Nodal structure of wave-functions with non-local potentials

Arnau Rios Huguet

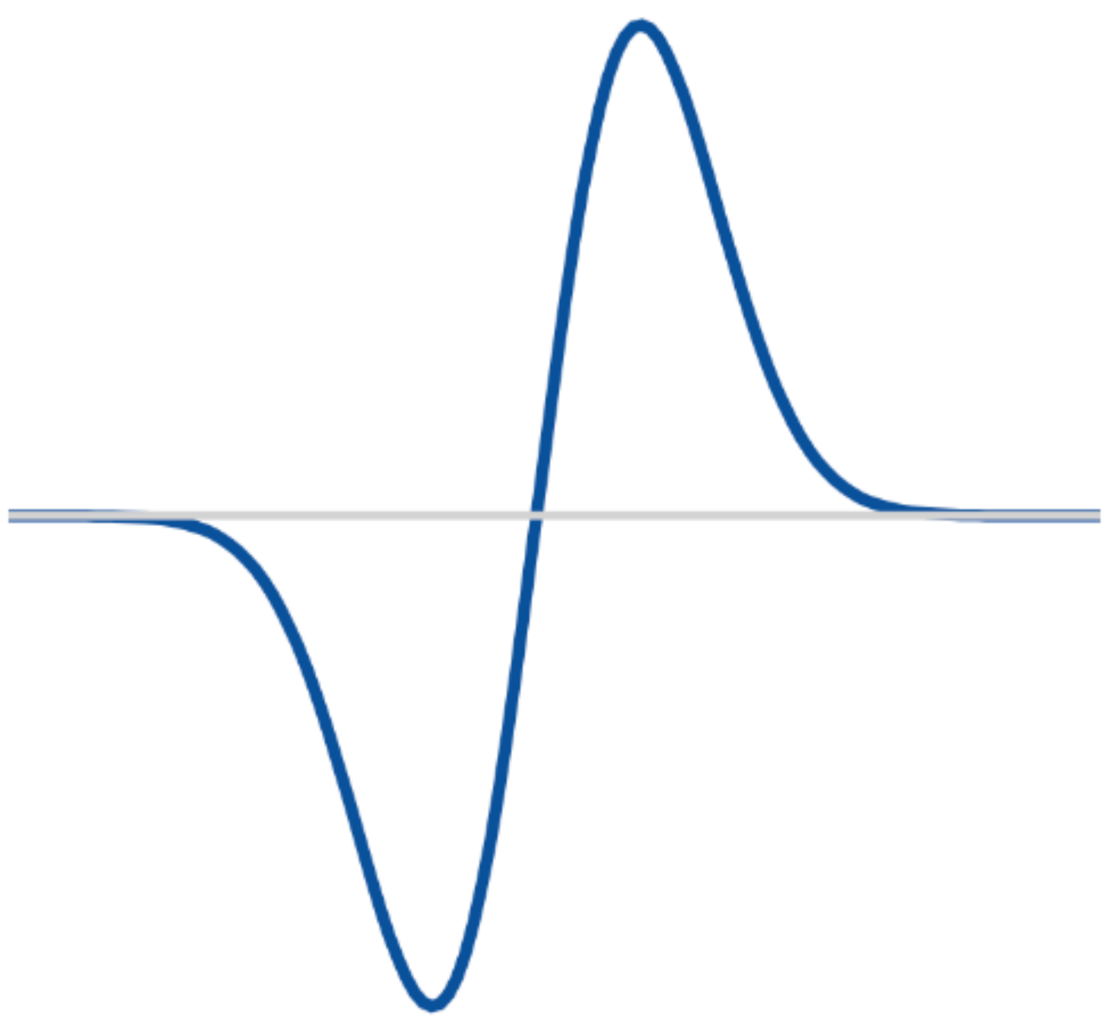
Senior Lecturer in Nuclear Theory

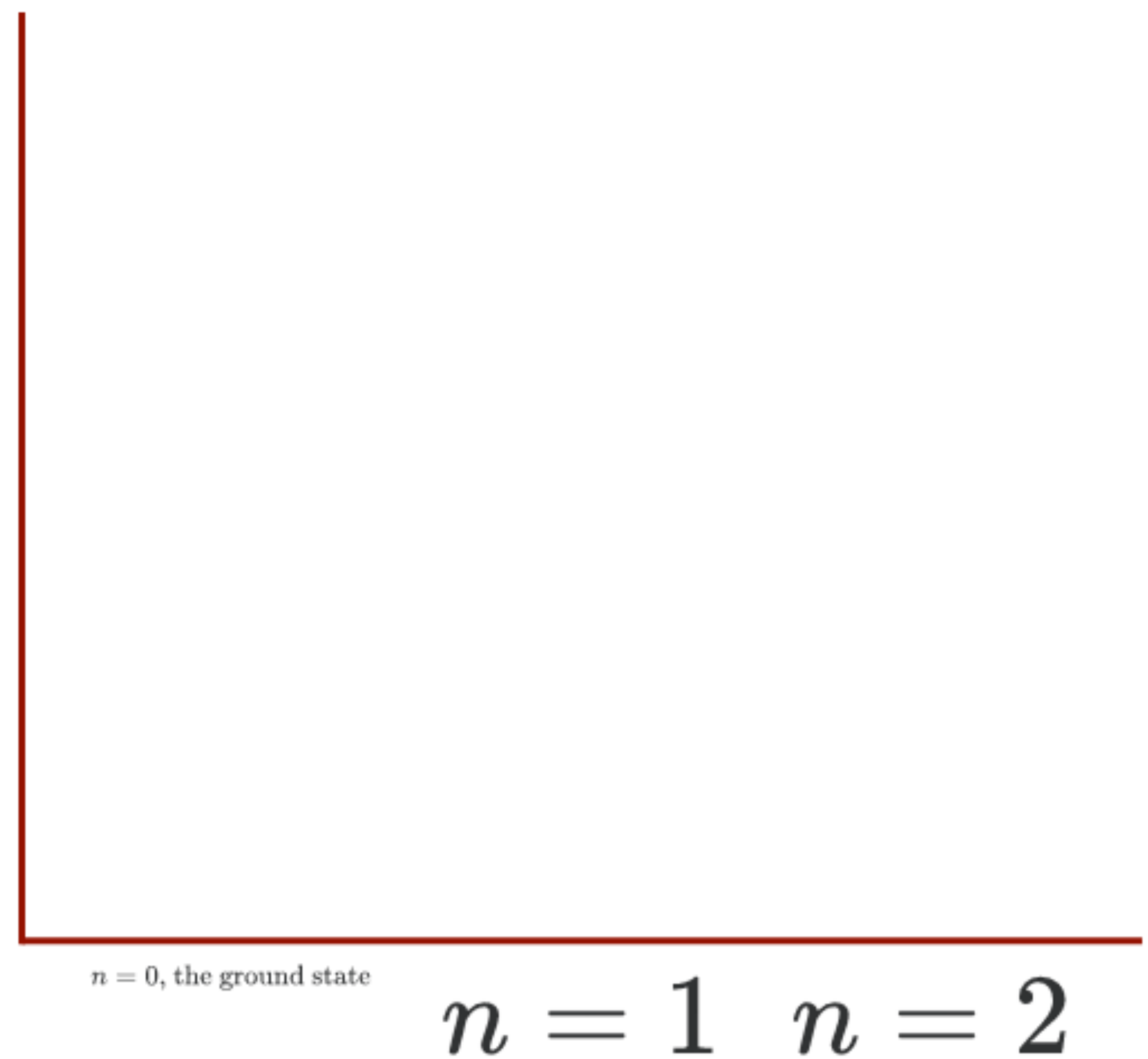
Department of Physics

University of Surrey

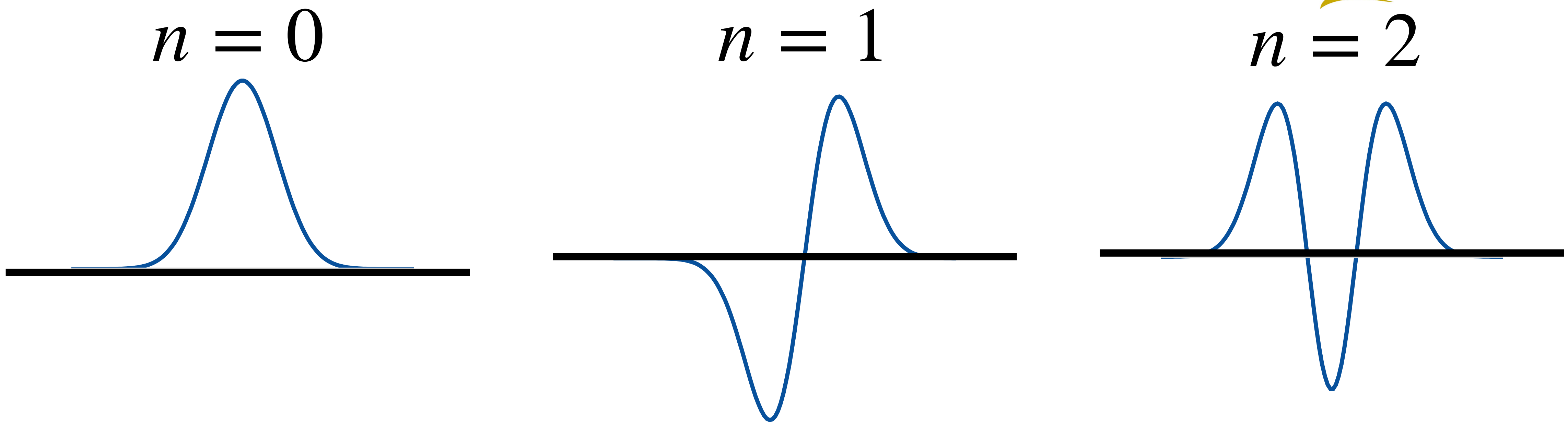
24 European Few Body Conference, 3 September 2019

This wavefunction is the result of one-dimensional local potential. What is its principal quantum number n?





The "nodes" theorem



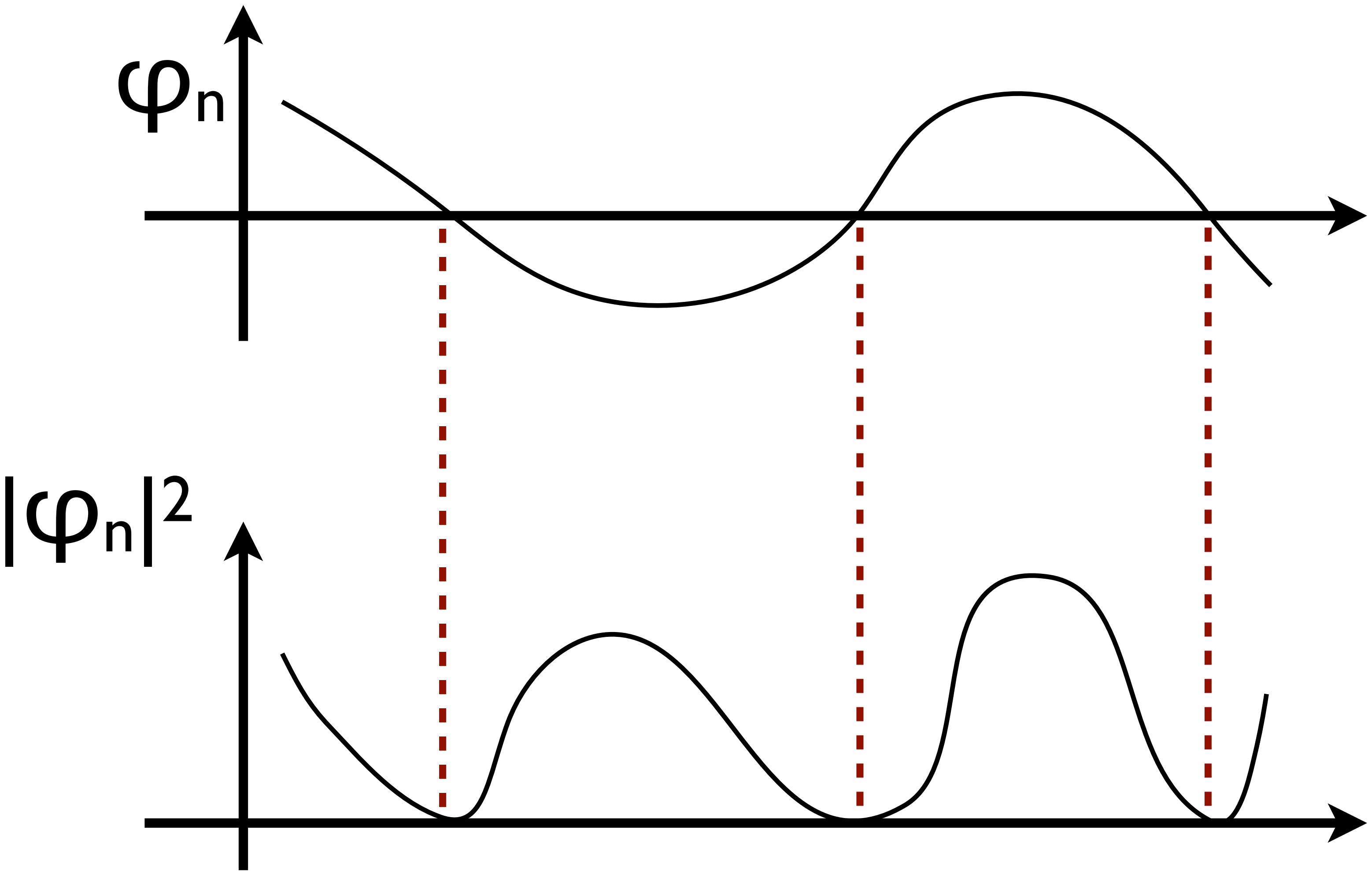
Nodes Theorem

With the energy eigenvalues ordered in a monotonic increasing sequence, the n^{th} eigenfunction $\psi_n(x)$ has n nodes

Messiah, *Quantum Mechanics*
Mandl, *Quantum Mechanics*

Quantum number	Number of nodes		
n	N_n	⇒	$N_n = n$

Why nodes?

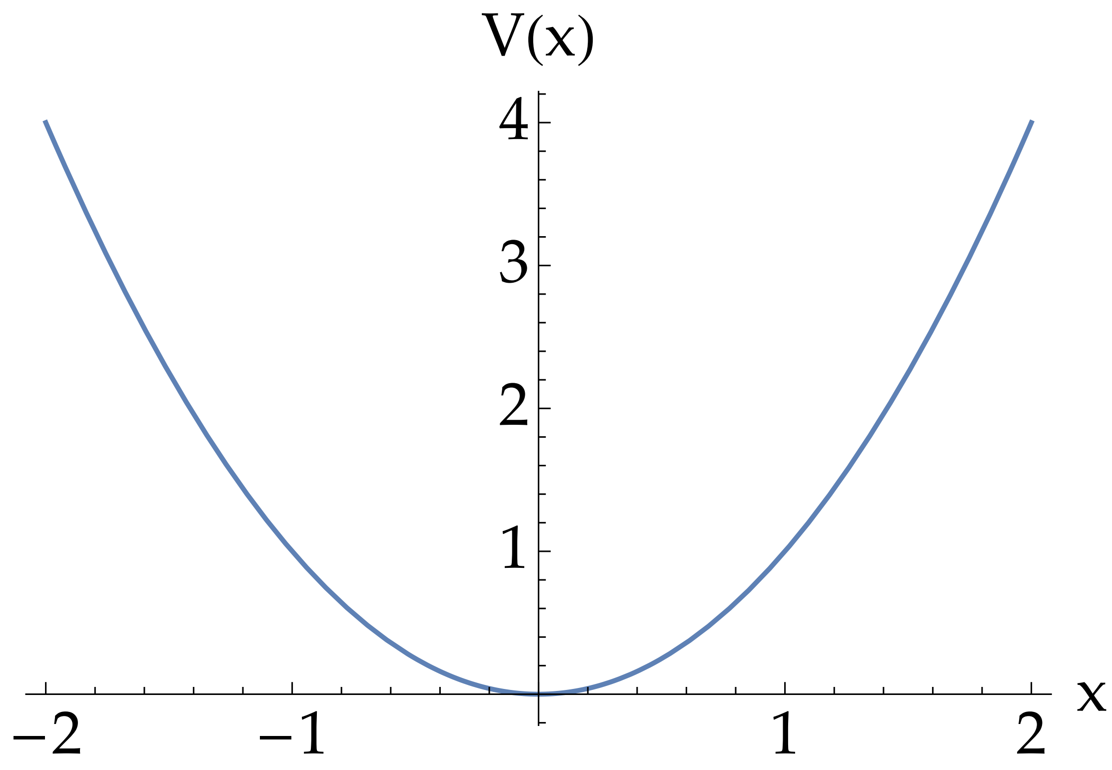


- Nodes in wave-functions associated to **low probability** regions
- Nodal structure is **physically relevant** in chemistry
- Many-body nodal structure for **Monte Carlo**
- Mathematical physics **interest**

Why non-local potentials?

