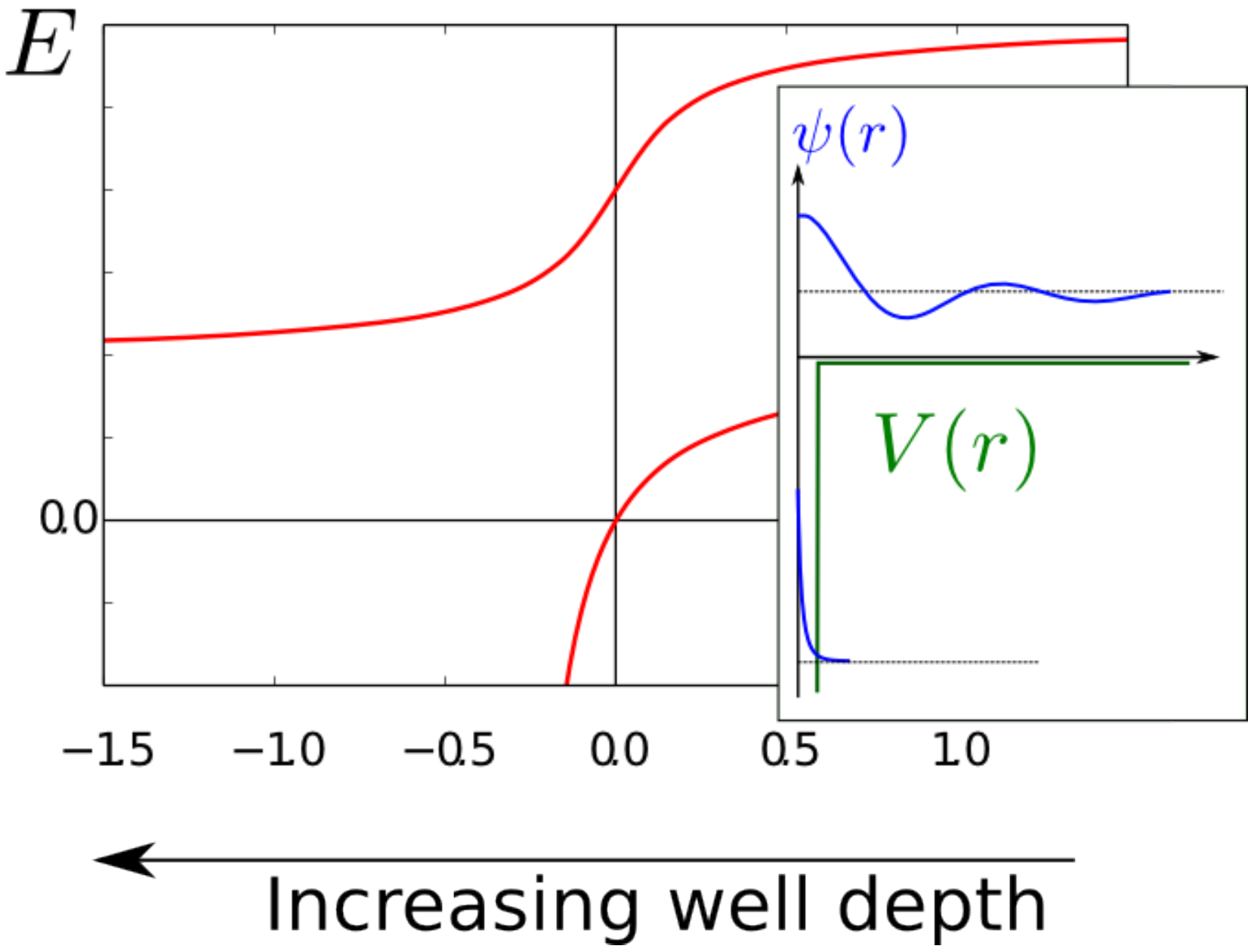

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