Pseudoψence

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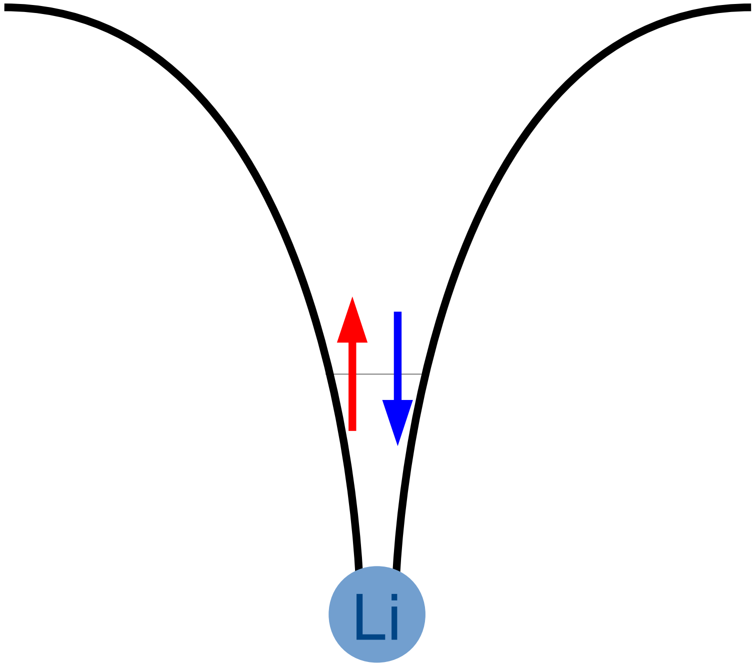
Evaluating the energy

$$
\begin{aligned}
E = \int \hat{KE}\, \bar{\psi}_{\vec{r}}\, \psi_{\vec{r}} \\
+ V_{\text{e-i}}(\vec{r} - \vec{r}\,')\, n_{\vec{r}\,'}\, \bar{\psi}_{\vec{r}}\, \psi_{\vec{r}} \\
+ V_{\text{e-e}}(\vec{r} - \vec{r}\,')\, \bar{\psi}_{\vec{r}}\, \bar{\psi}_{\vec{r}\,'}\, \psi_{\vec{r}\,'}\, \psi_{\vec{r}}
\end{aligned}
$$

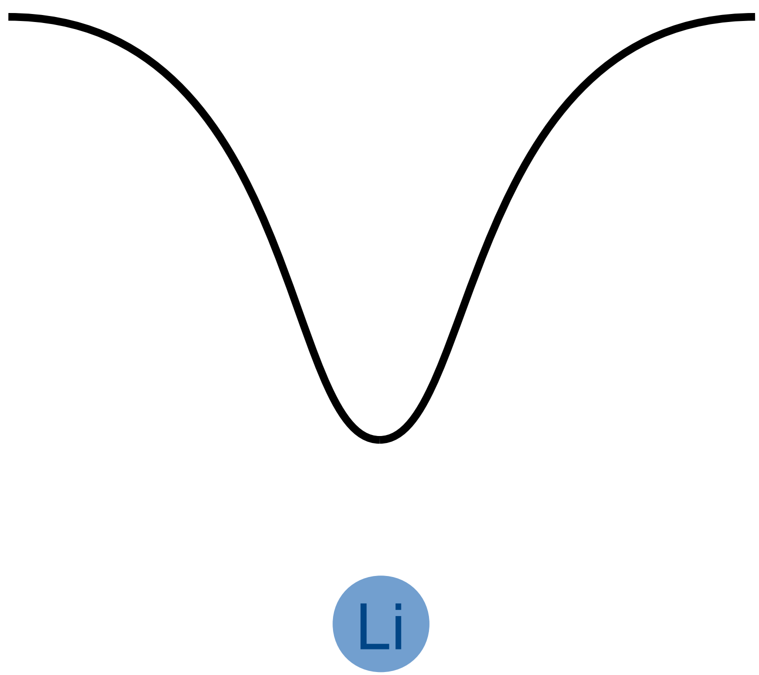
Pseudopotential for atoms

$$E = \int \hat{KE}\,\bar{\psi}_{\vec{r}}\,\psi_{\vec{r}} + V_{\text{e-i}}(\vec{r}-\vec{r}\,')\,n_{\vec{r}\,'}\,\bar{\psi}_{\vec{r}}\,\psi_{\vec{r}} + V_{\text{e-e}}(\vec{r}-\vec{r}\,')\,\bar{\psi}_{\vec{r}}\,\bar{\psi}_{\vec{r}\,'}\,\psi_{\vec{r}\,'}\,\psi_{\vec{r}}$$