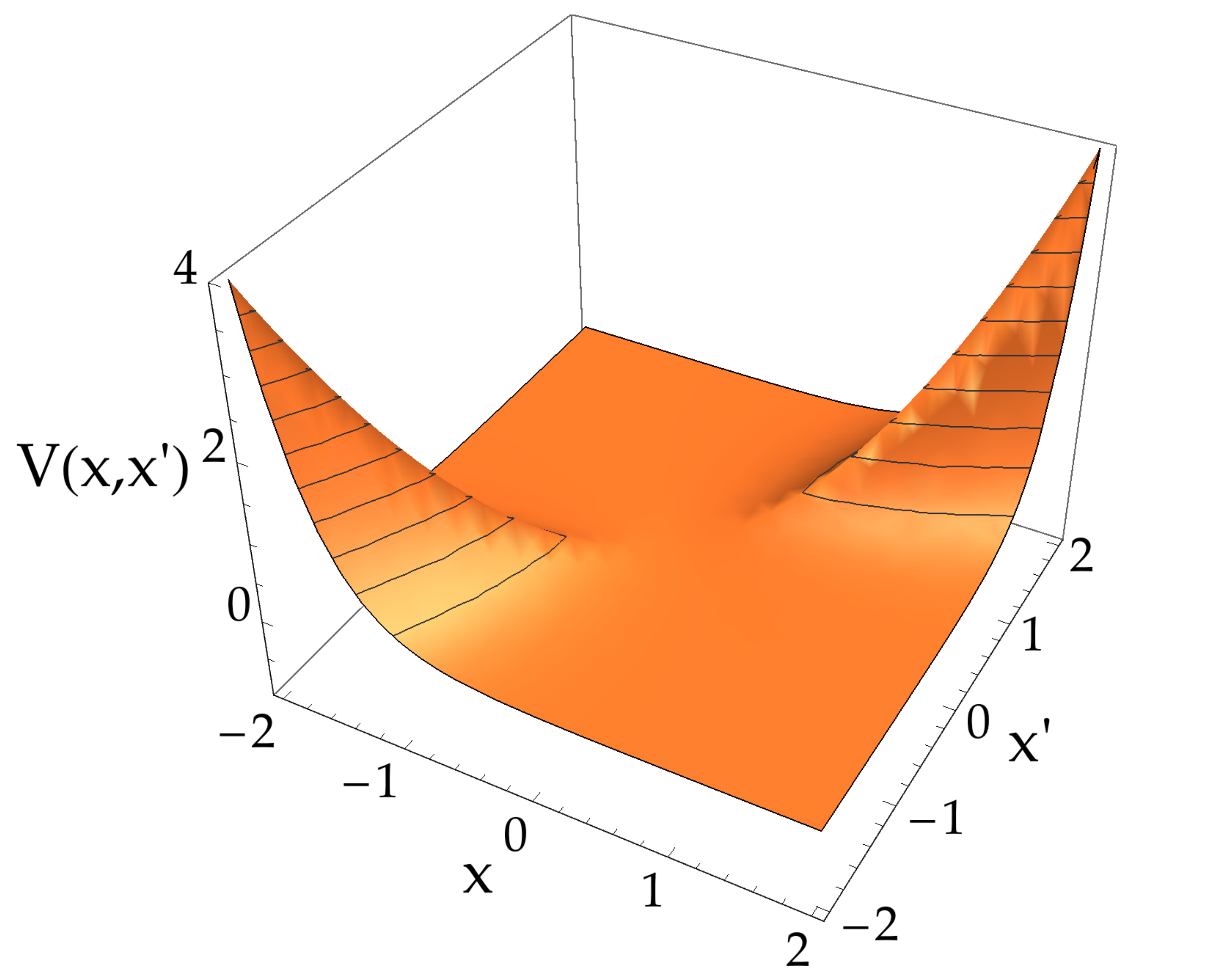
Local

$$\left[\frac{\hat{p}^2}{2m} + V(x)\right]\psi_n(x) = \epsilon_n \psi_n(x)$$



Non-local

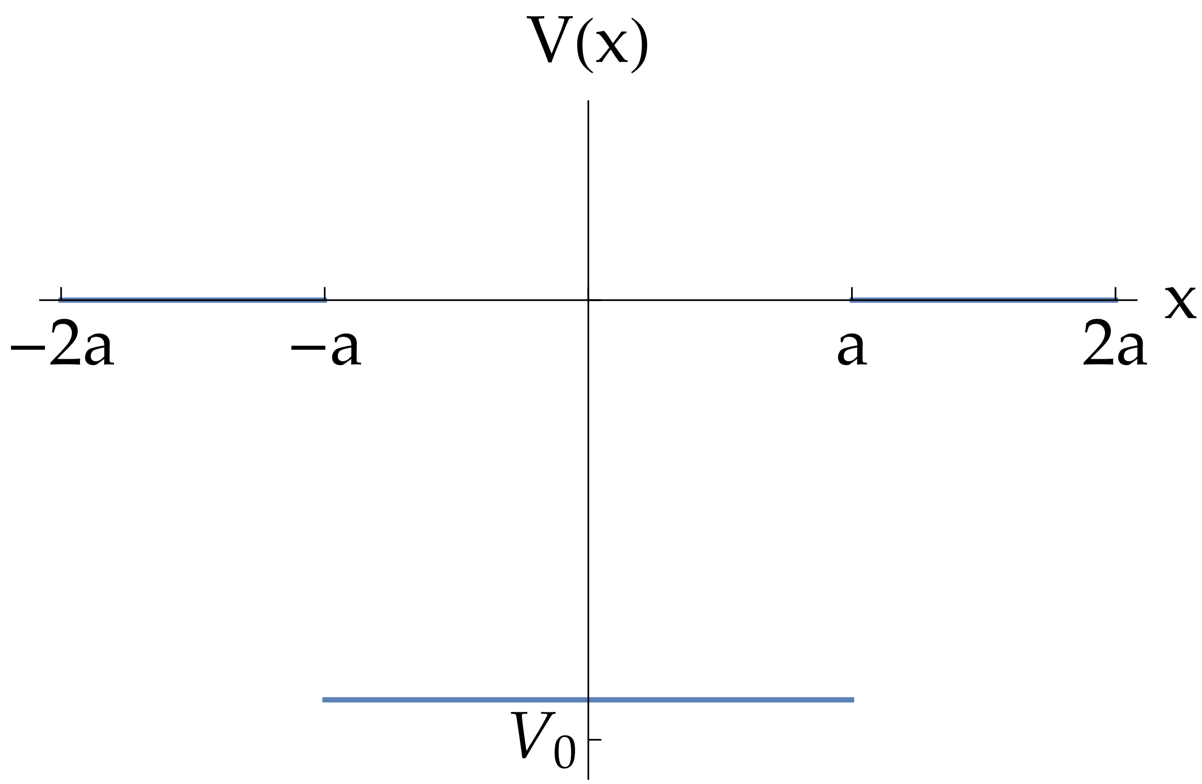
$$\frac{\hat{p}^2}{2m}\psi_n(x) + \int d\bar{x} V(x,\bar{x})\psi_n(\bar{x}) = \epsilon_n \psi_n(x)$$



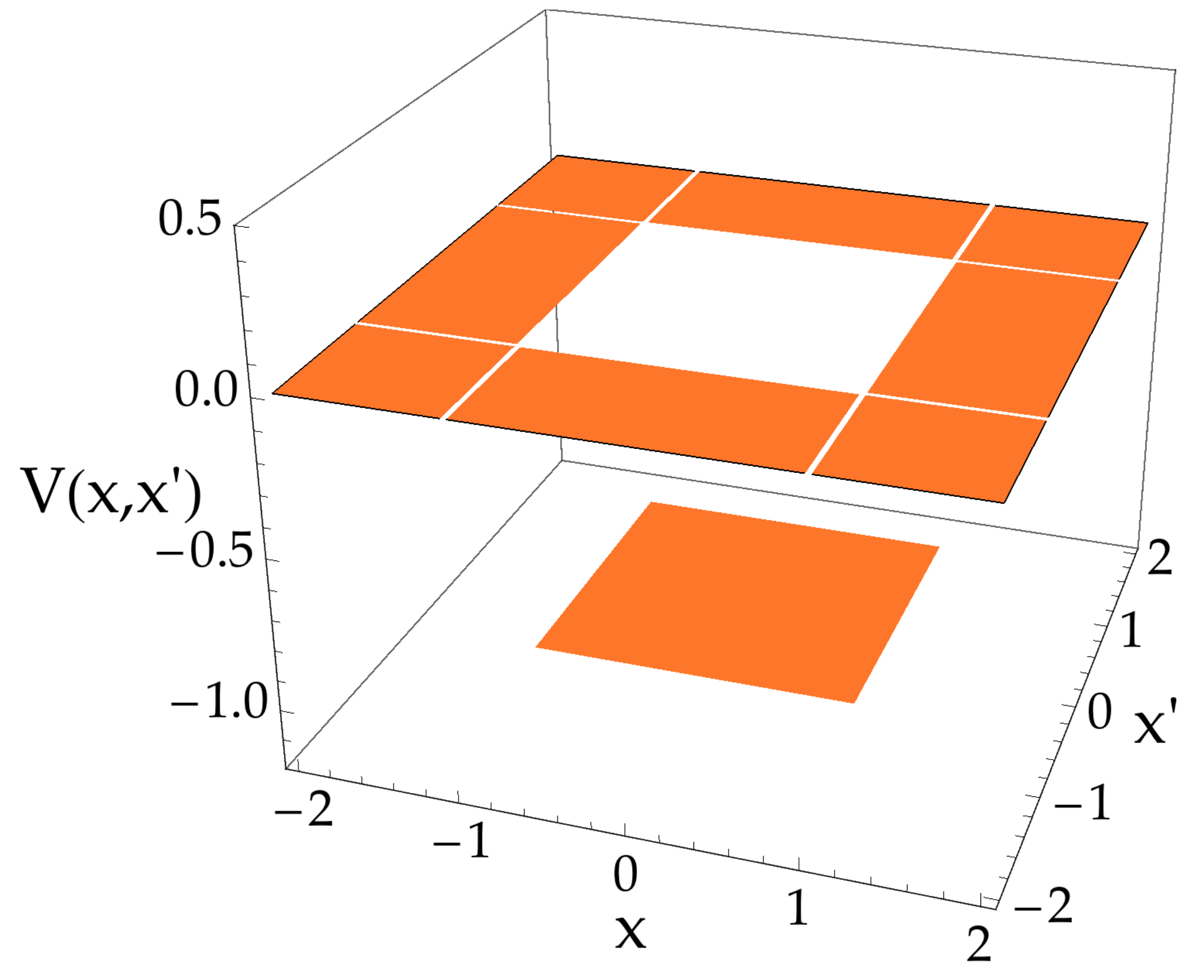
- **Nuclear** interactions are **non-local** by nature (**OPE**)
- **Non-locality arises naturally** in many-body (**exchange**)

Non-local square well

Local well



Non-local well



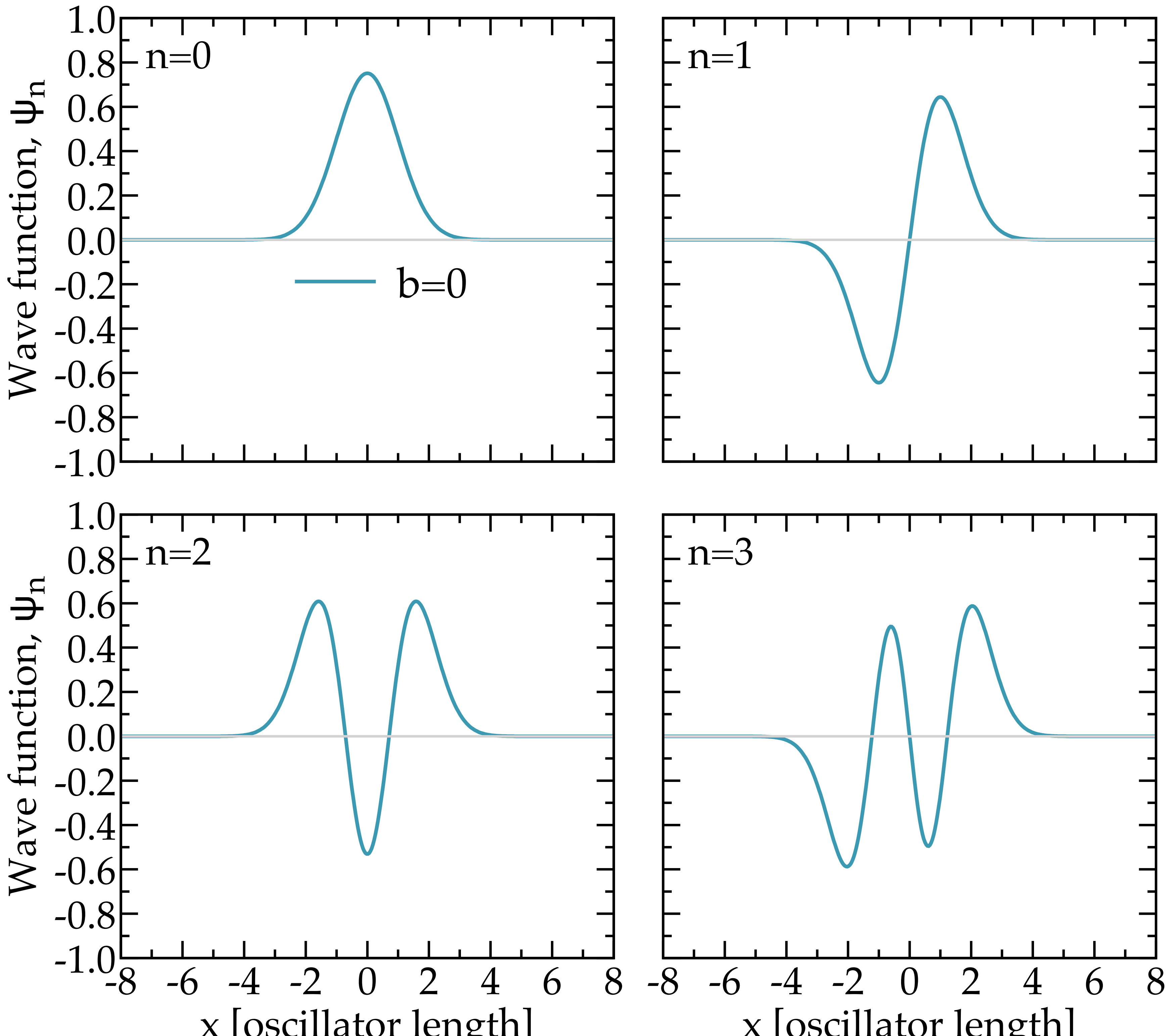
- Number of bound states depends on depth of well
- At least one bound state for all V_0 and a