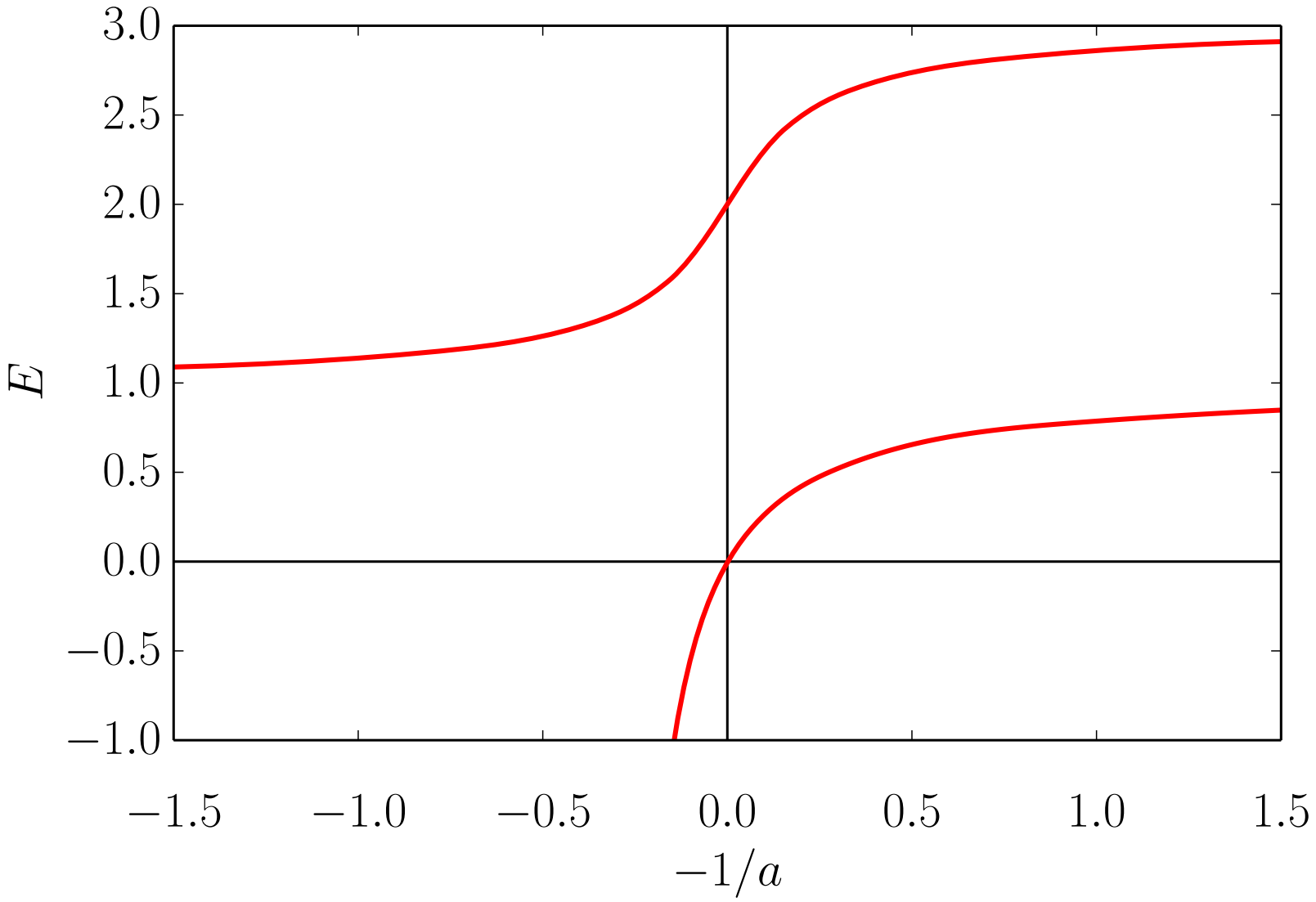
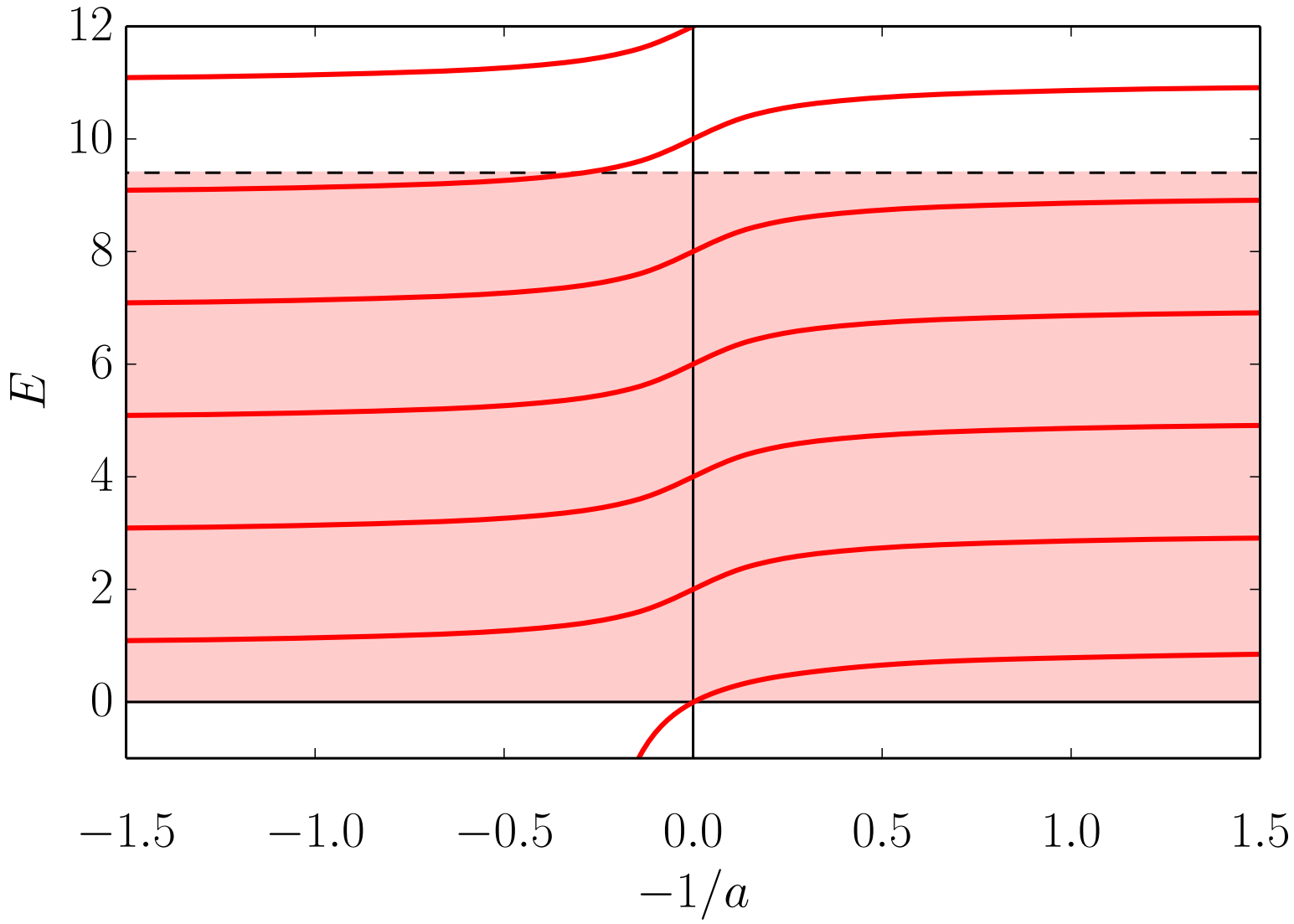