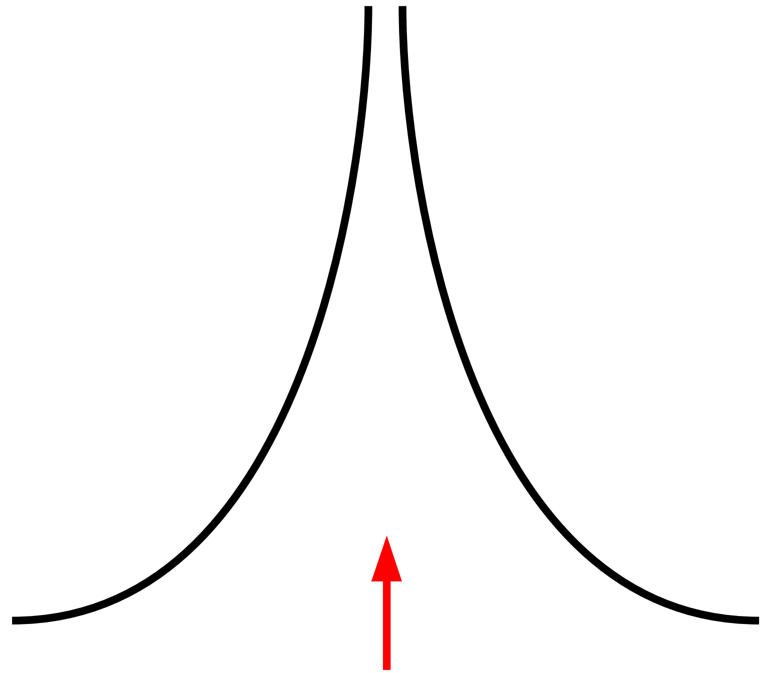
Pseudopotential for atoms

$$
\begin{aligned}
E = \int & \hat{KE}\, \bar{\psi}_{\vec{r}}\, \psi_{\vec{r}} \\
& + V_{\text{e-i}}\left(\vec{r} - \vec{r}\,'\right) n_{\vec{r}\,'}\, \bar{\psi}_{\vec{r}}\, \psi_{\vec{r}} \\
& + V_{\text{e-e}}\left(\vec{r} - \vec{r}\,'\right) \bar{\psi}_{\vec{r}}\, \bar{\psi}_{\vec{r}\,'}\, \psi_{\vec{r}\,'}\, \psi_{\vec{r}}
\end{aligned}
$$



Pseudopotential for electrons

$$
\begin{aligned}
E = \int \hat{KE}\, & \bar{\psi}_{\vec{r}}\, \psi_{\vec{r}} \\
& + V_{\text{e-i}}(\vec{r} - \vec{r}\,')\, n_{\vec{r}\,'}\, \bar{\psi}_{\vec{r}}\, \psi_{\vec{r}} \\
& + V_{\text{e-e}}(\vec{r} - \vec{r}\,')\, \bar{\psi}_{\vec{r}}\, \bar{\psi}_{\vec{r}\,'}\, \psi_{\vec{r}\,'}\, \psi_{\vec{r}}
\end{aligned}
$$



Pseudopotential for electrons

$$E = \int \hat{KE}\, \bar{\psi}_{\vec{r}}\, \psi_{\vec{r}}$$
$$+ V_{\text{e-i}}(\vec{r} - \vec{r}\,')\, n_{\vec{r}\,'}\, \bar{\psi}_{\vec{r}}\, \psi_{\vec{r}}$$
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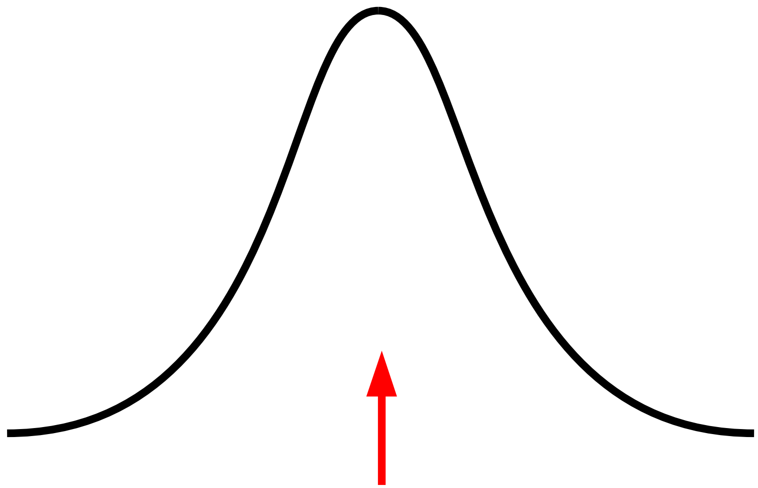


Pseudopotential for kinetic energy

$$E = \int \hat{KE}\, \bar{\psi}_{\vec{r}}\, \psi_{\vec{r}}$$
$$+ V_{\text{e-i}}(\vec{r} - \vec{r}\,')\, n_{\vec{r}\,'}\, \bar{\psi}_{\vec{r}}\, \psi_{\vec{r}}$$
$$+ V_{\text{e-e}}(\vec{r} - \vec{r}\,')\, \bar{\psi}_{\vec{r}}\, \bar{\psi}_{\vec{r}\,'}\, \psi_{\vec{r}\,'}\, \psi_{\vec{r}}$$

Pseudopotential for wave function

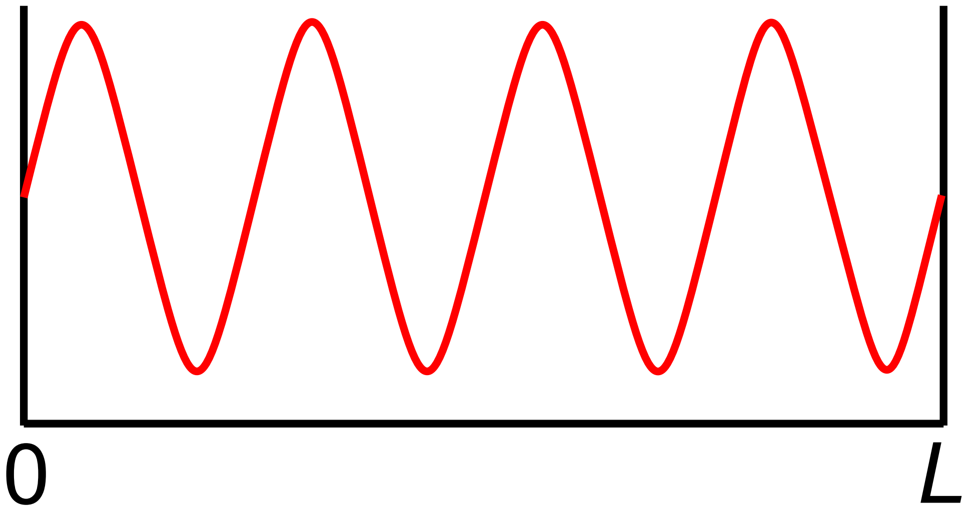
$$E = \int \hat{KE}\, \bar{\psi}_{\vec{r}}\, \psi_{\vec{r}} + V_{\text{e-i}}(\vec{r} - \vec{r}\,')\, n_{\vec{r}\,'}\, \bar{\psi}_{\vec{r}}\, \psi_{\vec{r}} + V_{\text{e-e}}(\vec{r} - \vec{r}\,')\, \bar{\psi}_{\vec{r}}\, \bar{\psi}_{\vec{r}\,'}\, \psi_{\vec{r}\,'}\, \psi_{\vec{r}}$$