- Only one bound state
- Nodeless state (analytical)
- Approaches Heaviside function as V_0 decreases

Nichols, *American Journal of Physics* **33** , 474 (1965)

Non-locality and wavefunctions

$$V(x) = x^2$$



Quantum number

$$n$$

Number of nodes

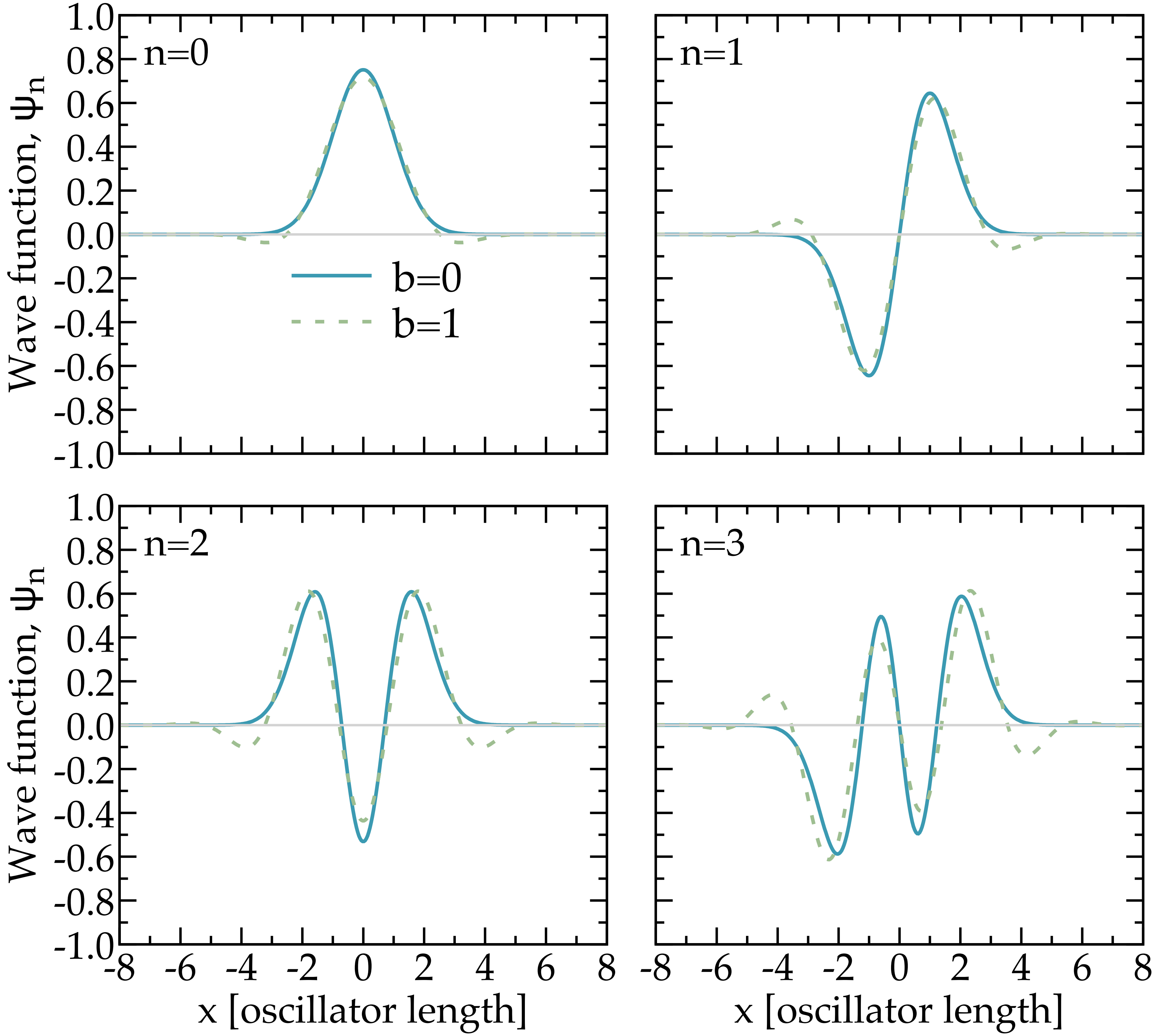
$$\mathcal{N}_n$$

$$\mathcal{N}_n = n$$

Hooverman, Nucl. Phys. A ***189****, 161-169 (1972)*

Non-locality and wavefunctions

$$V(x,x') = \left(\frac{x+x'}{2}\right)^2 \frac{\exp\left(-\frac{|x-x'|}{b}\right)}{2b}$$



Quantum number

$$n$$

Number of nodes

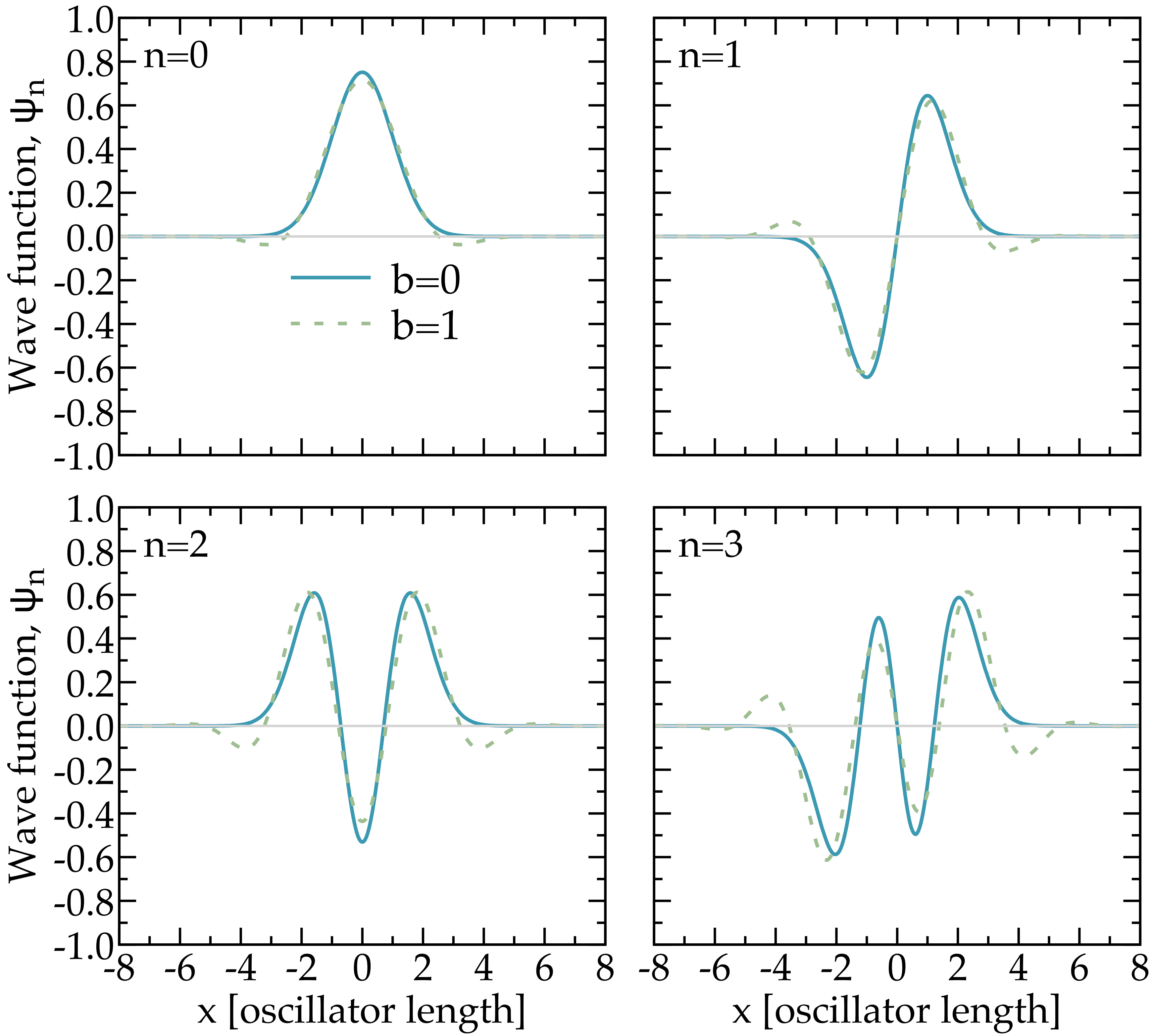
$$\mathcal{N}_n$$

$$\mathcal{N}_n = n$$

Hooverman, Nucl. Phys. A ***189****, 161-169 (1972)*

Non-locality and wavefunctions

$$V(x,x') = \left(\frac{x+x'}{2}\right)^2 \frac{\exp\left(-\frac{|x-x'|}{b}\right)}{2b}$$



Quantum number

$$n$$

Number of nodes

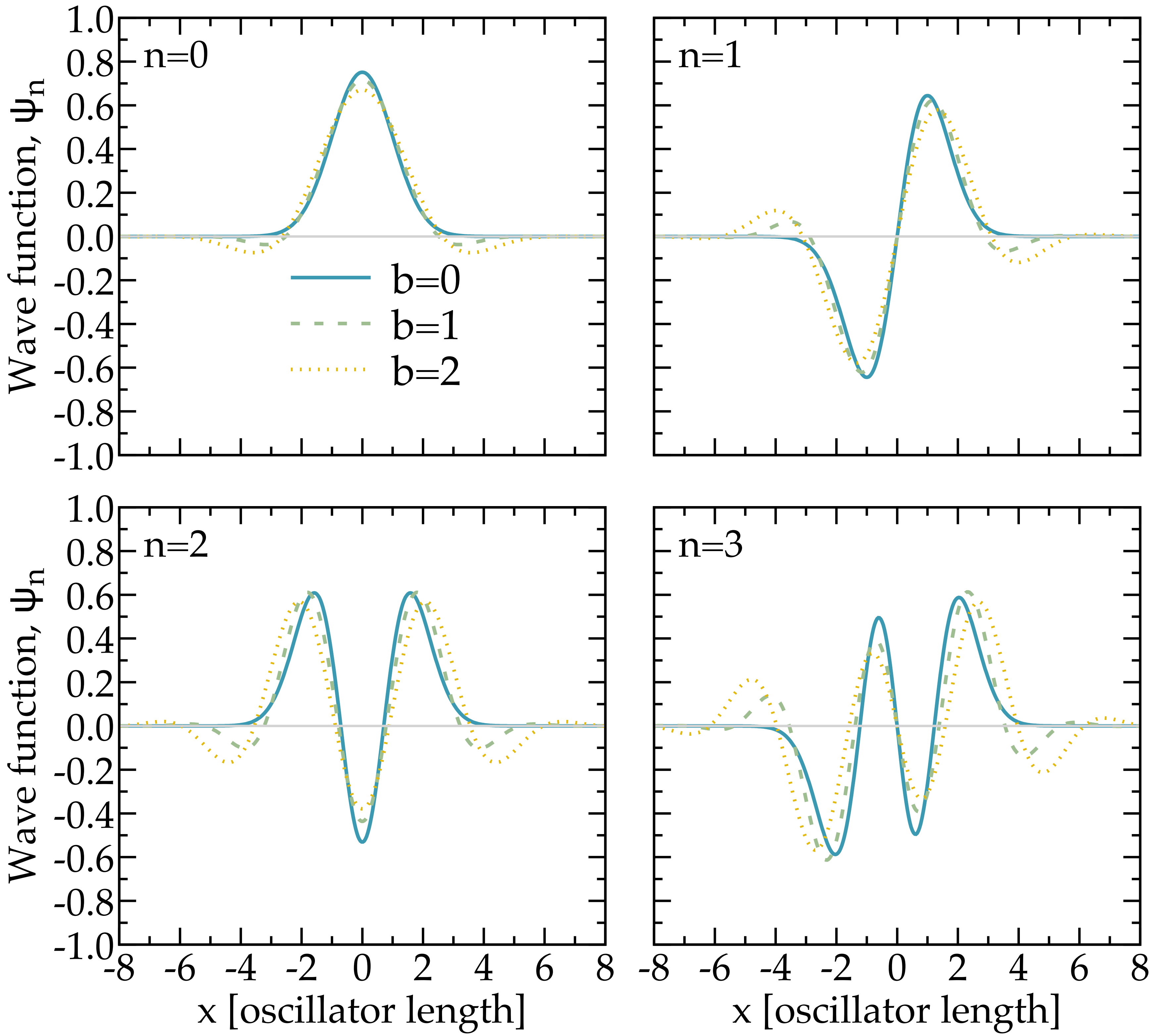
$$\mathcal{N}_n$$

$$\mathcal{N}_n \neq n$$

Hooverman, Nucl. Phys. A ***189,*** *161-169 (1972)*

Non-locality and wavefunctions

$$V(x,x') = \left(\frac{x+x'}{2}\right)^2 \frac{\exp\left(-\frac{|x-x'|}{b}\right)}{2b}$$



Quantum number

$$n$$

Number of nodes

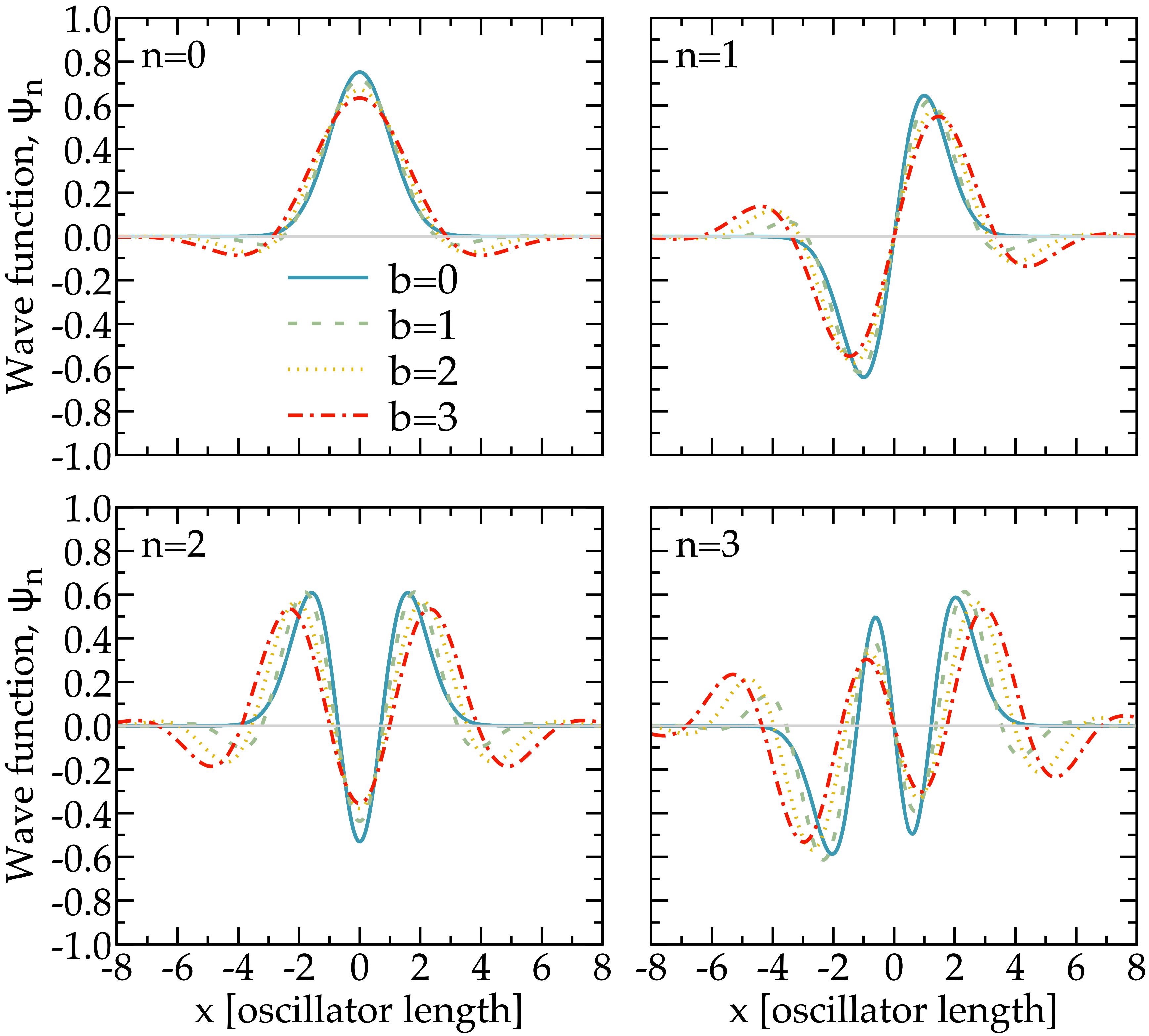
$$\mathcal{N}_n$$

$$\mathcal{N}_n \neq n$$

*Hooverman, Nucl. Phys. A **189**, 161-169 (1972)*

Non-locality and wavefunctions

$$V(x,x') = \left(\frac{x+x'}{2}\right)^2 \frac{\exp\left(-\frac{|x-x'|}{b}\right)}{2b}$$