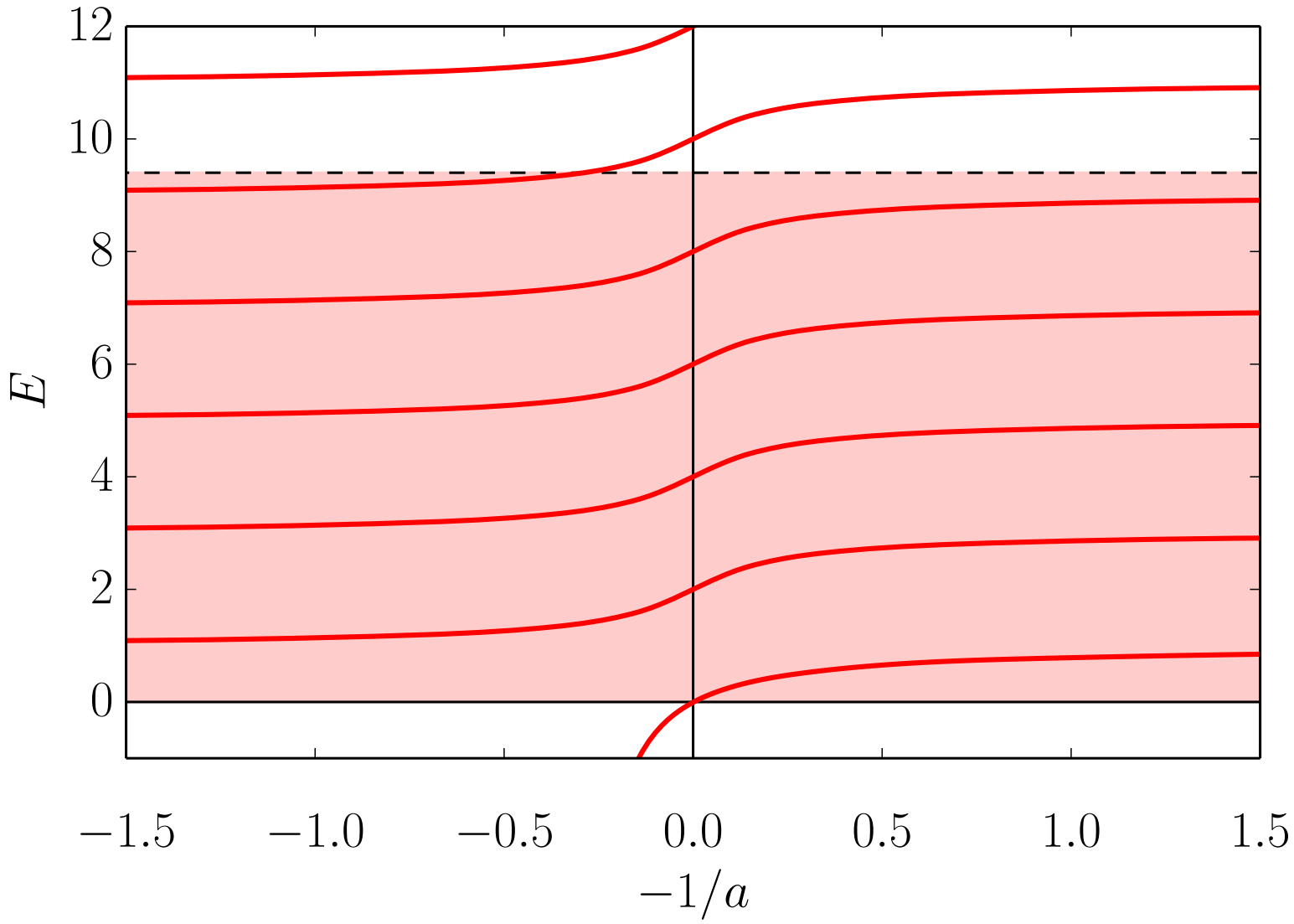
Pseudopotential requirements



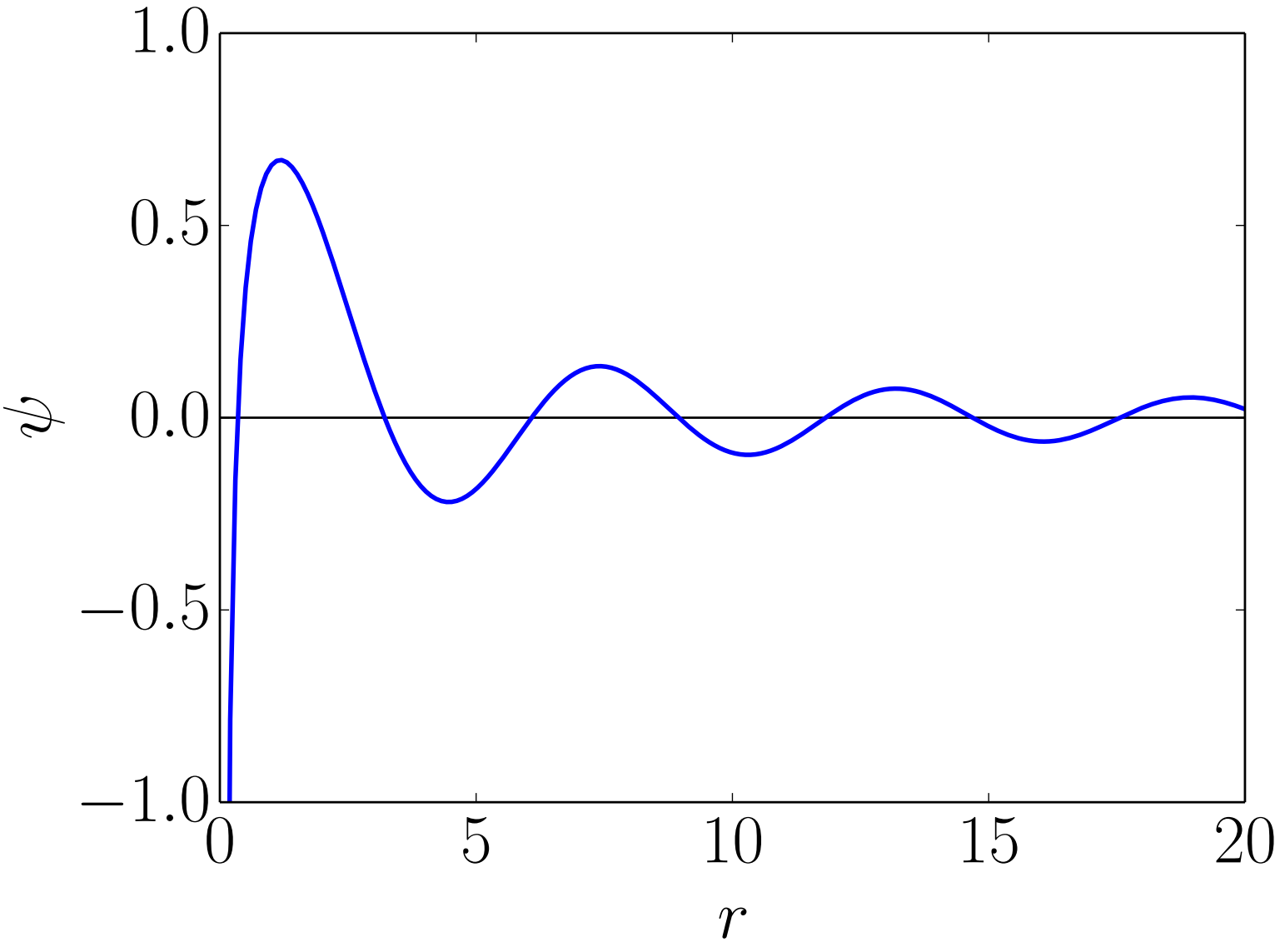
Building the pseudopotential

N. Trouiller and J.L Martins, *Efficient pseudopotentials for plane wave calculations*, PRB **43**, 1993 (1991)