Pseudopotential for wave function

$$E = \int \hat{KE}\, \bar{\psi}_{\vec{r}}\, \psi_{\vec{r}} + V_{\text{e-i}}(\vec{r} - \vec{r}\,')\, n_{\vec{r}\,'}\, \bar{\psi}_{\vec{r}}\, \psi_{\vec{r}} + V_{\text{e-e}}(\vec{r} - \vec{r}\,')\, \bar{\psi}_{\vec{r}}\, \bar{\psi}_{\vec{r}\,'}\, \psi_{\vec{r}\,'}\, \psi_{\vec{r}}$$

$$N = \int \bar{\psi}_{\vec{r}}\, \psi_{\vec{r}}$$

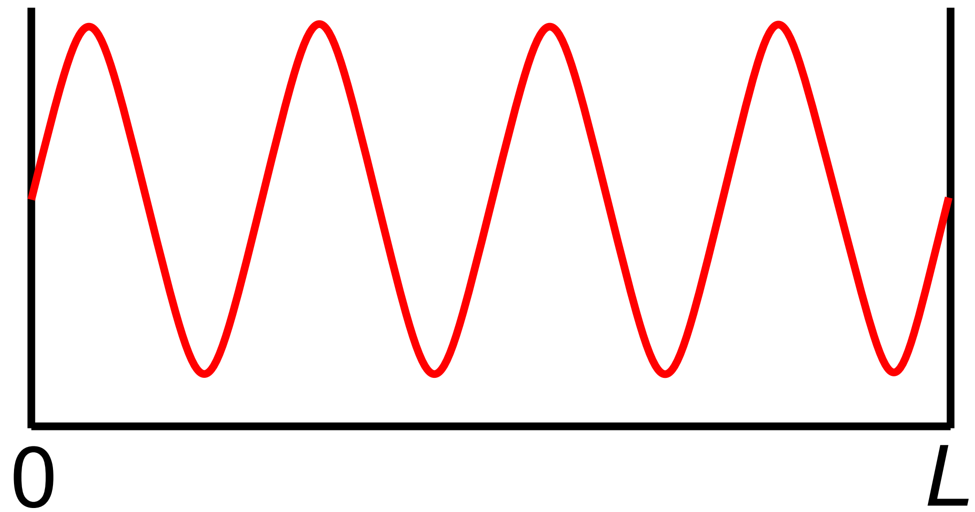
Particle in a box



$$\psi = A \sin\left(8\pi \frac{x}{L}\right)$$

$$E = -\int \bar{\psi} \frac{\nabla^2}{2} \psi \, dx \quad \longleftrightarrow \quad \sin^2 x$$

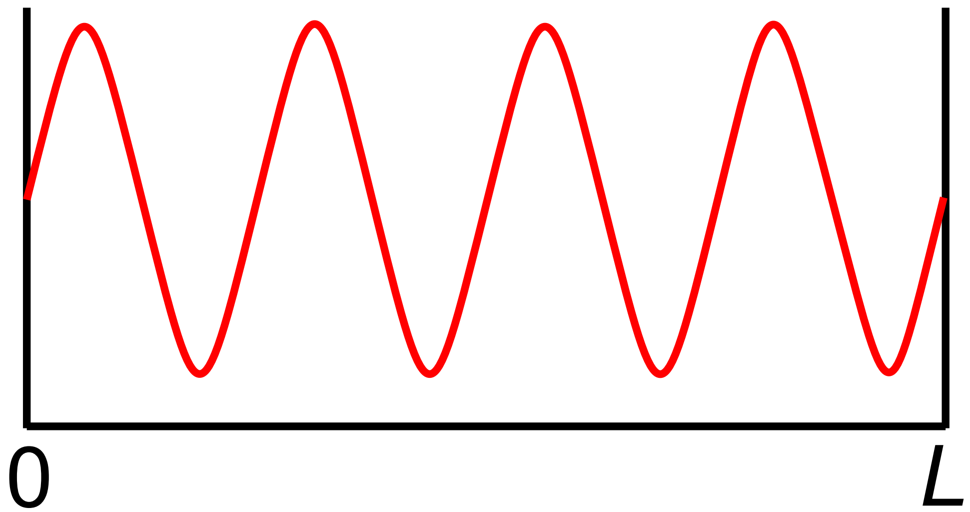
Particle in a box



$$\psi = A\sin\left(8\pi\frac{x}{L}\right)$$

$$E = -\int \bar{\psi}\,\frac{\nabla^2}{2}\,\psi\,dx$$
$$= \frac{32\pi^2 A^2}{L^2}\int \sin^2\left(8\pi\frac{x}{L}\right)dx$$