Quantum number

$$n$$

Number of nodes

$$\mathcal{N}_n$$

$$\mathcal{N}_n \neq n$$

*Hooverman, Nucl. Phys. A **189**, 161-169 (1972)*

Non-local potentials

UNIVERSITY OF SURREY

Nuclear Physics **A189** (1972) 161—169; © *North-Holland Publishing Co., Amsterdam*

ANOMALOUS NODES IN THE BOUND STATE WAVE FUNCTIONS FOR NON-LOCAL POTENTIALS

R. H. HOOVERMAN
Department of Physics, Union College, Schenectady, NY 12308

Received 14 February 1972

We conclude that the *additional nodes are a phenomenon that can generally be expected whenever the kernel of a non-local potential has positive sign and sufficiently large non-locality.*

Hooverman, Nucl. Phys. A ***189*** *155-160, ibid 161-169 (1972)*

- Does **number of nodes** always increase?
- Does potential need to be **repulsive**?
- Is there a relation between principal quantum numbers and number of nodes in non-local case?

$$\left[\frac{\hat{p}^2}{2m} + V(x)\right]\psi_n(x) = \epsilon_n \psi_n(x)$$

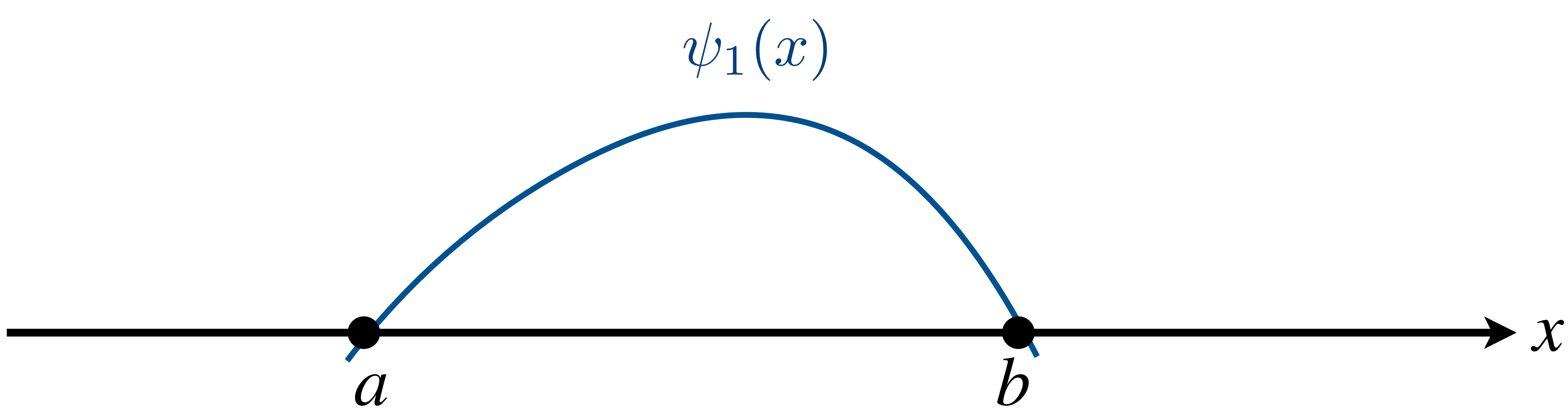
- Define Wronskian $\mathcal{W}(\psi_1, \psi_2) = \psi_1(x)\psi_2'(x) - \psi_2(x)\psi_1'(x)$

- W for two independent solutions satisfies:

$$\mathcal{W}(\psi_1, \psi_2)|_b^a = (\epsilon_1 - \epsilon_2)\int_a^b dx\, \psi_1 \psi_2$$

- Consider a and b two consecutive nodes of ψ_1

$$\epsilon_2 > \epsilon_1 \qquad \psi_2(b)\psi_1'(b) - \psi_2(a)\psi_1'(a) = (\epsilon_2 - \epsilon_1)\int_a^b dx\, \psi_1 \psi_2$$



$$\left[\frac{\hat{p}^2}{2m} + V(x)\right]\psi_n(x) = \epsilon_n \psi_n(x)$$

UNIVERSITY OF SURREY

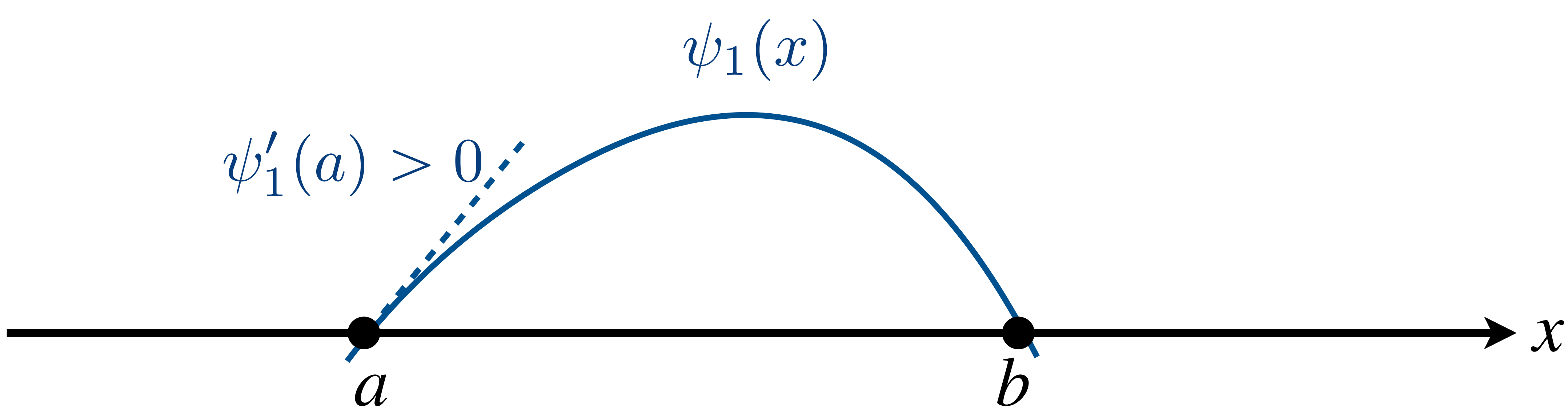
- Define Wronskian $\mathcal{W}(\psi_1, \psi_2) = \psi_1(x)\psi_2'(x) - \psi_2(x)\psi_1'(x)$

- W for two independent solutions satisfies:

$$\mathcal{W}(\psi_1, \psi_2)|_b^a = (\epsilon_1 - \epsilon_2)\int_a^b dx\, \psi_1 \psi_2$$

- Consider a and b two consecutive nodes of ψ_1

$\epsilon_2 > \epsilon_1$ $$\psi_2(b)\psi_1'(b) - \psi_2(a)\psi_1'(a) = (\epsilon_2 - \epsilon_1)\int_a^b dx\, \psi_1 \psi_2$$



$$\left[\frac{\hat{p}^2}{2m} + V(x)\right]\psi_n(x) = \epsilon_n \psi_n(x)$$

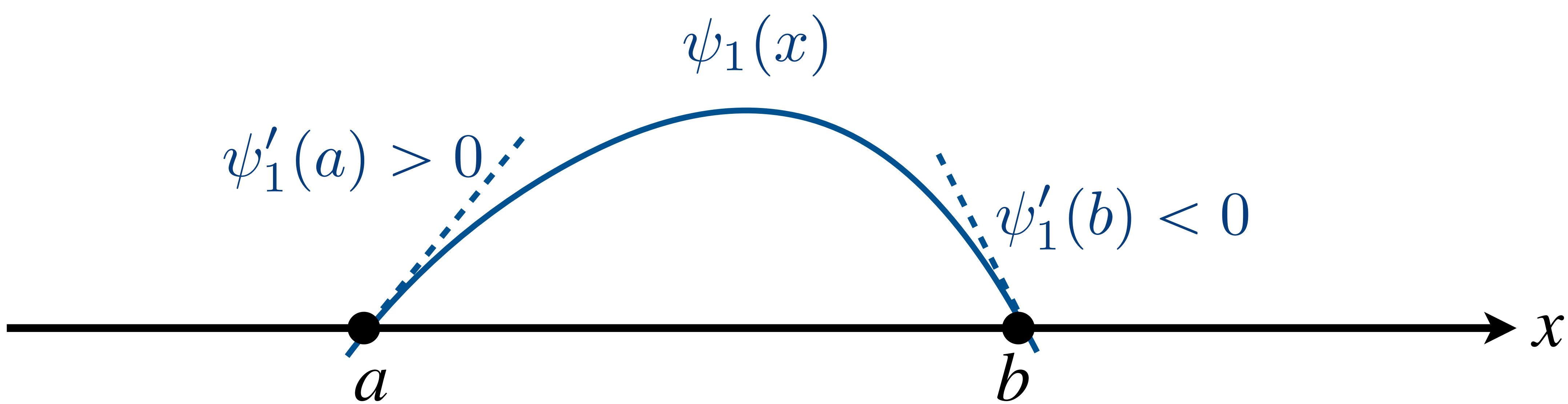
- Define Wronskian $\mathcal{W}(\psi_1, \psi_2) = \psi_1(x)\psi_2'(x) - \psi_2(x)\psi_1'(x)$

- W for two independent solutions satisfies:

$$\mathcal{W}(\psi_1, \psi_2)\big|_b^a = (\epsilon_1 - \epsilon_2)\int_a^b dx\, \psi_1 \psi_2$$

- Consider a and b two consecutive nodes of ψ_1

$$\epsilon_2 > \epsilon_1 \qquad \psi_2(b)\psi_1'(b) - \psi_2(a)\psi_1'(a) = (\epsilon_2 - \epsilon_1)\int_a^b dx\, \psi_1 \psi_2$$



$$\left[\frac{\hat{p}^2}{2m} + V(x)\right]\psi_n(x) = \epsilon_n \psi_n(x)$$

UNIVERSITY OF SURREY

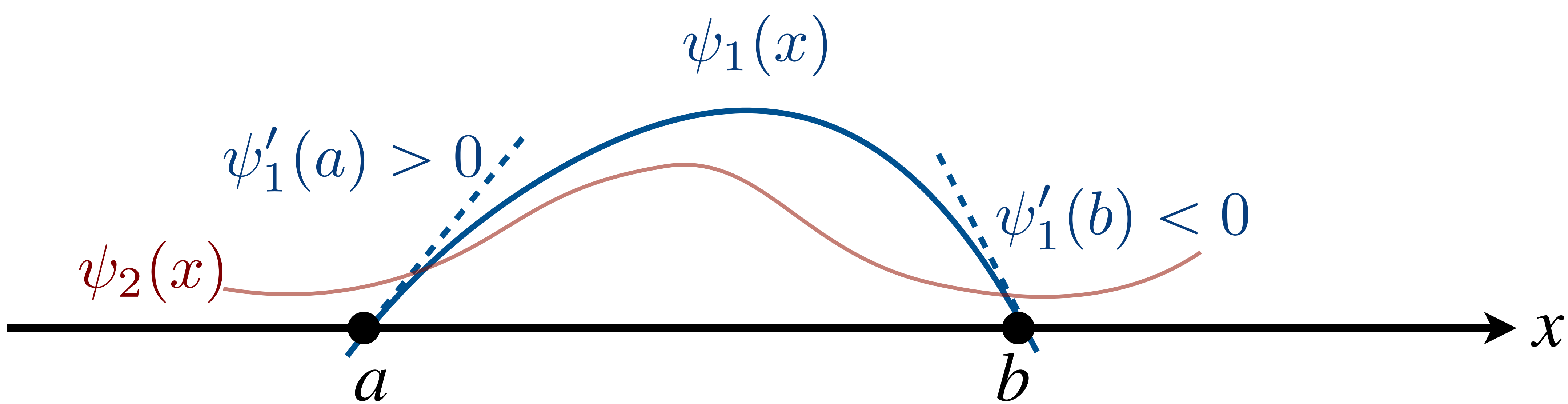
- Define Wronskian $\mathcal{W}(\psi_1, \psi_2) = \psi_1(x)\psi_2'(x) - \psi_2(x)\psi_1'(x)$

- W for two independent solutions satisfies:

$$\mathcal{W}(\psi_1, \psi_2)|_b^a = (\epsilon_1 - \epsilon_2)\int_a^b dx\, \psi_1 \psi_2$$

- Consider a and b two consecutive nodes of ψ_1

$\epsilon_2 > \epsilon_1$ $\quad \psi_2(b)\psi_1'(b) - \psi_2(a)\psi_1'(a) = (\epsilon_2 - \epsilon_1)\int_a^b dx\, \psi_1 \psi_2$



$$\left[\frac{\hat{p}^2}{2m} + V(x)\right]\psi_n(x) = \epsilon_n \psi_n(x)$$

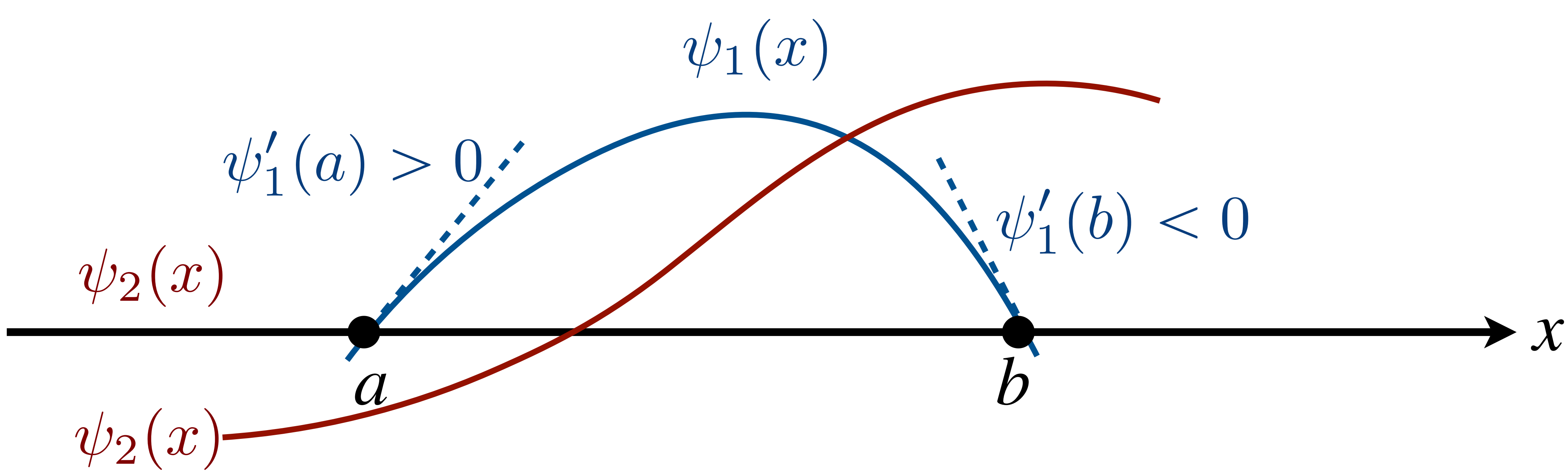
- Define Wronskian $\mathcal{W}(\psi_1, \psi_2) = \psi_1(x)\psi_2'(x) - \psi_2(x)\psi_1'(x)$