Pseudopotential requirements



Building the pseudo-wavefunction



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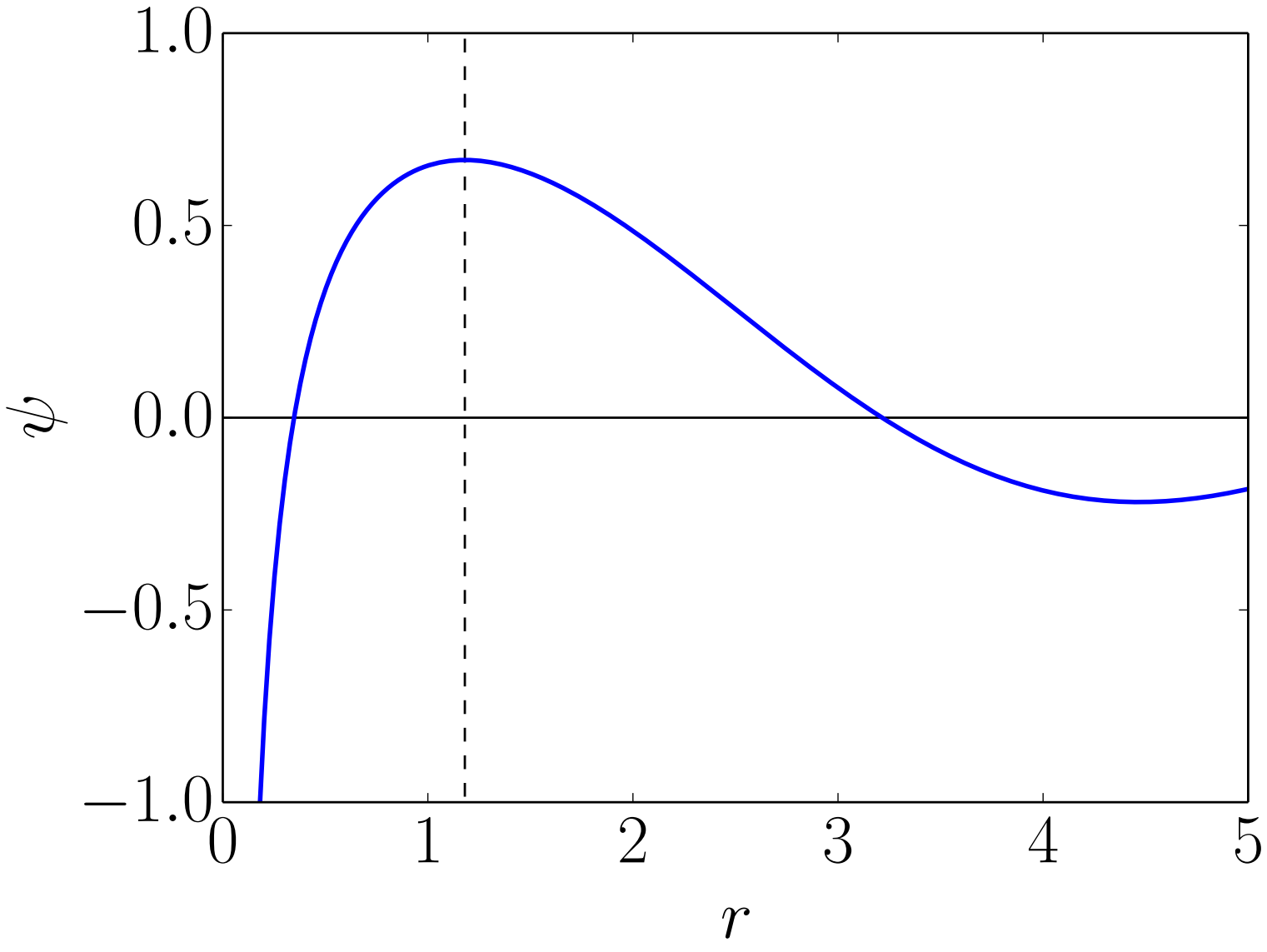
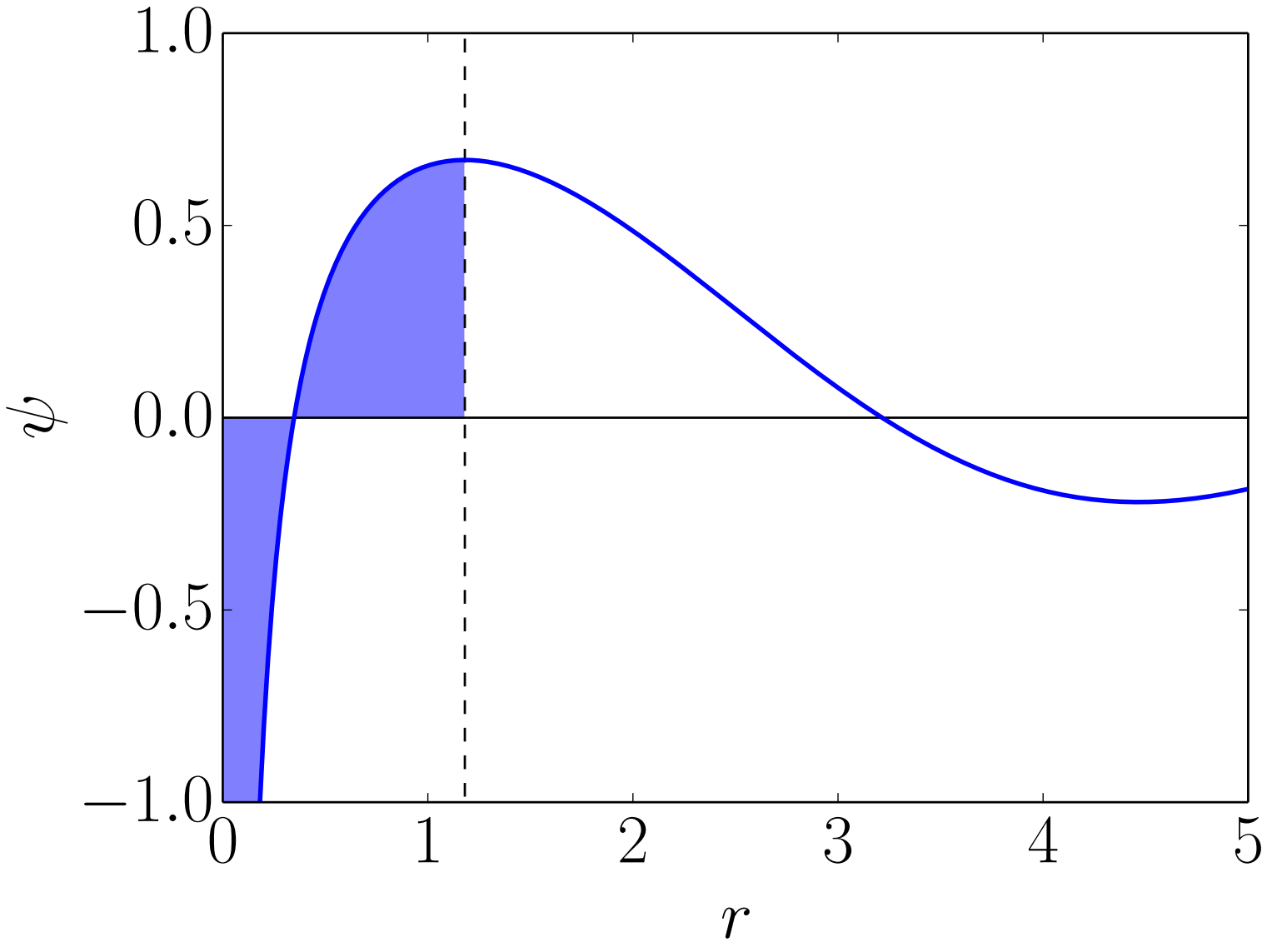