Particle in a box



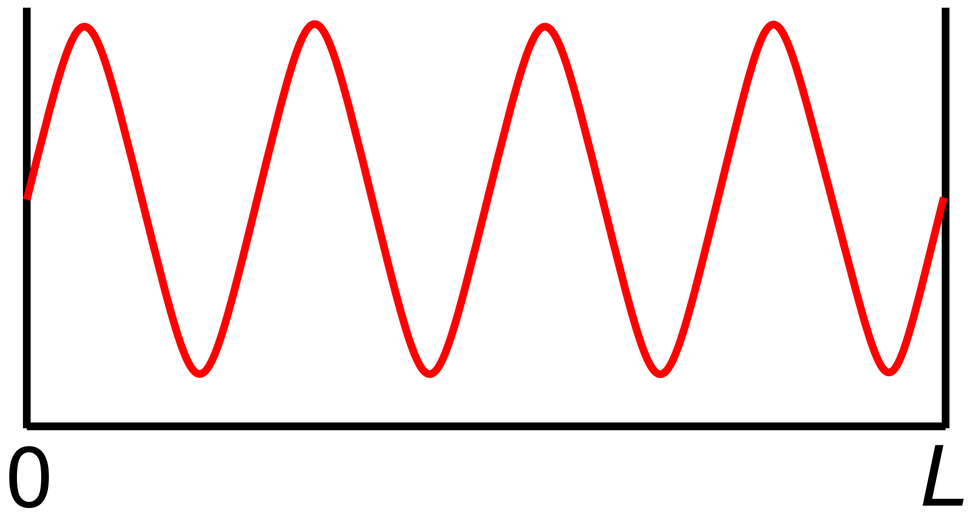
$$\psi = A \sin\left(8\pi \frac{x}{L}\right)$$

$$E = -\int \bar{\psi} \frac{\nabla^2}{2} \psi \, dx$$

$$= \frac{32\pi^2 A^2}{L^2} \int \sin^2\left(8\pi \frac{x}{L}\right) dx$$

$$\langle \sin^2 \rangle = \frac{1}{2}$$

Particle in a box



$$\psi = A\sin\left(8\pi\frac{x}{L}\right)$$

$$E = -\int \bar{\psi}\frac{\nabla^2}{2}\psi\,dx$$
$$= \frac{32\pi^2 A^2}{L^2}\int \sin^2\left(8\pi\frac{x}{L}\right)dx$$
$$= \frac{16\pi^2 A^2}{L}$$

Particle in a box

$$E = \langle \sin^2 \rangle$$

$$\langle \sin^2 \rangle = \frac{1}{2}$$

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$$\cos^2 + \sin^2 = 1$$

Particle in a box

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$$\cos^2 + \sin^2 = 1$$

$$\frac{d}{dx} \sin x = \cos x$$

Particle in a box

$$-\bar{\psi}\frac{\nabla^2}{2}\psi \quad \rightarrow \quad \frac{k^2}{2}\sin^2(kx)$$

$$(\nabla\bar{\psi})(\nabla\psi) \quad \rightarrow \quad \frac{k^2}{2}\cos^2(kx)$$

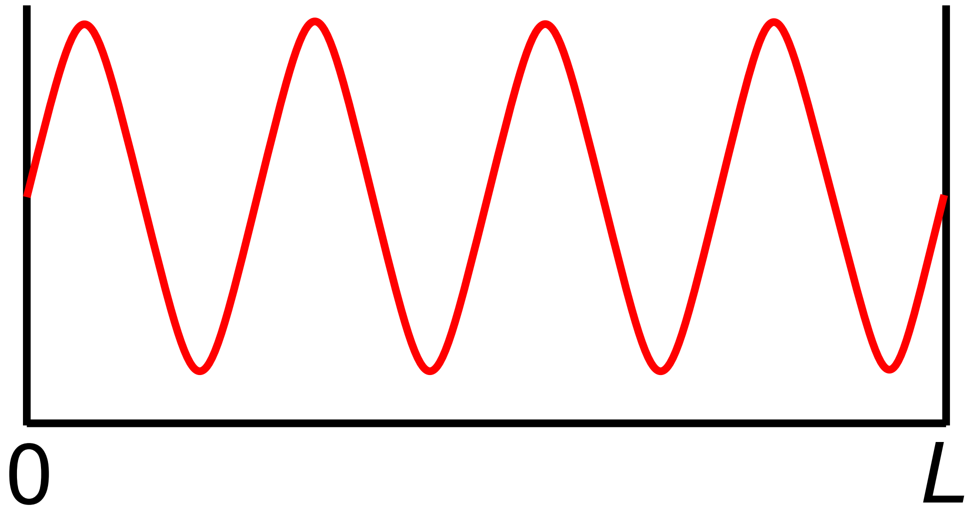
Particle in a box

$$-\bar{\psi}\frac{\nabla^2}{2}\psi \quad \rightarrow \quad \frac{k^2}{2}\sin^2(kx)$$

$$(\nabla\bar{\psi})(\nabla\psi) \quad \rightarrow \quad \frac{k^2}{2}\cos^2(kx)$$

$$E = \frac{1}{2}\int -\bar{\psi}\nabla^2\psi\, dx \rightarrow \frac{1}{4}\int (\nabla\bar{\psi})(\nabla\psi) - \bar{\psi}\nabla^2\psi\, dx$$

Particle in a box



$$\psi = A\sin\left(8\pi\frac{x}{L}\right)$$

$$E = \frac{1}{4}\int(\nabla\bar{\psi})(\nabla\psi) - \bar{\psi}\nabla^2\psi\,dx$$
$$= \frac{16\pi^2 A^2}{L^2}\int \cos^2\left(8\pi\frac{x}{L}\right) + \sin^2\left(8\pi\frac{x}{L}\right)dx$$
$$= \frac{16\pi^2 A^2}{L}$$