- W for two independent solutions satisfies:

$$\mathcal{W}(\psi_1, \psi_2)|_b^a = (\epsilon_1 - \epsilon_2)\int_a^b dx\, \psi_1 \psi_2$$

- Consider a and b two consecutive nodes of ψ_1

$$\epsilon_2 > \epsilon_1 \qquad \psi_2(b)\psi_1'(b) - \psi_2(a)\psi_1'(a) = (\epsilon_2 - \epsilon_1)\int_a^b dx\, \psi_1 \psi_2$$



$$\frac{\hat{p}^2}{2m}\psi_n(x) + \int d\bar{x} V(x,\bar{x})\psi_n(\bar{x}) = \epsilon_n \psi_n(x)$$

UNIVERSITY OF SURREY

- Define Wronskian $\mathcal{W}(\psi_1, \psi_2) = \psi_1(x)\psi_2'(x) - \psi_2(x)\psi_1'(x)$

- W for two independent solutions satisfies:

$$\mathcal{W}(\psi_1,\psi_2)|_b^a = (\epsilon_1 - \epsilon_2)\int_a^b dx\, \psi_1\psi_2 + \int_a^b dx \int d\bar{x} V(x,\bar{x})\left\{\psi_1(x)\psi_2(\bar{x}) - \psi_2(x)\psi_1(\bar{x})\right\}$$

- Consider a and b two consecutive nodes of ψ_1

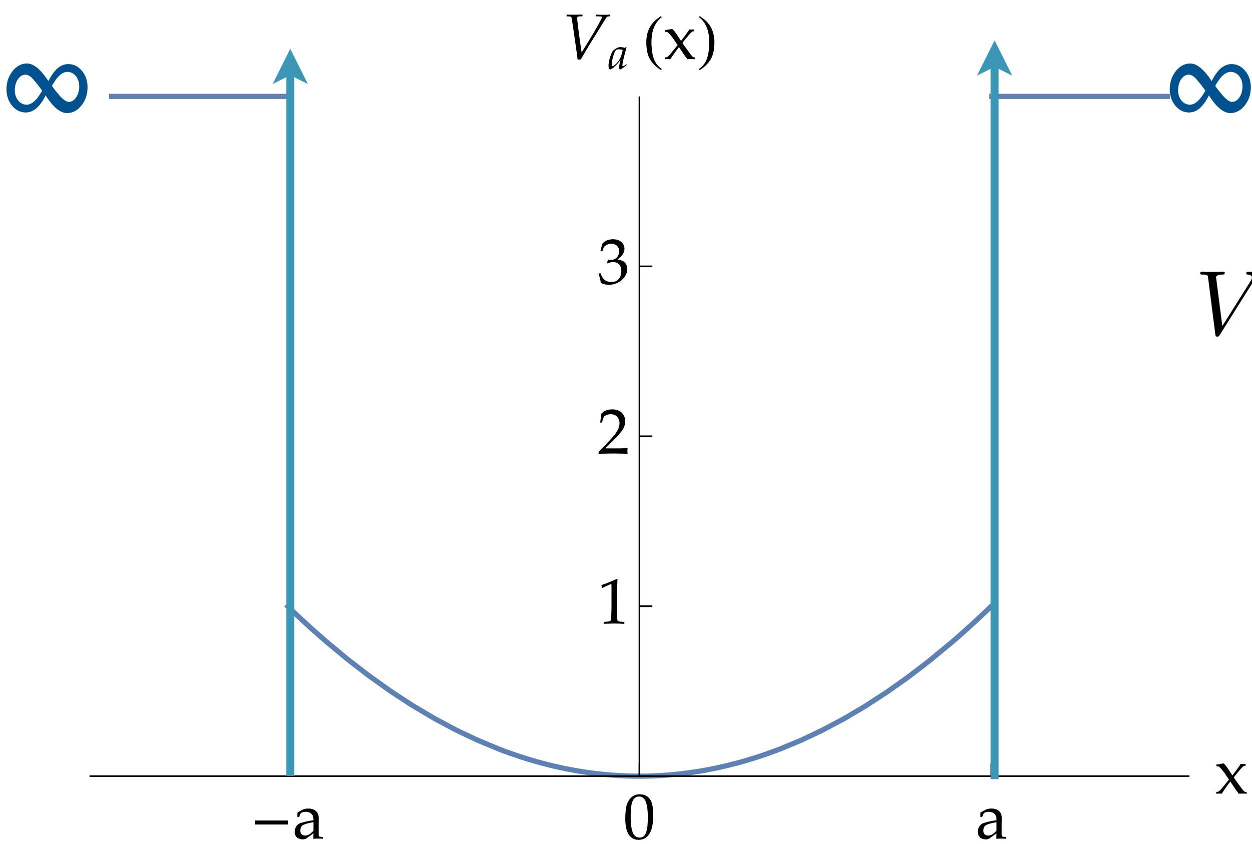
$$\epsilon_2 > \epsilon_1 \quad \psi_2(b)\psi_1'(b) - \psi_2(a)\psi_1'(a) = (\epsilon_2 - \epsilon_1)\int_a^b dx\, \psi_1\psi_2 + \int_a^b dx \int d\bar{x} V(x,\bar{x})\left\{\psi_1(x)\psi_2(\bar{x}) - \psi_2(x)\psi_1(\bar{x})\right\}$$

Proof 2
Continuous procedure

$$\left[\frac{\hat{p}^2}{2m} + V(x)\right]\psi_n(x) = \epsilon_n \psi_n(x)$$

UNIVERSITY OF SURREY

- Define family of potentials:



$$V_a(x) = \begin{cases} V(x), & -a < x < a \\ \infty, & |x| > a \end{cases}$$

- For sufficiently small a eigenfunctions are known

$$\psi_n(x) = \begin{cases} A\cos\left(\frac{n\pi}{2a}x\right), & n = 0, 2, 4, \cdots \\ A\sin\left(\frac{n\pi}{2a}x\right), & n = 1, 3, 5, \cdots \end{cases}$$

- Increase a - can we develop new nodes?

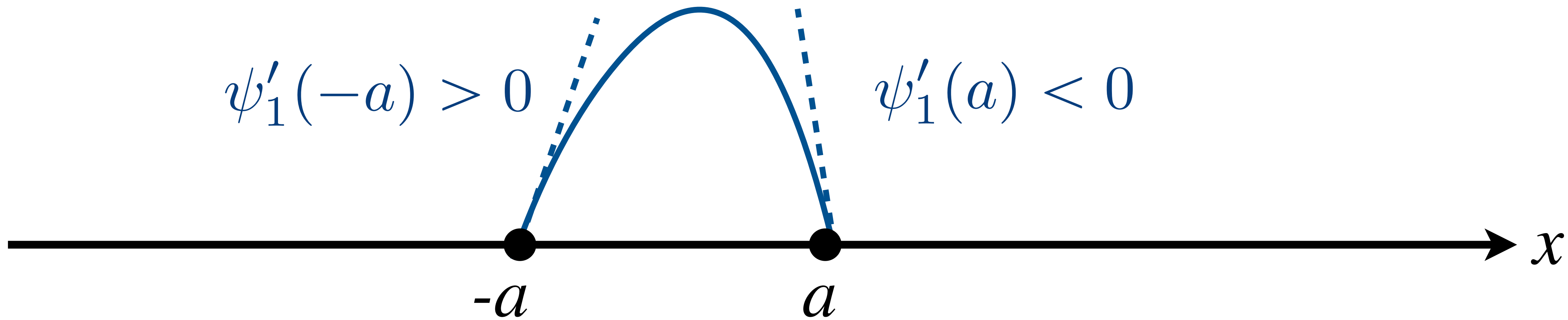
Moriconi, American Journal of Physics ***75****, 284 (2007)*