Norm conservation

$$\left.\frac{\partial \tan(\delta_{PP})}{\partial E}\right|_{r=c} = \left.\frac{\partial \tan(\delta_{\text{true}})}{\partial E}\right|_{r=c}$$

Norm conservation



Building the pseudo-wavefunction

- Norm conservation
- The pseudo-wavefunction must join smoothly onto the wavefunction at the cutoff: at least two derivatives must match.

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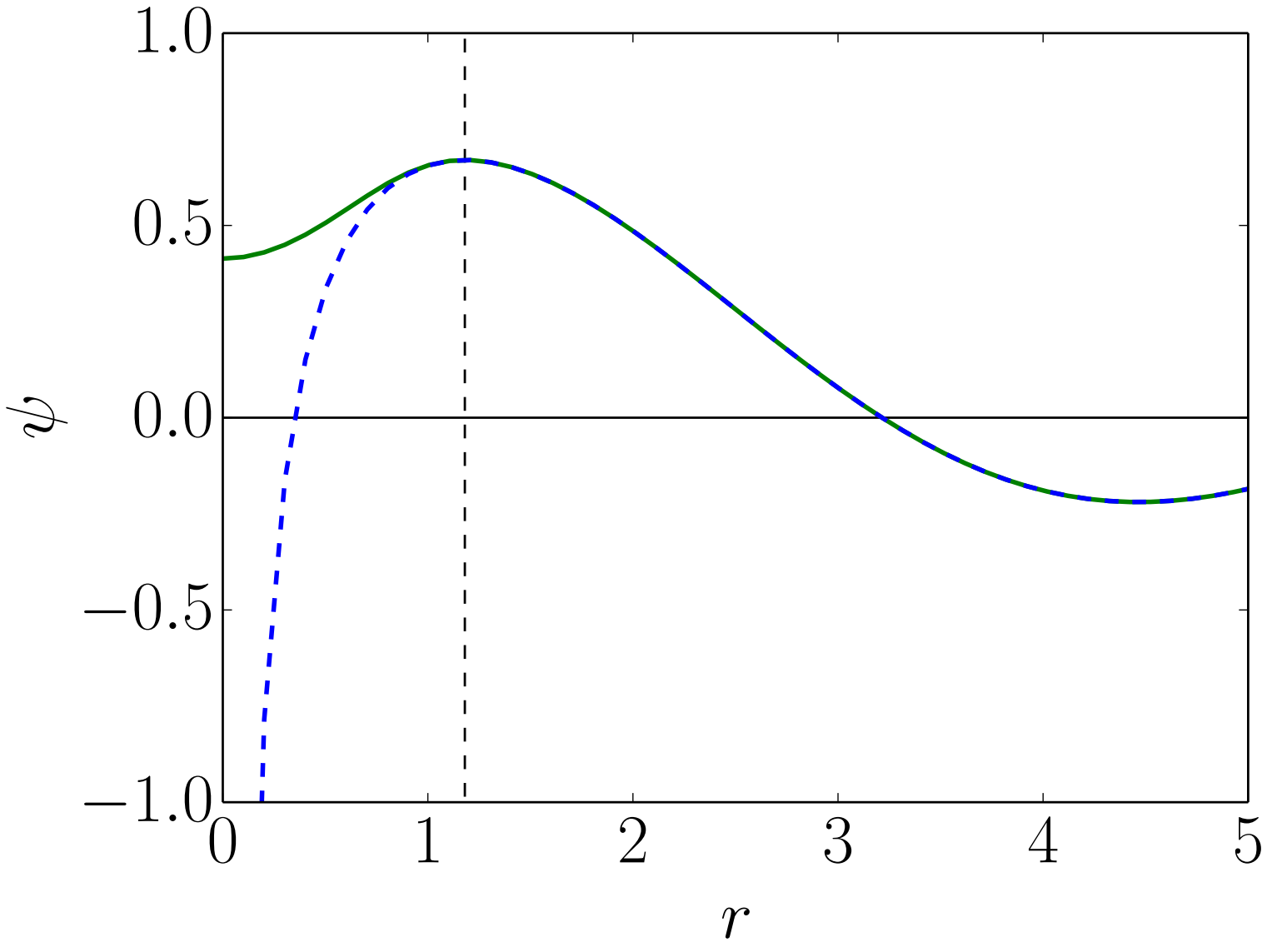
Functional form of the pseudo-wavefunction

$$\psi_{PP} = \begin{cases} e^{p(r)} & r \leqslant c \\ \psi_{\text{true}} & r > c \end{cases}$$