Wave function normalization

$$N = \int \bar{\psi}\,\psi\, dx \rightarrow \frac{1}{2}\int \bar{\psi}\,\psi + \frac{(\nabla\bar{\psi})(\nabla\psi)}{k^2}\, dx$$

$$k^2 = \frac{-\nabla^2\psi}{\psi}$$

Pseudoψence

$$E = \int \hat{KE}\, \bar{\psi}_{\vec{r}}\, \psi_{\vec{r}} + V_{\text{e-i}}(\vec{r} - \vec{r}\,')\, n_{\vec{r}}\, \bar{\psi}_{\vec{r}}\, \psi_{\vec{r}} + V_{\text{e-e}}(\vec{r} - \vec{r}\,')\, \bar{\psi}_{\vec{r}}\, \bar{\psi}_{\vec{r}\,'}\, \psi_{\vec{r}\,'}\, \psi_{\vec{r}}$$

$$N = \int \bar{\psi}_{\vec{r}}\, \psi_{\vec{r}}$$

Pseudoψence

$$E = \frac{\int \bar{\psi}\,\hat{H}\,\psi\,dr}{\int \bar{\psi}\,\psi} = \int_{\bar{\psi}\,\psi} \frac{\bar{\psi}\,\hat{H}\,\psi}{\bar{\psi}\,\psi}\,dr$$

Pseudoψence

$$E = \frac{\int \bar{\psi} \hat{H} \psi \, dr}{\int \bar{\psi} \psi} = \int_{\bar{\psi}\psi} \frac{\bar{\psi} \hat{H} \psi}{\bar{\psi} \psi} dr$$

$$\psi = A \sin\left(8 \pi \frac{x}{L}\right)$$

$$E = \int_{\bar{\psi}\psi} \frac{16 \pi^2 A^2}{L^2} dx$$

Pseudoψence

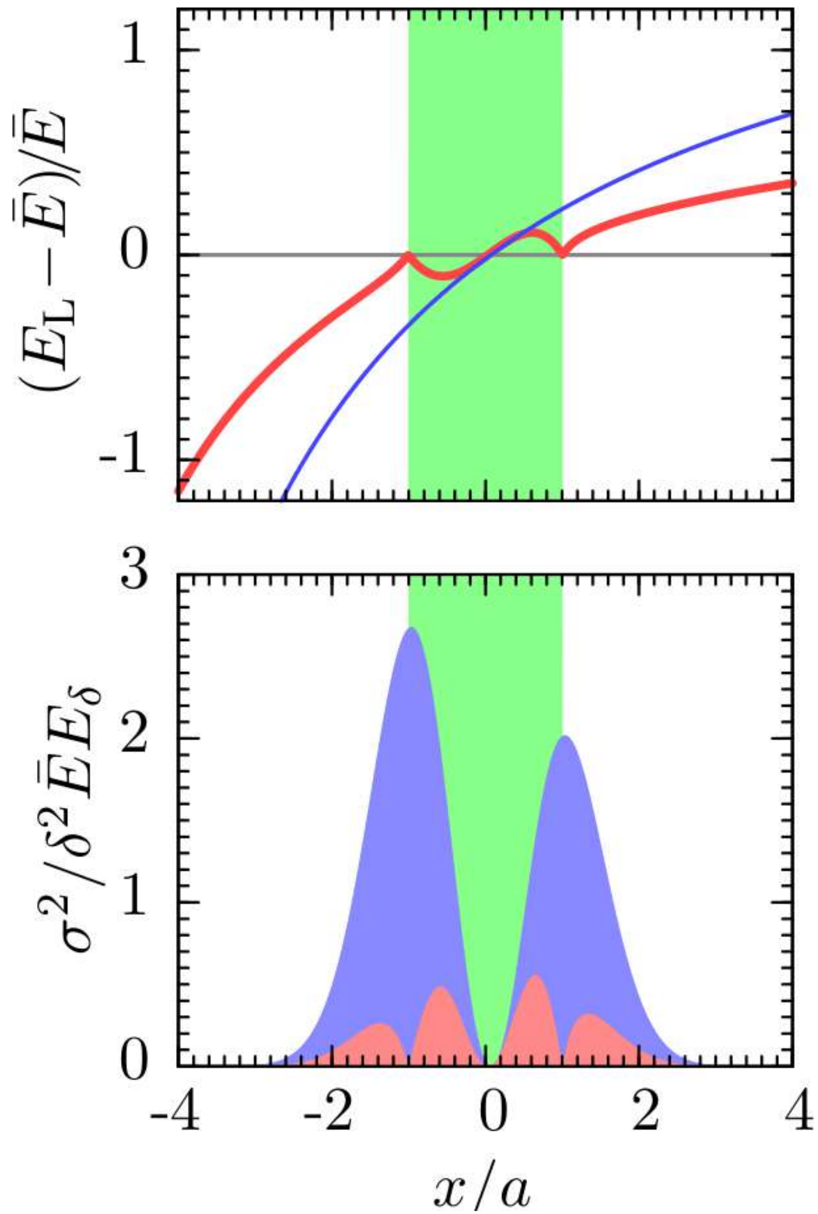
$$\psi = A\sin\left(\sqrt{2E_T}\,x\right)$$

$$\sigma^2 = \int \left(\frac{\bar{\psi} H \psi}{\bar{\psi}\psi} - E\right)^2 \bar{\psi}\psi\, dx$$