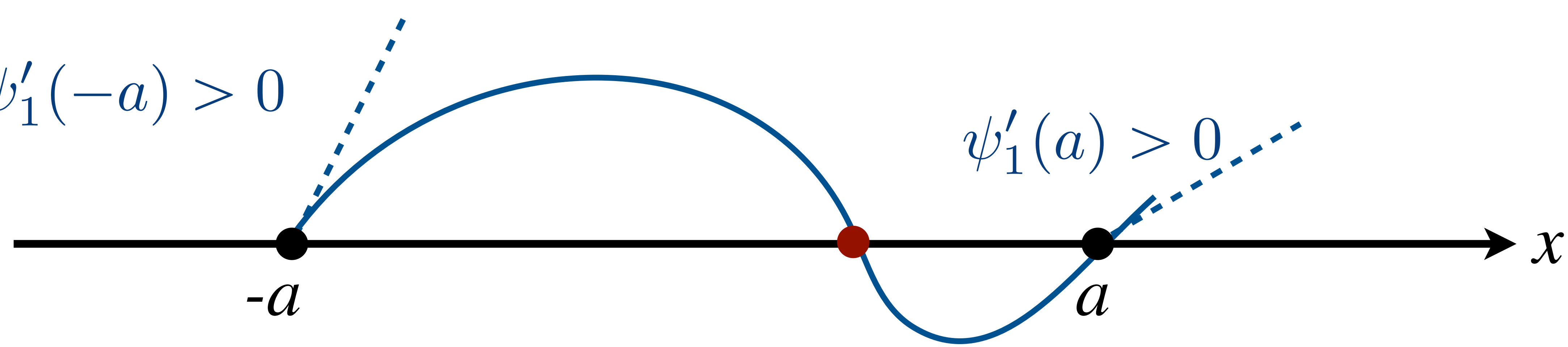
Proof 2

$$\left[\frac{\hat{p}^2}{2m} + V(x)\right]\psi_n(x) = \epsilon_n \psi_n(x)$$

UNIVERSITY OF SURREY

Case 1: one derivative changes sign

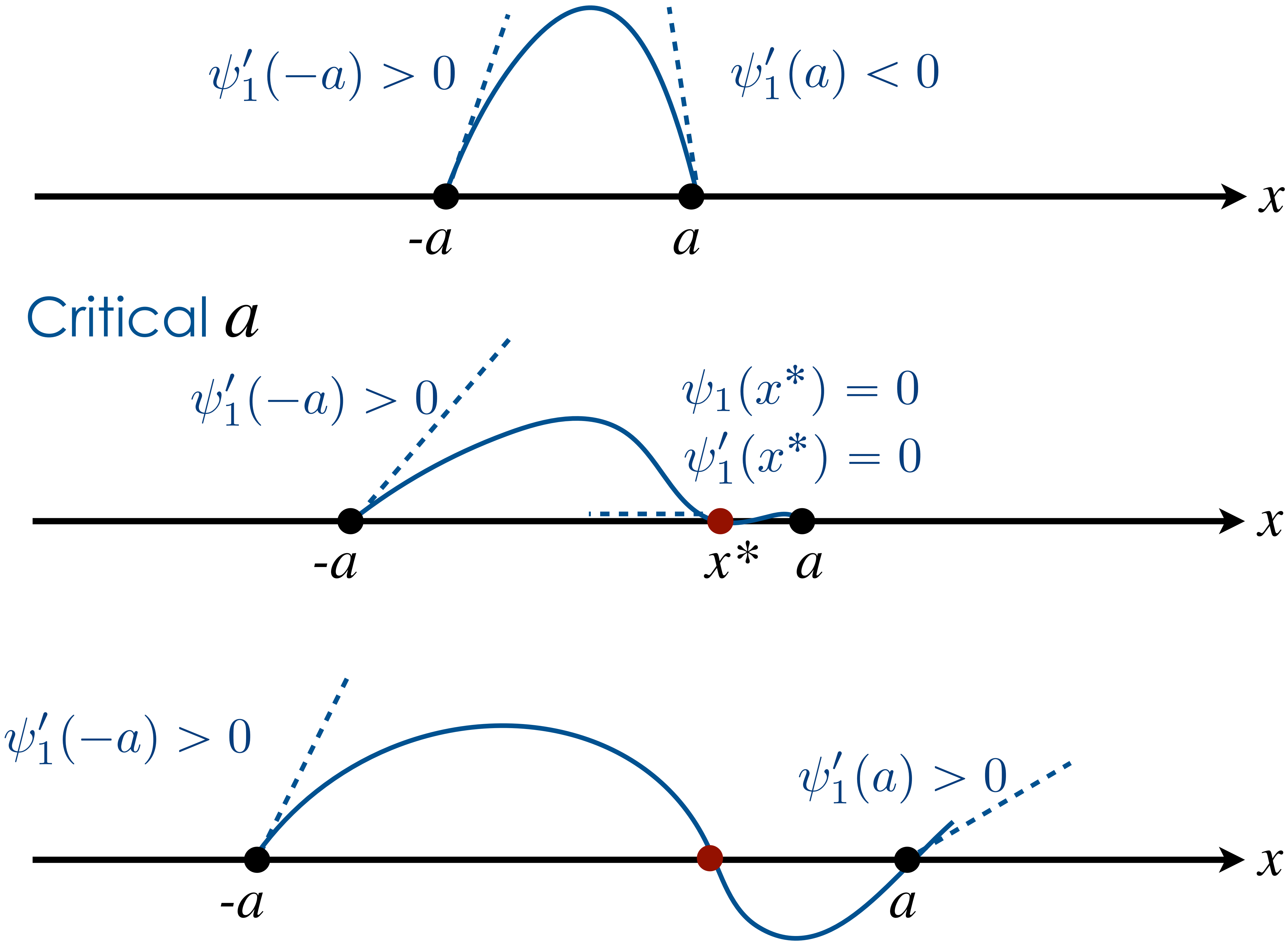




Proof 2

$$\left[\frac{\hat{p}^2}{2m} + V(x)\right]\psi_n(x) = \epsilon_n \psi_n(x)$$

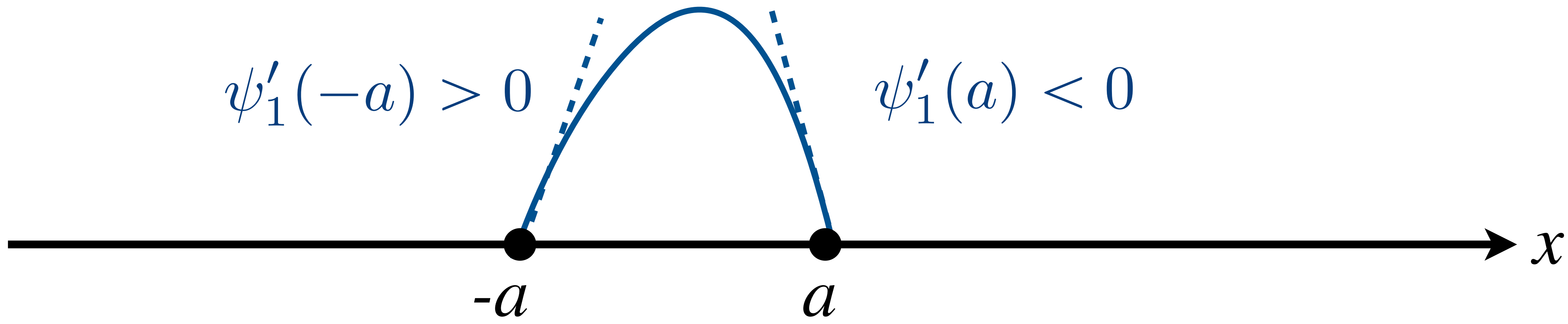
Case 1: one derivative changes sign

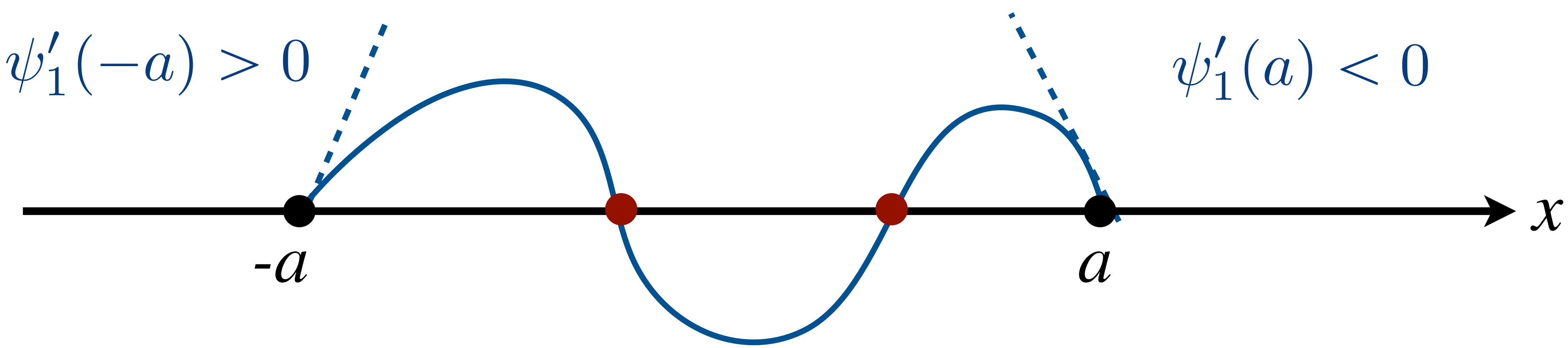


Proof 2

$$\left[\frac{\hat{p}^2}{2m}+V(x)\right]\psi_n(x)=\epsilon_n\psi_n(x)$$

Case 2: no change of sign

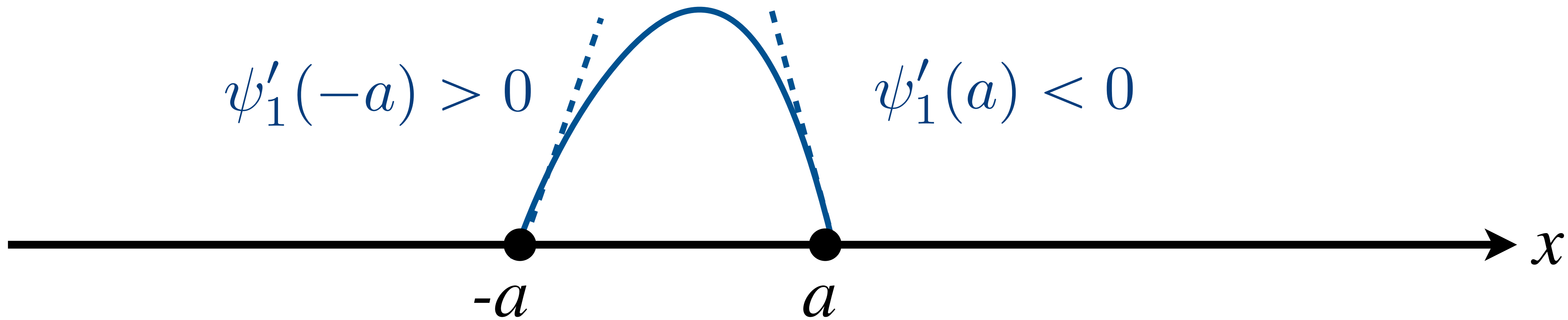




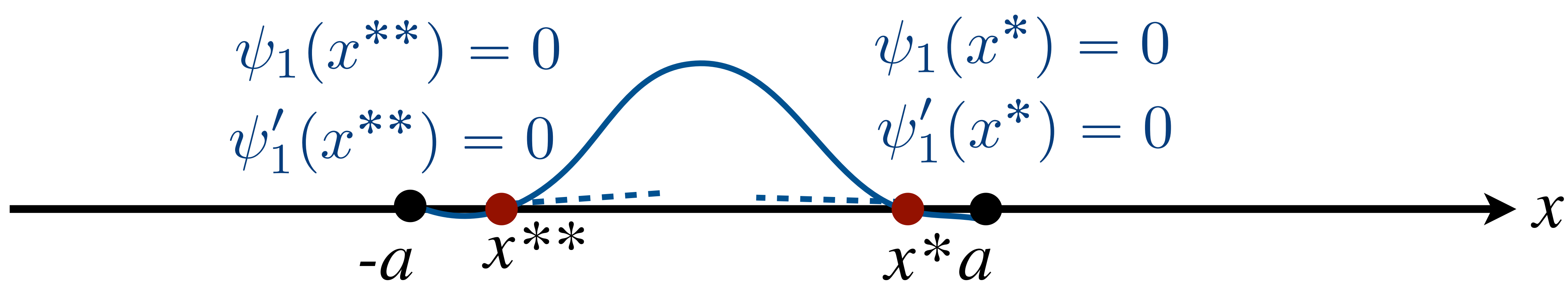
Proof 2

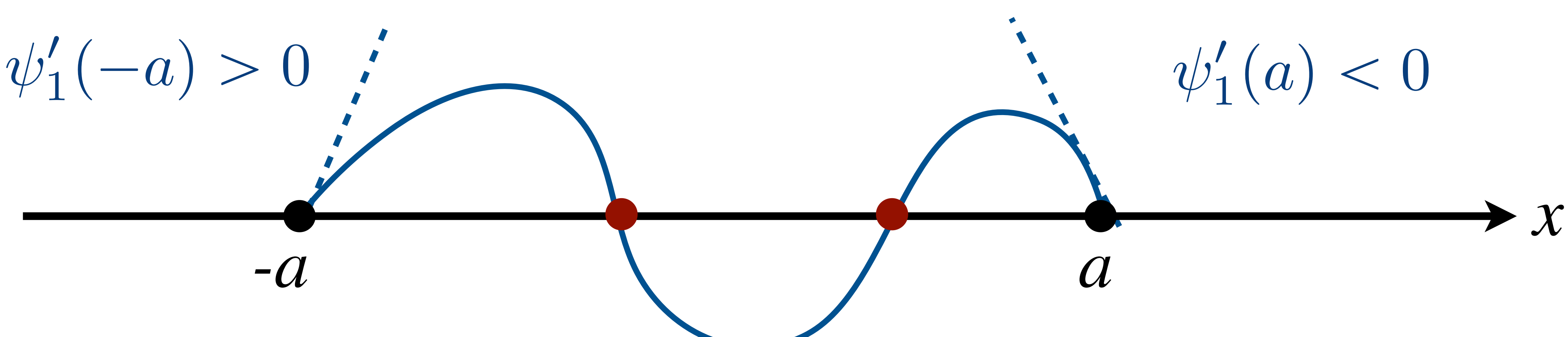
$$\left[\frac{\hat{p}^2}{2m} + V(x)\right]\psi_n(x) = \epsilon_n \psi_n(x)$$

Case 2: no change of sign



Critical a



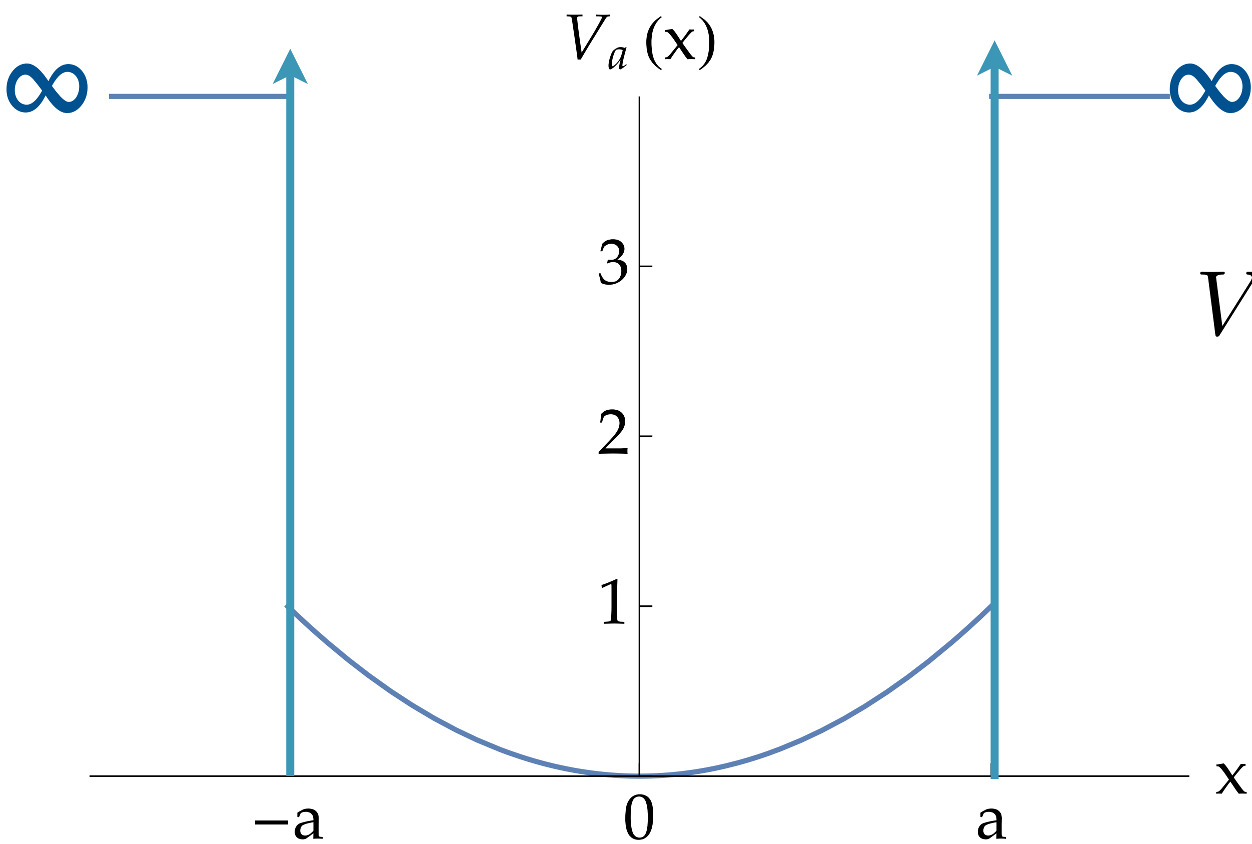


Proof 2

$$\left[\frac{\hat{p}^2}{2m} + V(x)\right]\psi_n(x) = \epsilon_n \psi_n(x)$$

UNIVERSITY OF SURREY

- Define family of potentials:



$$V_a(x) = \begin{cases} V(x), & -a < x < a \\ \infty, & |x| > a \end{cases}$$

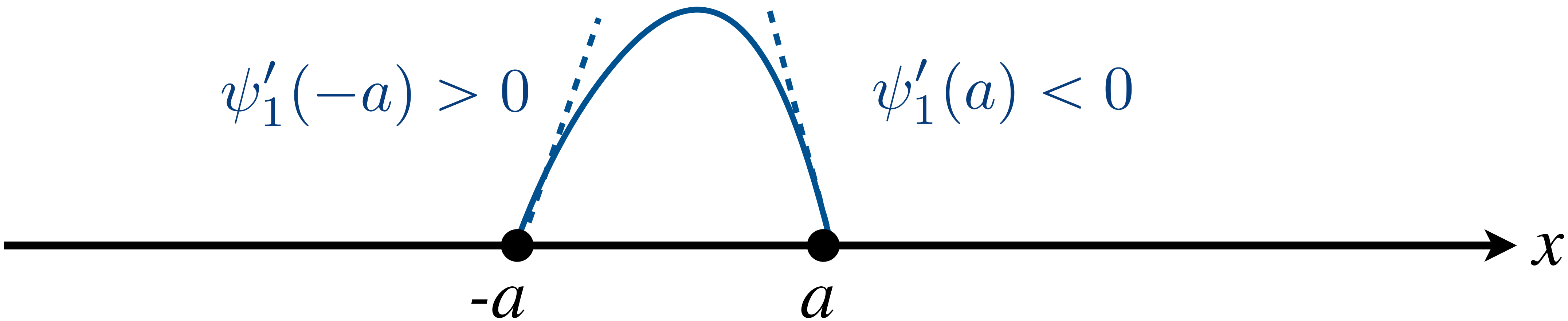
- In taking a→∞, we **cannot** generate new nodes
- Number of nodes same as infinite well

$$\mathcal{N}_n = n$$

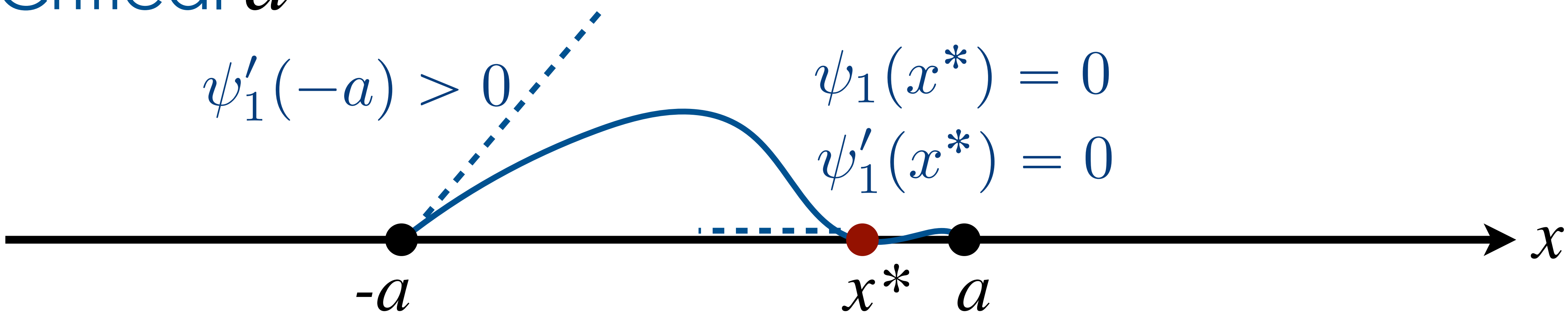
*Moriconi, American Journal of Physics **75**, 284 (2007)*

Proof 2: non-local case

Case 1: one derivative changes sign



Critical a



$$\frac{\hat{p}^2}{2m}\psi_n(x) + \int d\bar{x} V(x,\bar{x})\psi_n(\bar{x}) = \epsilon_n \psi_n(x)$$