$$p(r) = a_0 + a_2 r^2 + a_4 r^4 + \sum_{i=6} a_i r^i$$

Building the pseudo-wavefunction

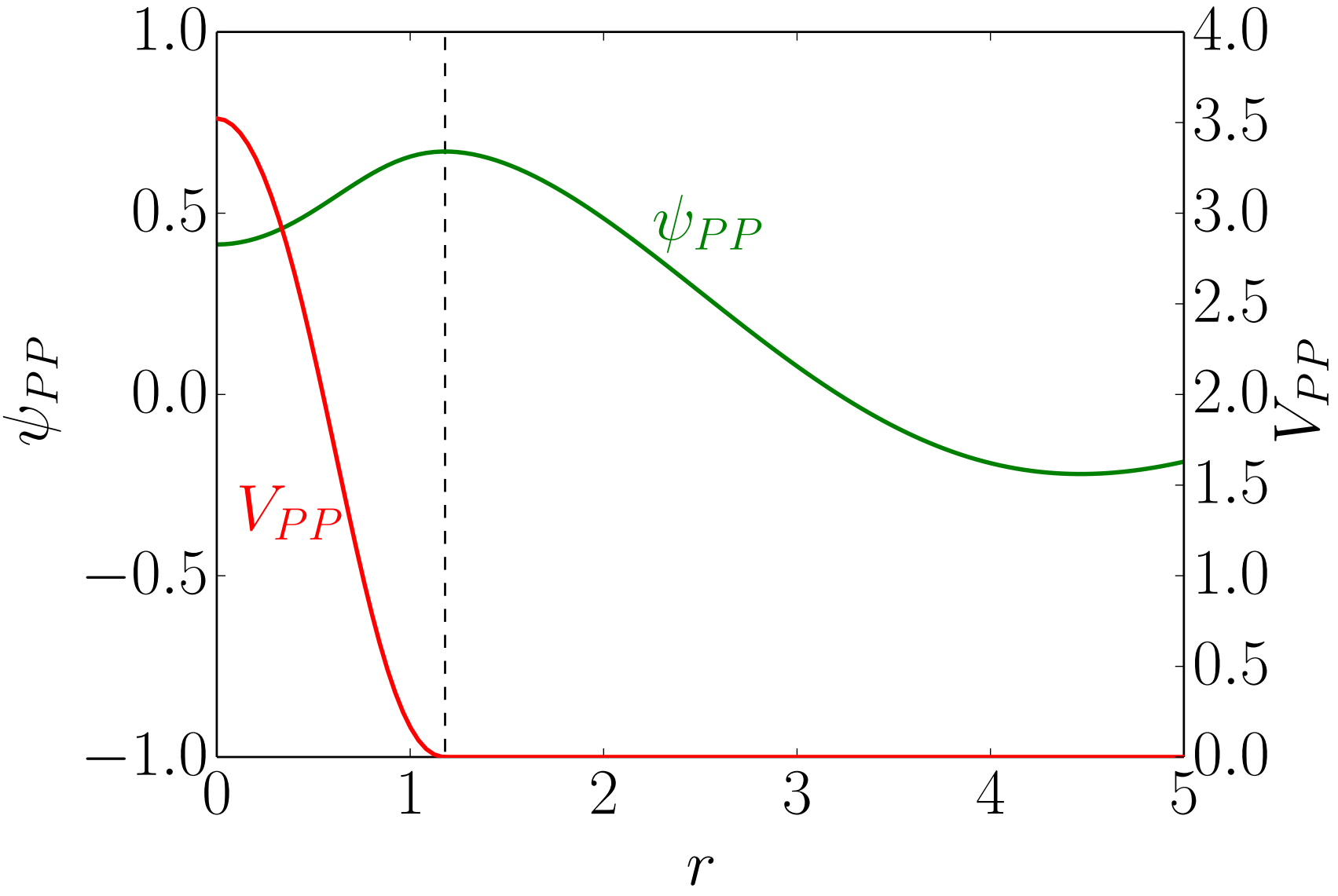


Building the pseudopotential

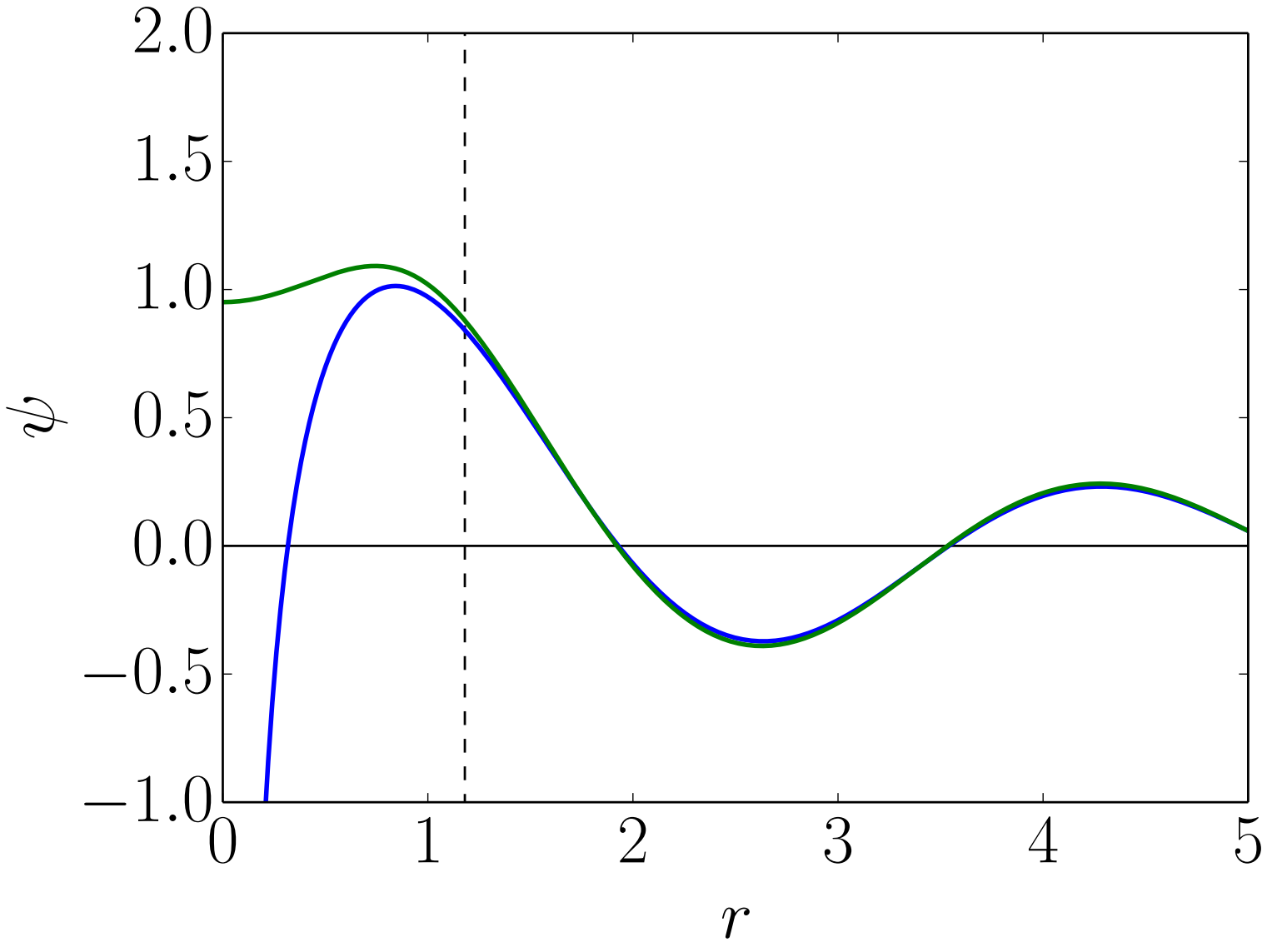
Invert the Schrödinger equation

$$V(r) = E + \frac{1}{2} \cdot \frac{\nabla^2 \psi}{\psi}$$

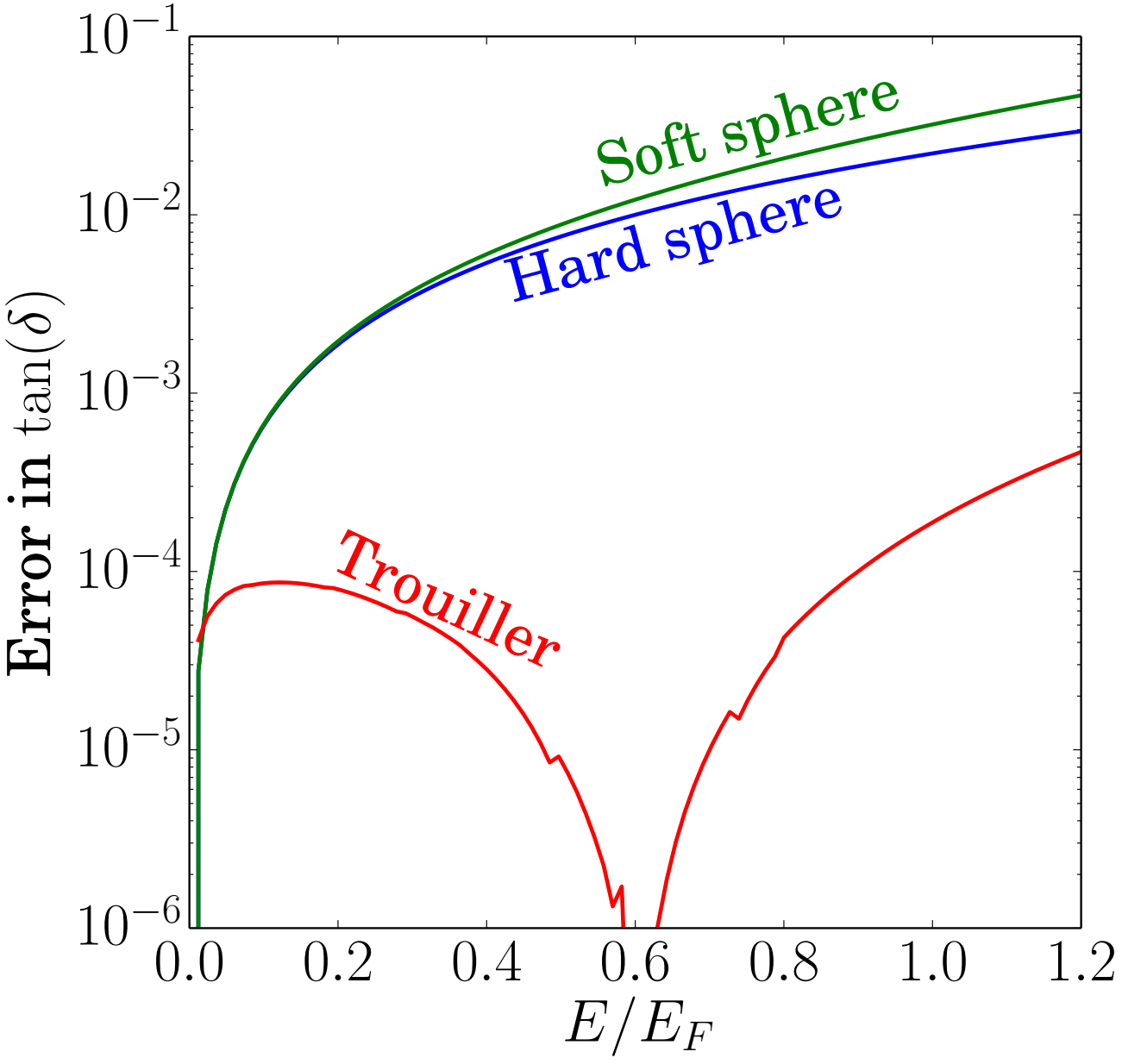
Building the pseudopotential



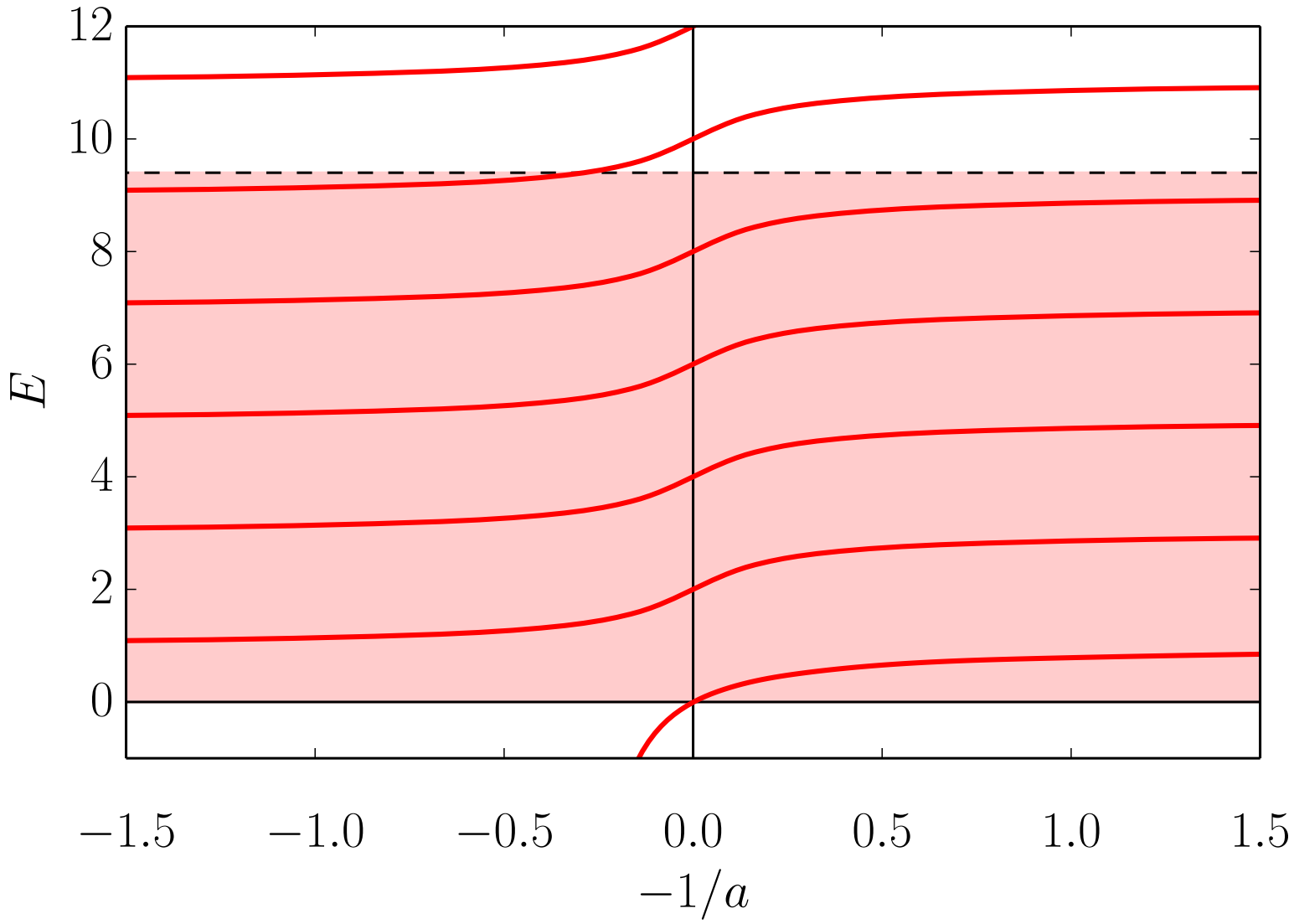