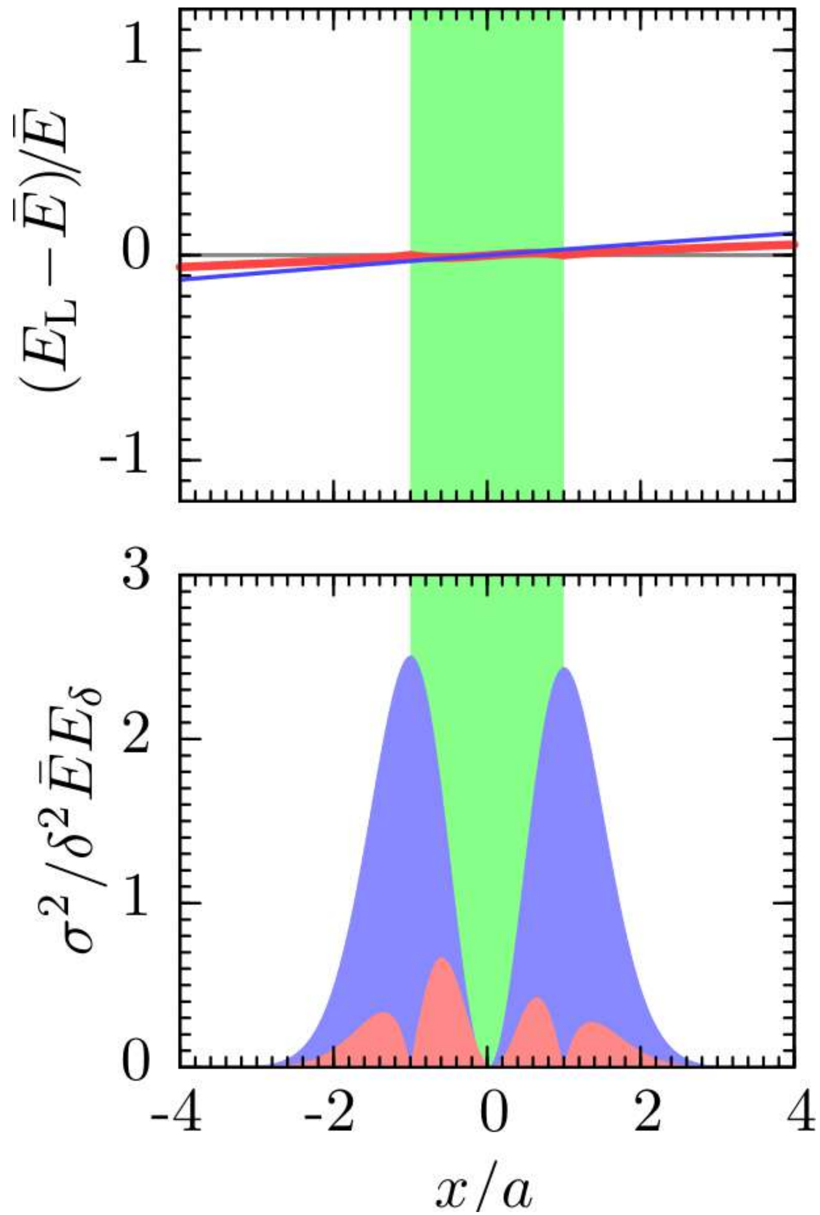
$$\sigma^2(\chi) = \left(\frac{E_T}{1-\chi+\chi E_T/E} - E\right)^2 \left(1-\chi+\chi E_T/E\right)$$