A generic family of potentials

UNIVERSITY OF SURREY

- Start from (solvable) **local** Hamiltonian

$$\left[\frac{\hat{p}^2}{2m} + V(x)\right]\psi_n(x) = \epsilon_n \psi_n(x)$$

- Add **non-local** hamiltonian of form

$$V_k(x,x') = \alpha_k \psi_k(x)^* \psi_k(x')$$

- Solution to the problem is then **analytical**

$$\left[\frac{\hat{p}^2}{2m} + V(x) + \int dx' V_k(x,x')\right]\tilde{\psi}_n(x) = \tilde{\epsilon}_n \tilde{\psi}_n(x)$$

$$\tilde{\psi}_n(x) = \psi_n(x)$$

$$\tilde{\epsilon}_n = \begin{cases} \epsilon_n, & n \neq k \\ \epsilon_k + \alpha_k, & n = k \end{cases}$$

Bulgac, *Nuclear Physics A* **487** 251 (1998)

Example: harmonic oscillator

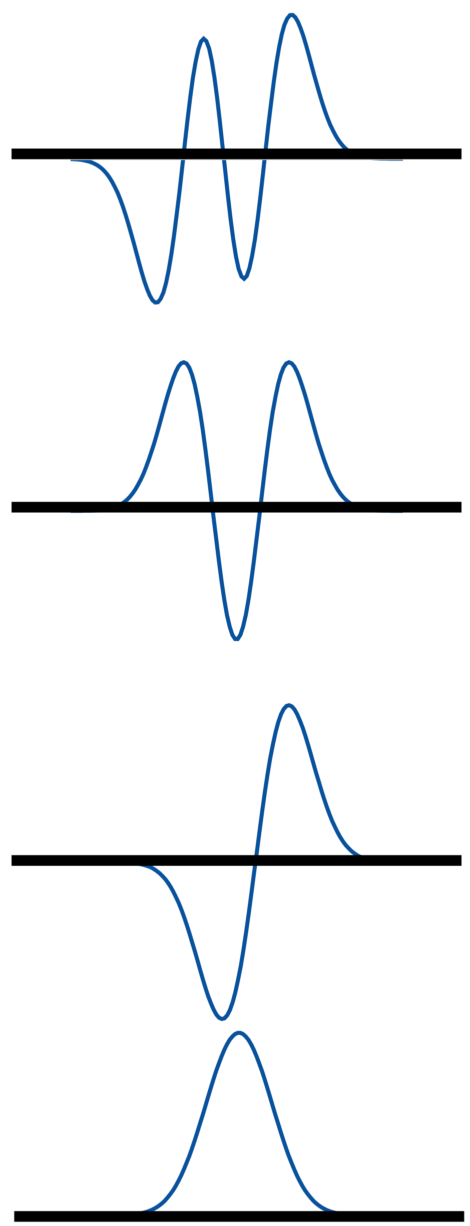
Local

$$n = 3,\ \epsilon_3 = \frac{7}{2}\hbar\omega$$

$$n = 2,\ \epsilon_2 = \frac{5}{2}\hbar\omega$$

$$n = 1,\ \epsilon_1 = \frac{3}{2}\hbar\omega$$

$$n = 0,\ \epsilon_0 = \frac{1}{2}\hbar\omega$$



Non-local

$$k = 0,\ \alpha_0 = \frac{1}{2}\hbar\omega$$

Example: harmonic oscillator

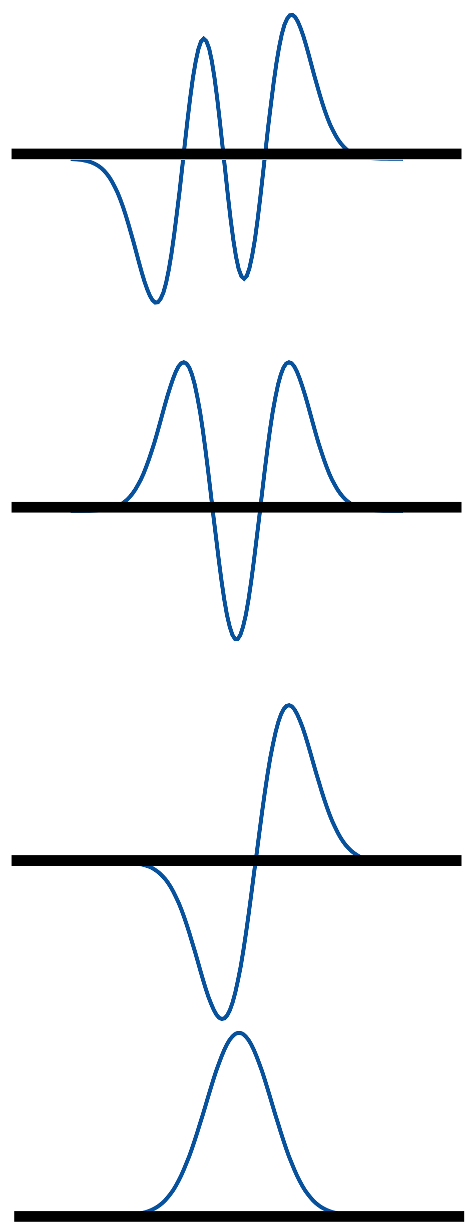
Local

$$n = 3,\ \epsilon_3 = \frac{7}{2}\hbar\omega$$

$$n = 2,\ \epsilon_2 = \frac{5}{2}\hbar\omega$$

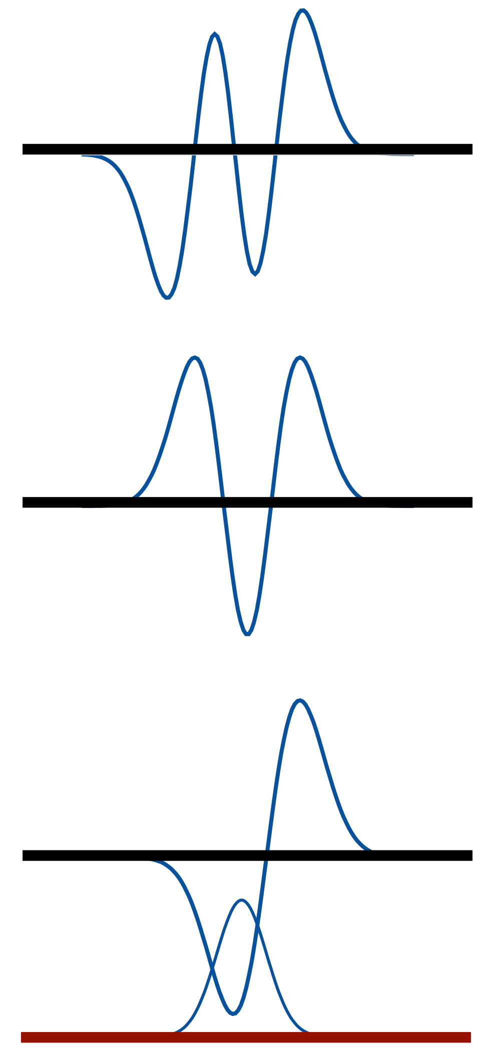
$$n = 1,\ \epsilon_1 = \frac{3}{2}\hbar\omega$$

$$n = 0,\ \epsilon_0 = \frac{1}{2}\hbar\omega$$



Non-local

$$k = 0,\ \alpha_0 = \frac{1}{2}\hbar\omega$$



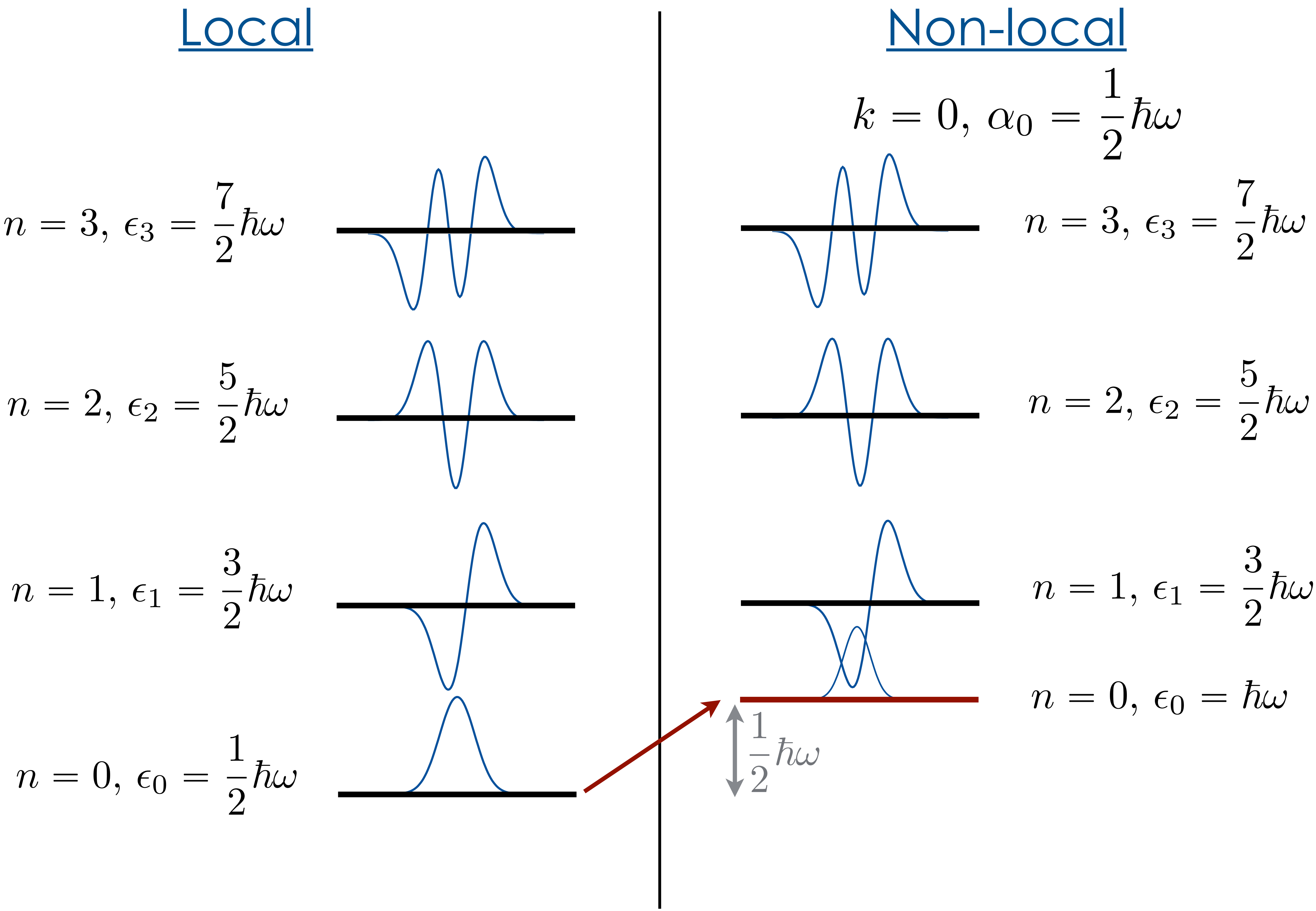
$$n = 3,\ \epsilon_3 = \frac{7}{2}\hbar\omega$$

$$n = 2,\ \epsilon_2 = \frac{5}{2}\hbar\omega$$

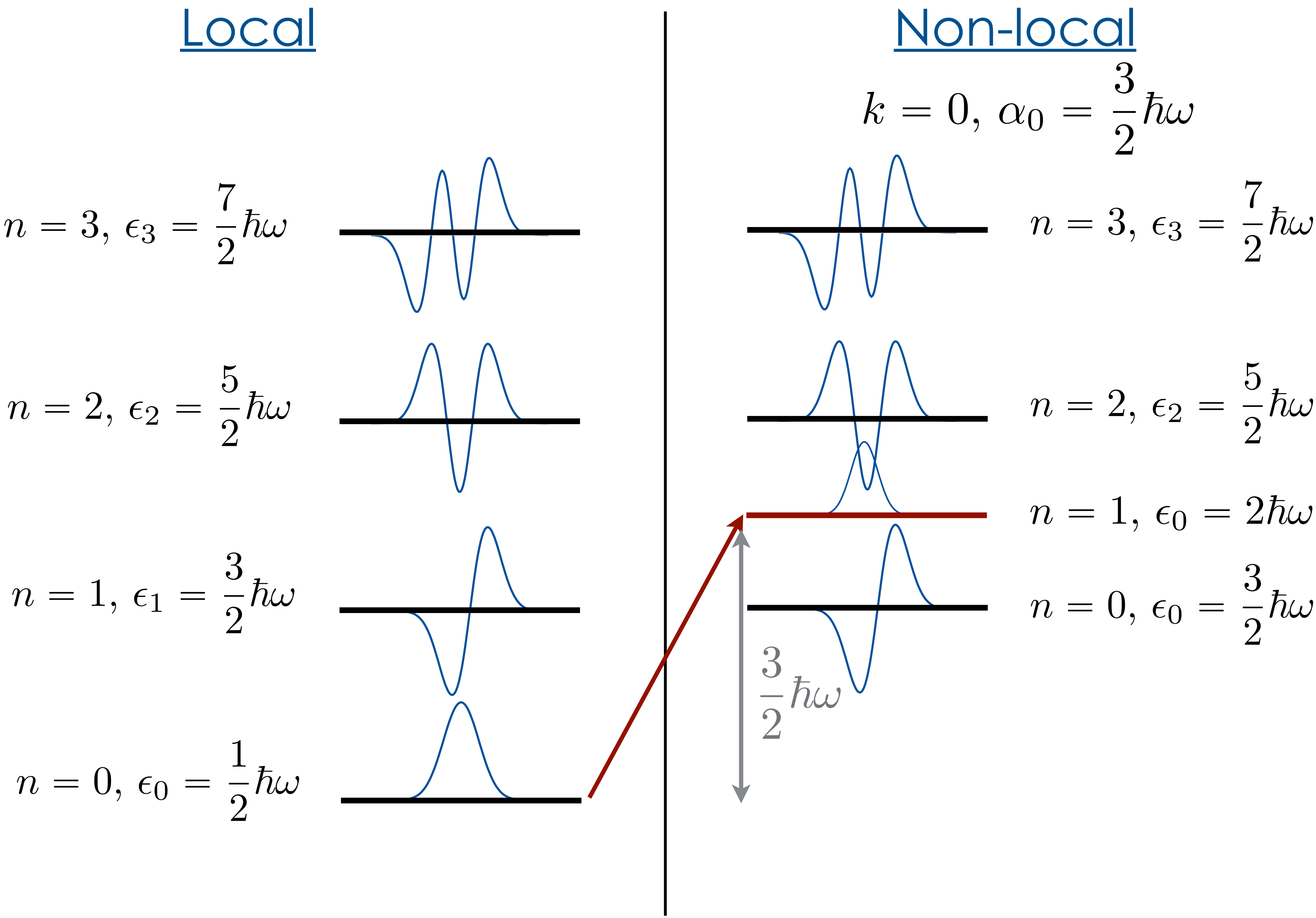
$$n = 1,\ \epsilon_1 = \frac{3}{2}\hbar\omega$$