Breaking the pseudopotential: $E = 2E_F$



Phase shifts



Pseudopotentials++



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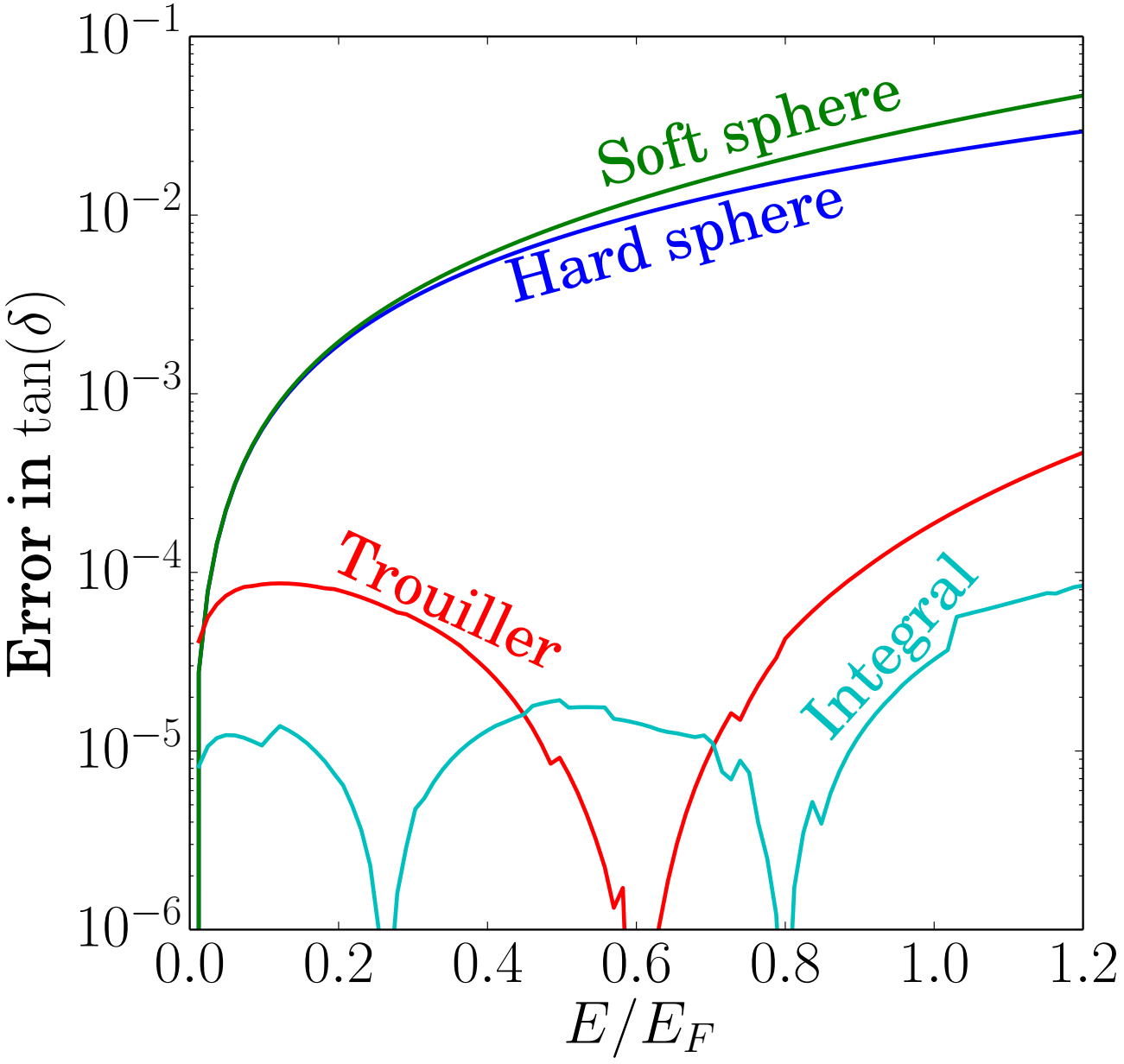

Applications

Ferromagnetism

We expect itinerant ferromagnetism to appear at sufficiently strong interactions.

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p-wave superconductivity

It is postulated that same-spin atoms feel a weak effective attraction.

Like-spin atoms may therefore form Cooper pairs.

Conclusion

- A good repulsive pseudopotential is necessary to model ultracold atomic gases at positive scattering length.

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- There is a lot of useful pseudopotential lore in the electronic structure literature.
- New pseudopotentials offer unprecedented opportunities to model exotic phenomena.