$$\frac{\sigma^2(1/2)}{\sigma^2(0)} = \frac{1}{4}$$

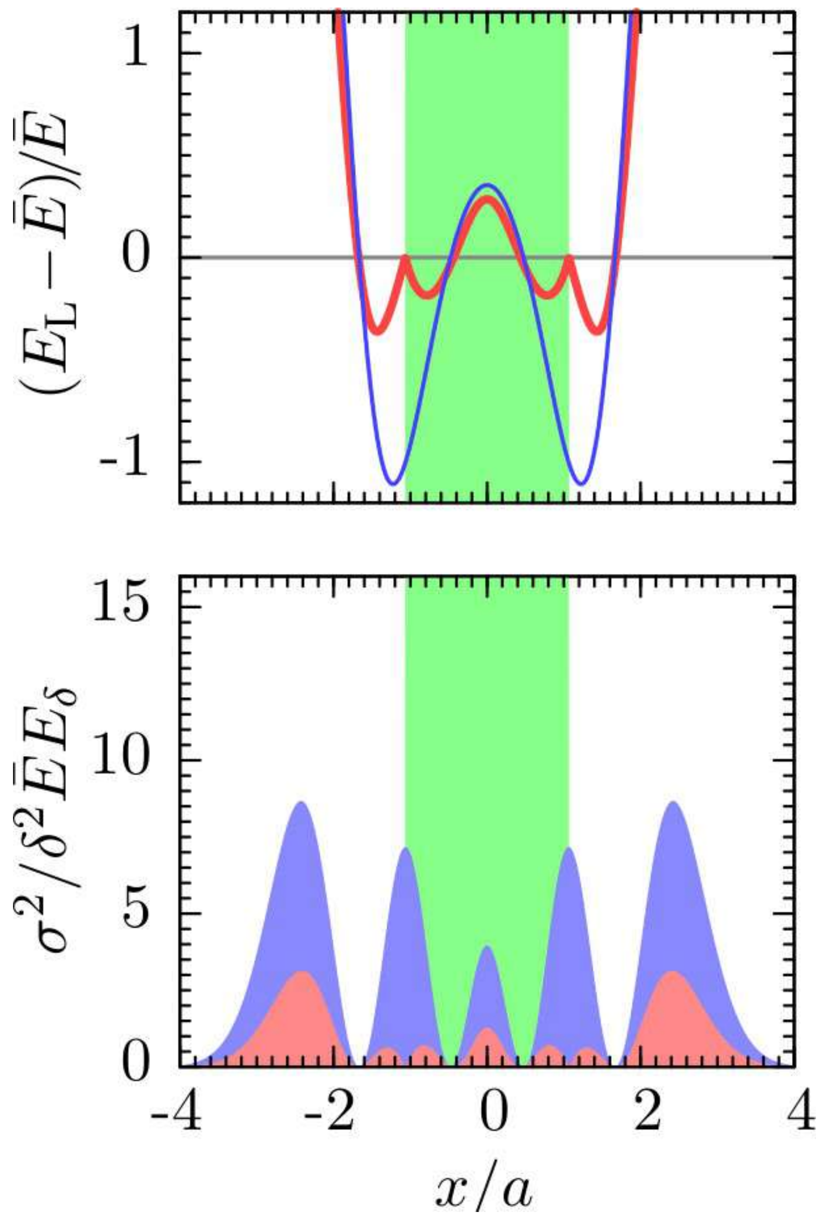
Results: Ψ_0+0.1Ψ_1



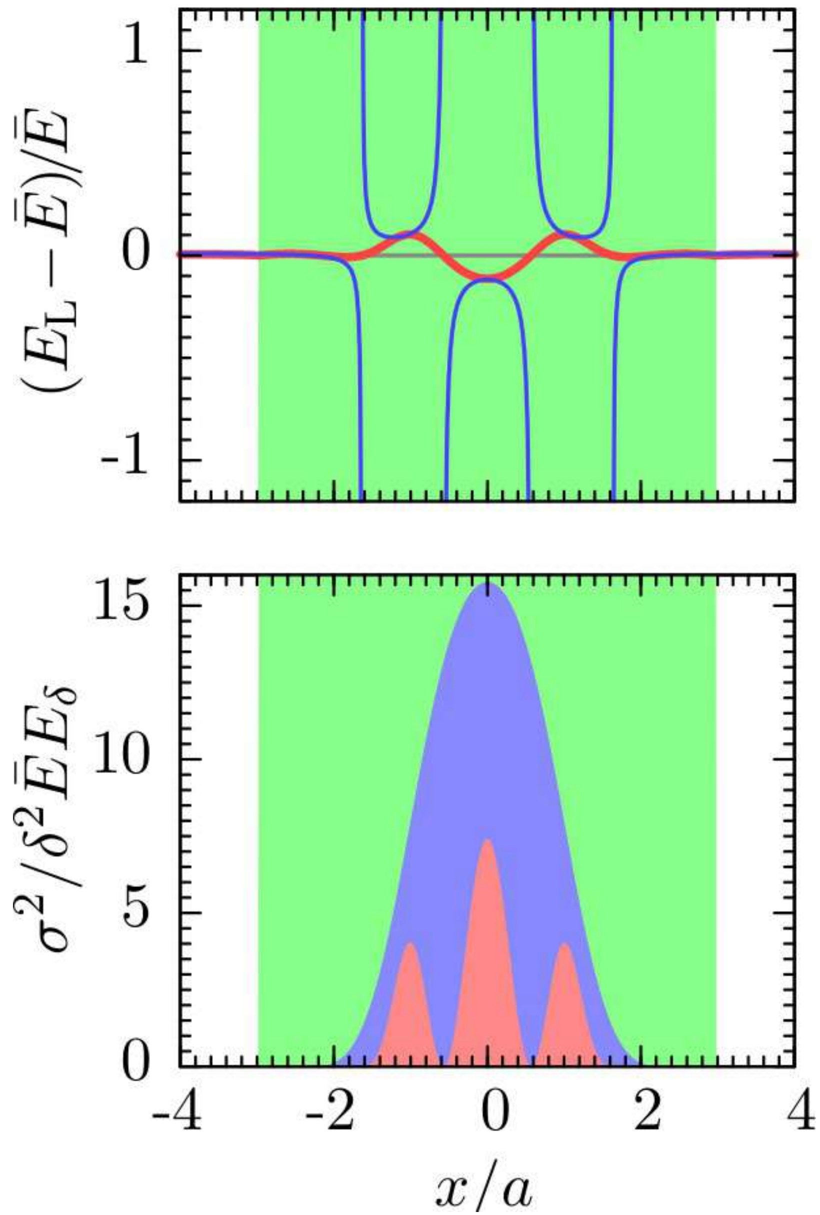
Results: $\Psi_0+0.01\Psi_1$



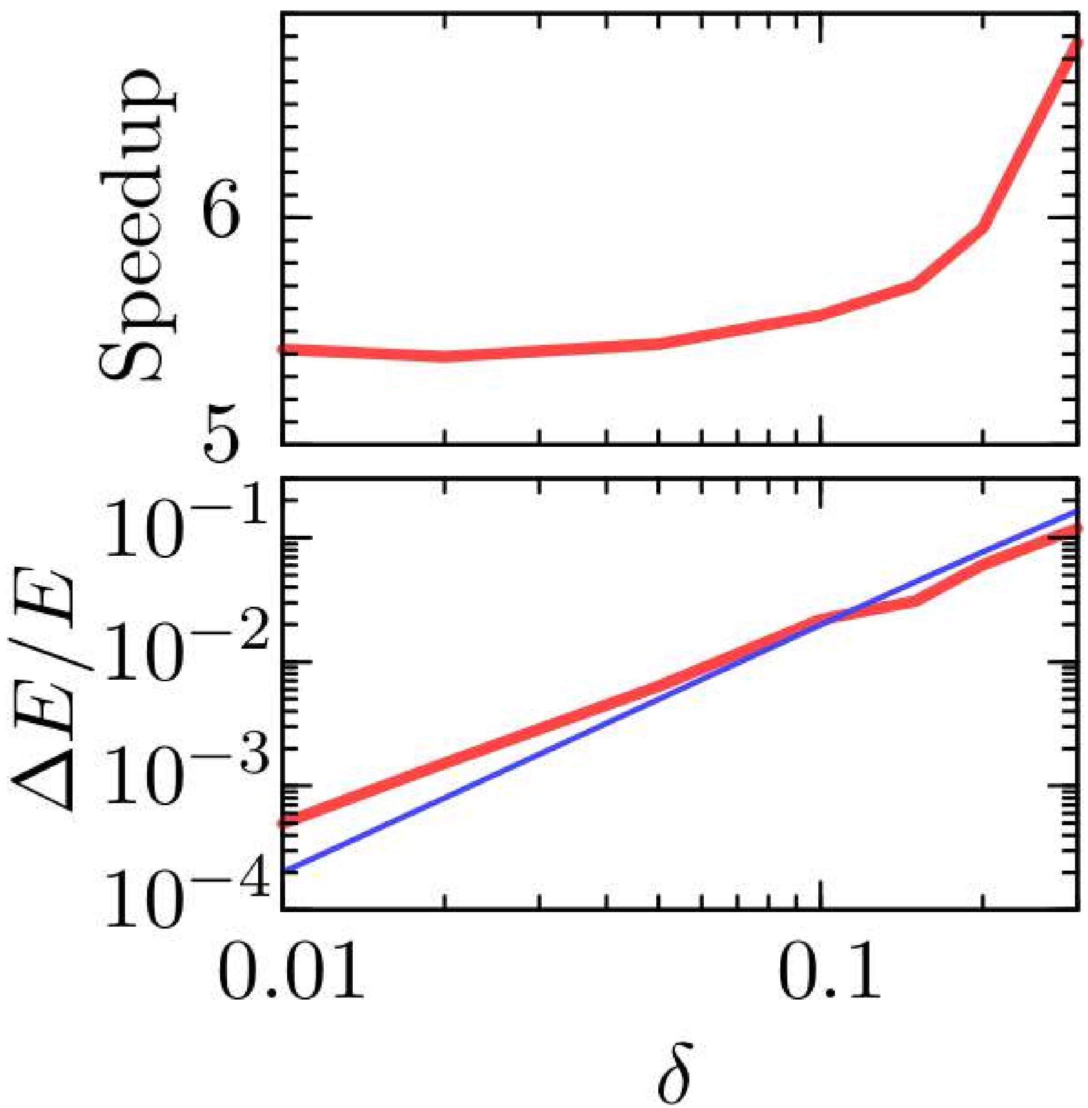
Results: $\Psi_0+0.1\Psi_4$