$$n = 0,\ \epsilon_0 = \hbar\omega$$

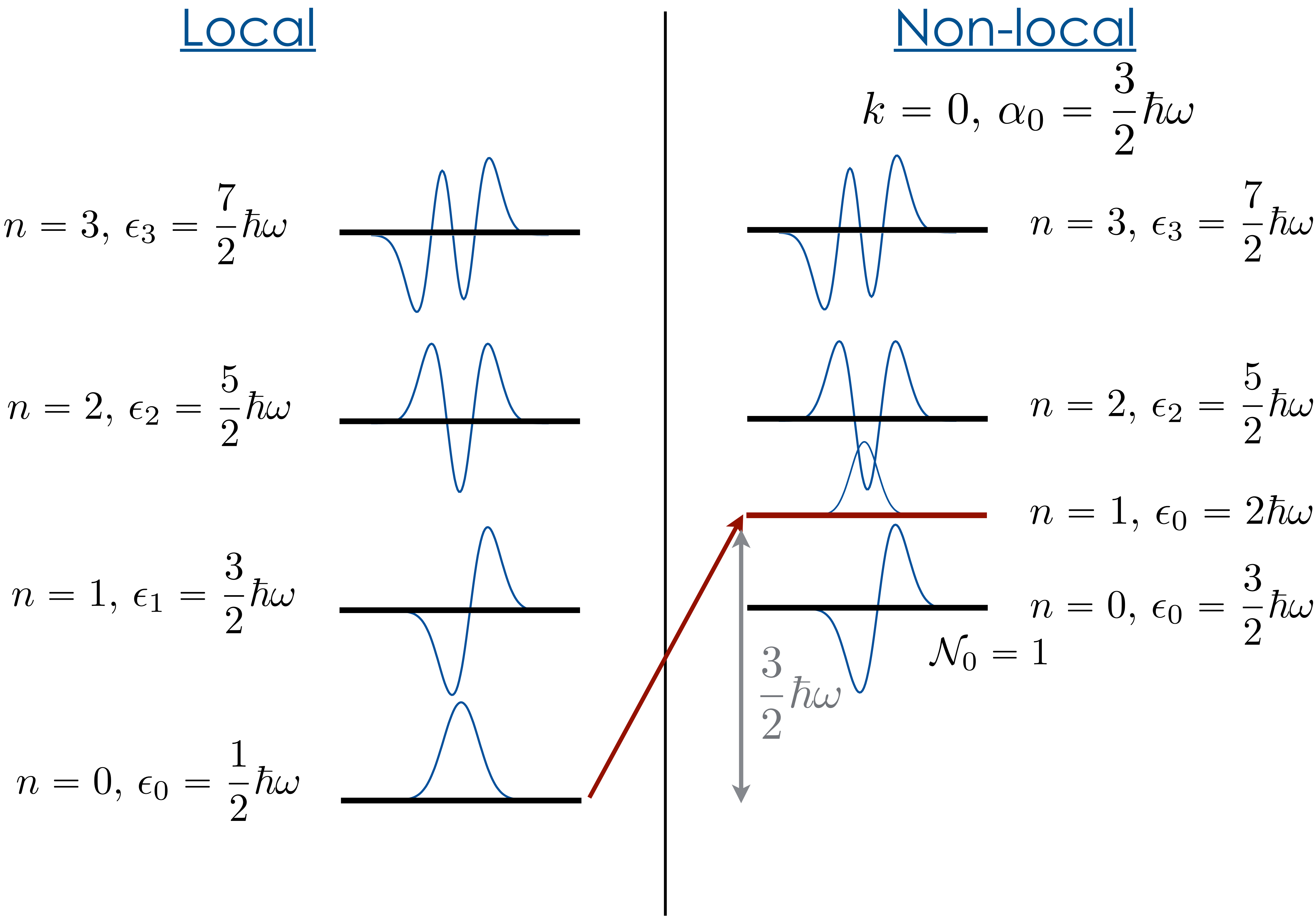
Example: harmonic oscillator



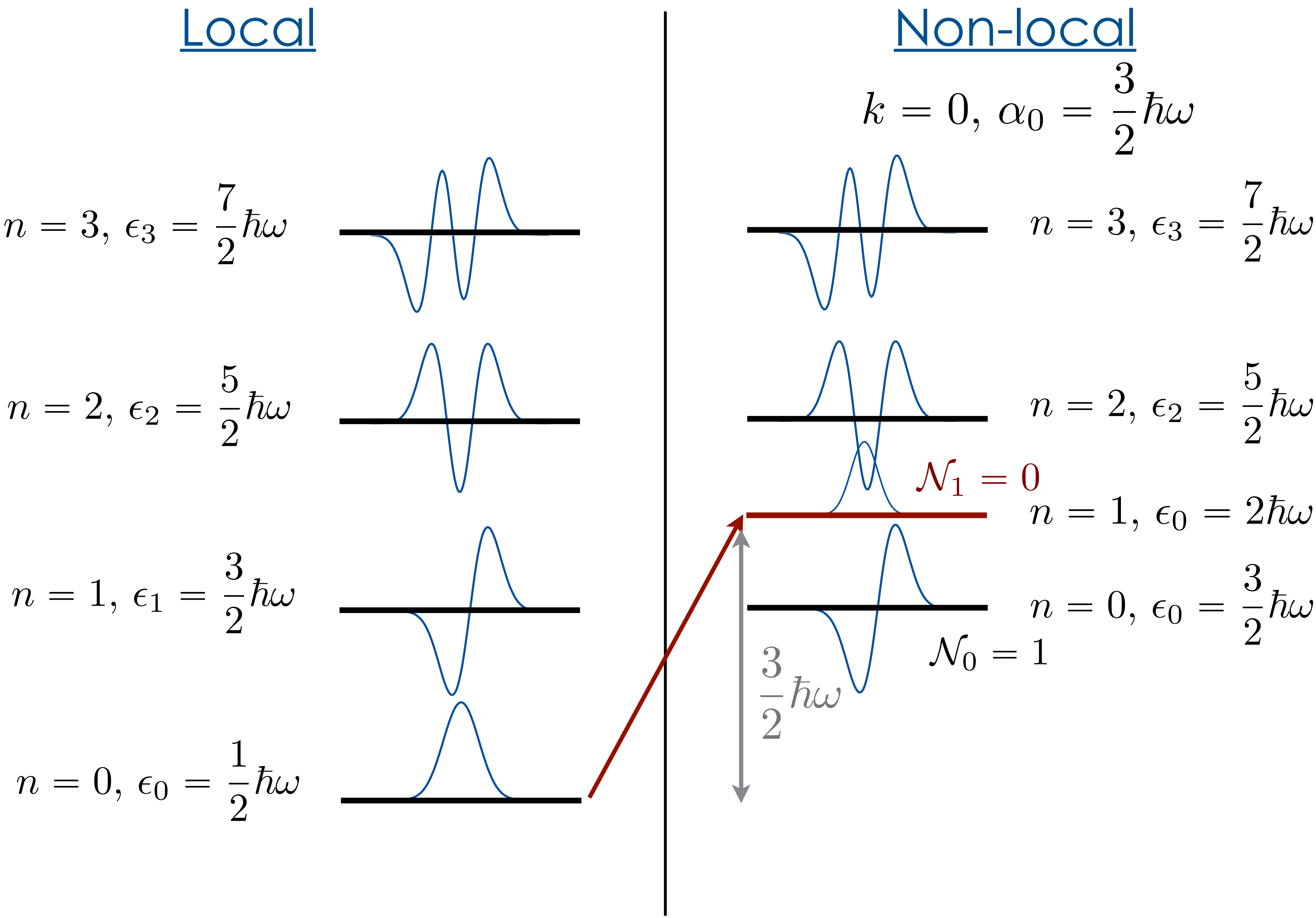
Example: harmonic oscillator



Example: harmonic oscillator

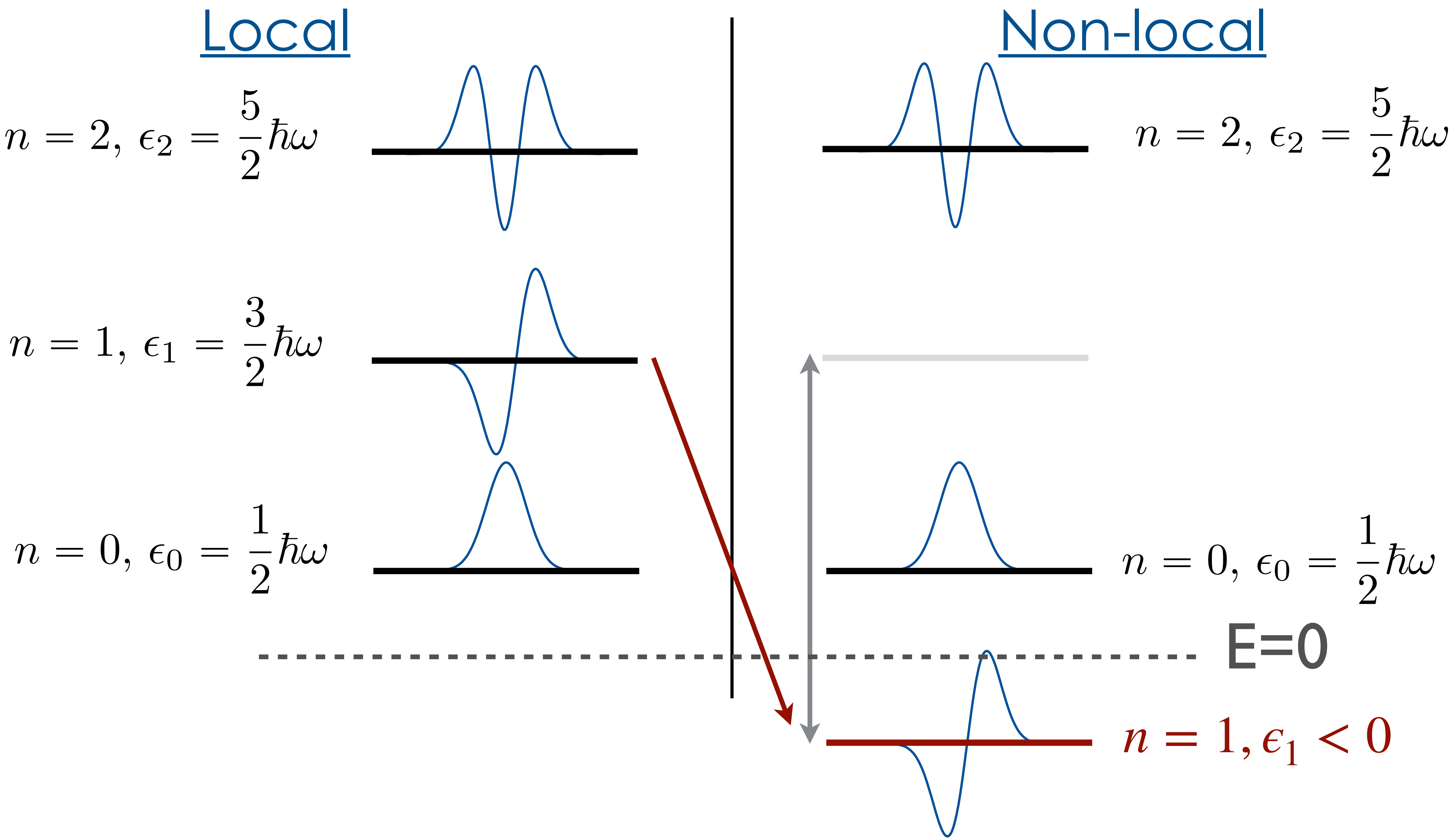


Example: harmonic oscillator



What can one do now?

- Dial $\alpha_k<0$ to get attractive non-local term
- Changes number of nodes too

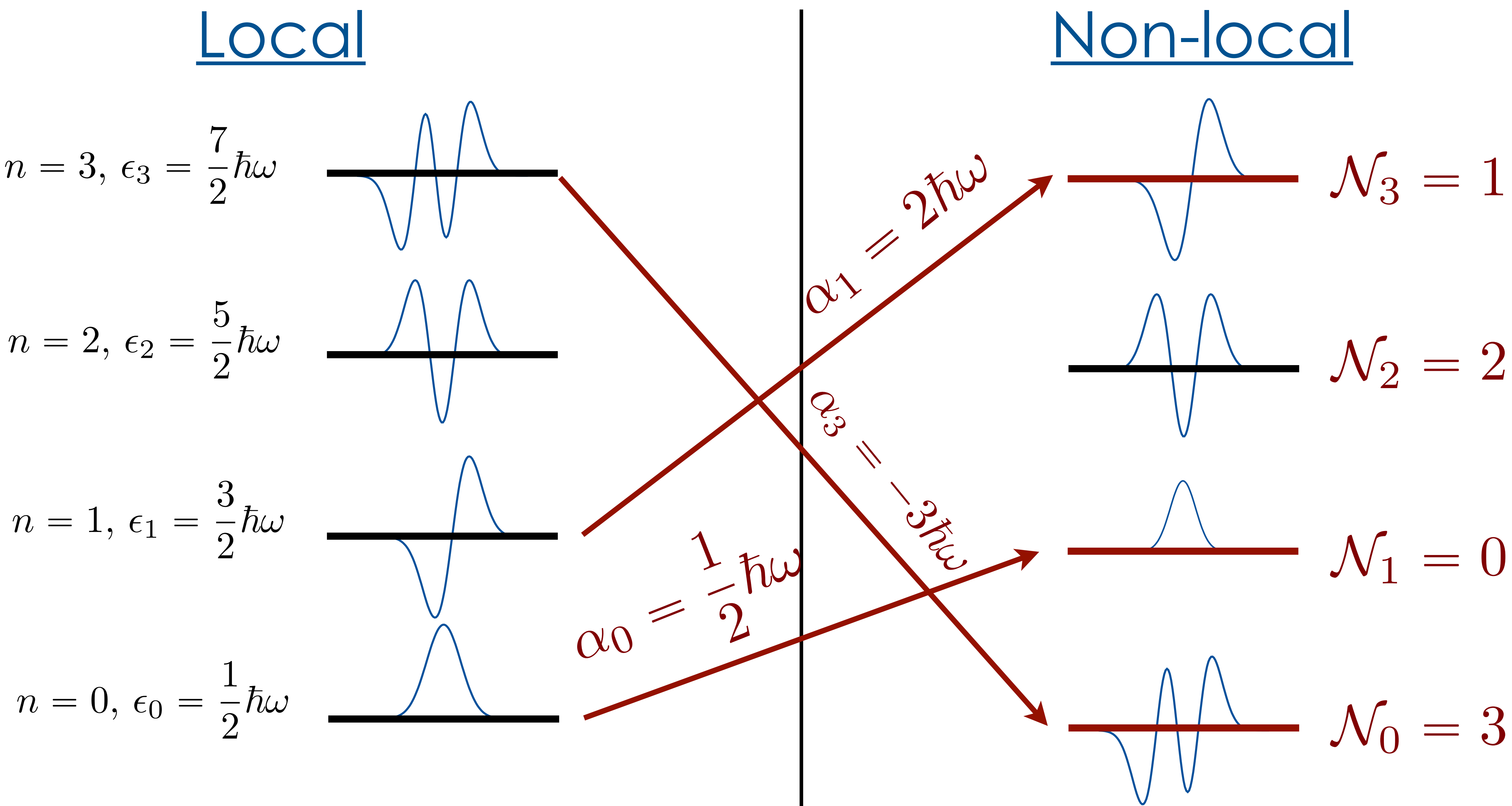


What can one do now?

- We can add more than one non-local potential:

$$\tilde{V}(x,x') = \sum_k \alpha_k \psi_k(x)^* \psi_k(x')$$

- One can **reorder** spectrum **at will**



Conclusion & outlook

Conclusion

*For a generic family of rank-n separable non-local potentials, there is **no** relation between **number of nodes** and **quantum number***

Conclusion & outlook

UNIVERSITY OF SURREY

Conclusion

*For a generic family of rank-n separable non-local potentials, there is **no** relation between **number of nodes** and **quantum number***

Outlook

- *Is this a feature specific to **rank-n** separable potentials?*
- *Are there **subsets of potentials** where connections can be drawn?*
- *Are there results of **integro-differential equation theory** that can be used here?*