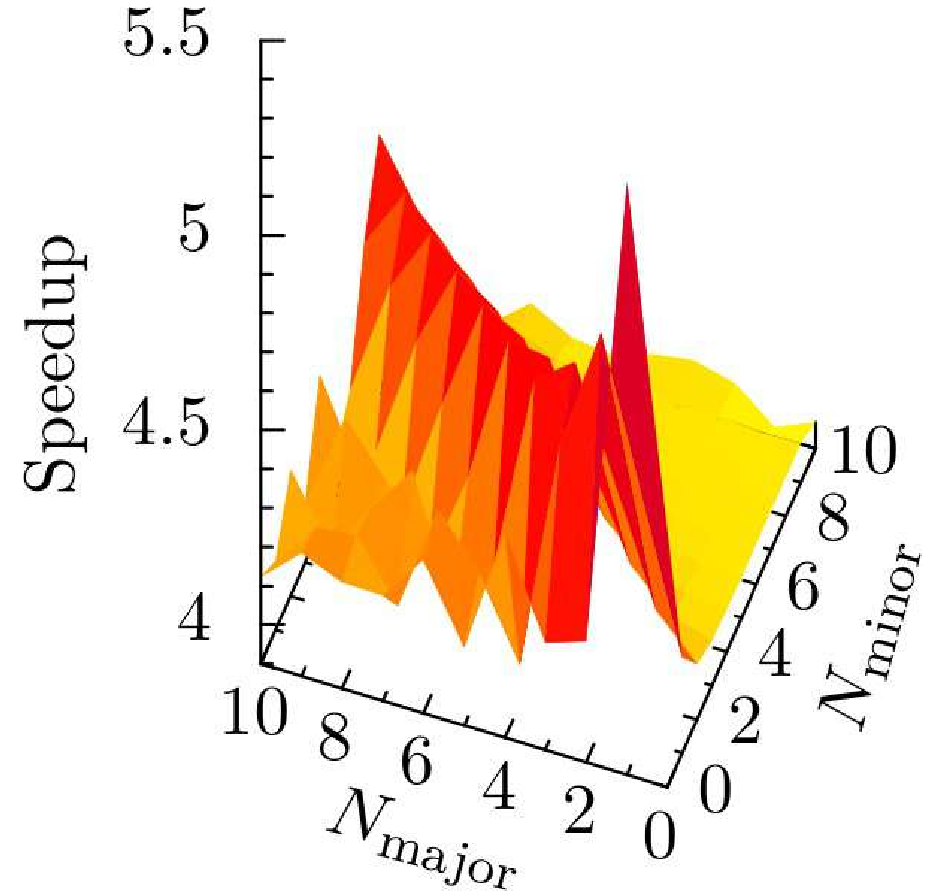
Results: $\Psi_4+0.1\Psi_0$



Results: $\Psi_0+\delta\Psi_1$



Results: $\Psi_{\text{major}}+\delta\Psi_{\text{minor}}$



Summary

Pseudized the wave function

Accelerates numerical calculations by a factor of 64 in 3D