Experimental Physics 3 - Em-Waves,Optics, Quantum mechanics

Lecture 28

Prof. Dr. Frank Cichos
WS 2022/23

Some dates in January and February

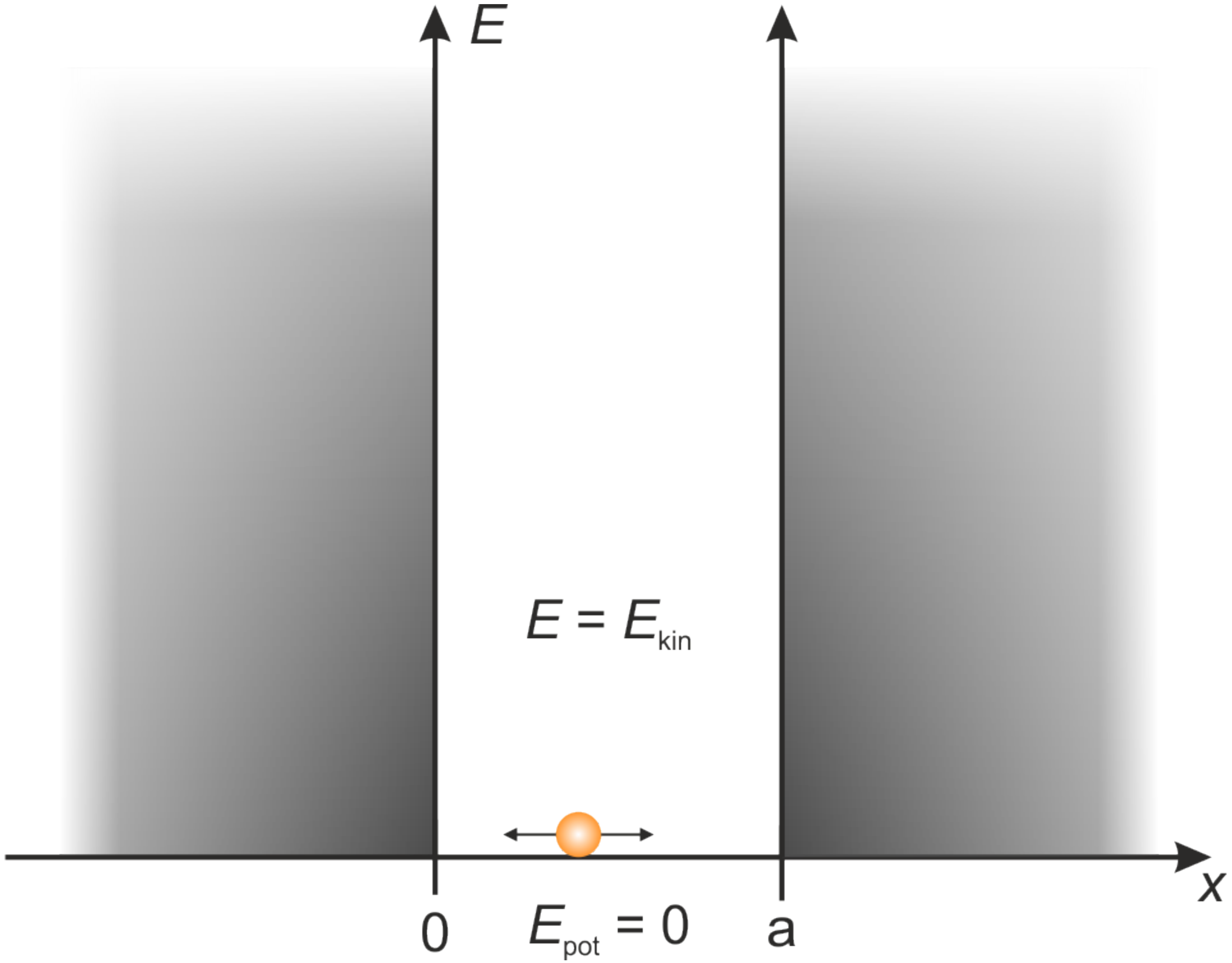
Mo	Tu	We	Th	Fr	Sa	Su
						1
2	3	4	5	6	7	8
9	10	11	12 Submission sheet 11	13	14	15
16	17	18	19 Submission mock exam	20	21	22
23	24	25	26 Submission sheet 12	27	28	29
30	31 Last Tuesday seminar	1	2 Last Thursday seminar Last lecture	3		

Exam: February 20, 2023, 9 am - 12 pm, 1 (one) DIN A4 page lettered

Re-exam: March 27, 2023, 9 am - 12 pm

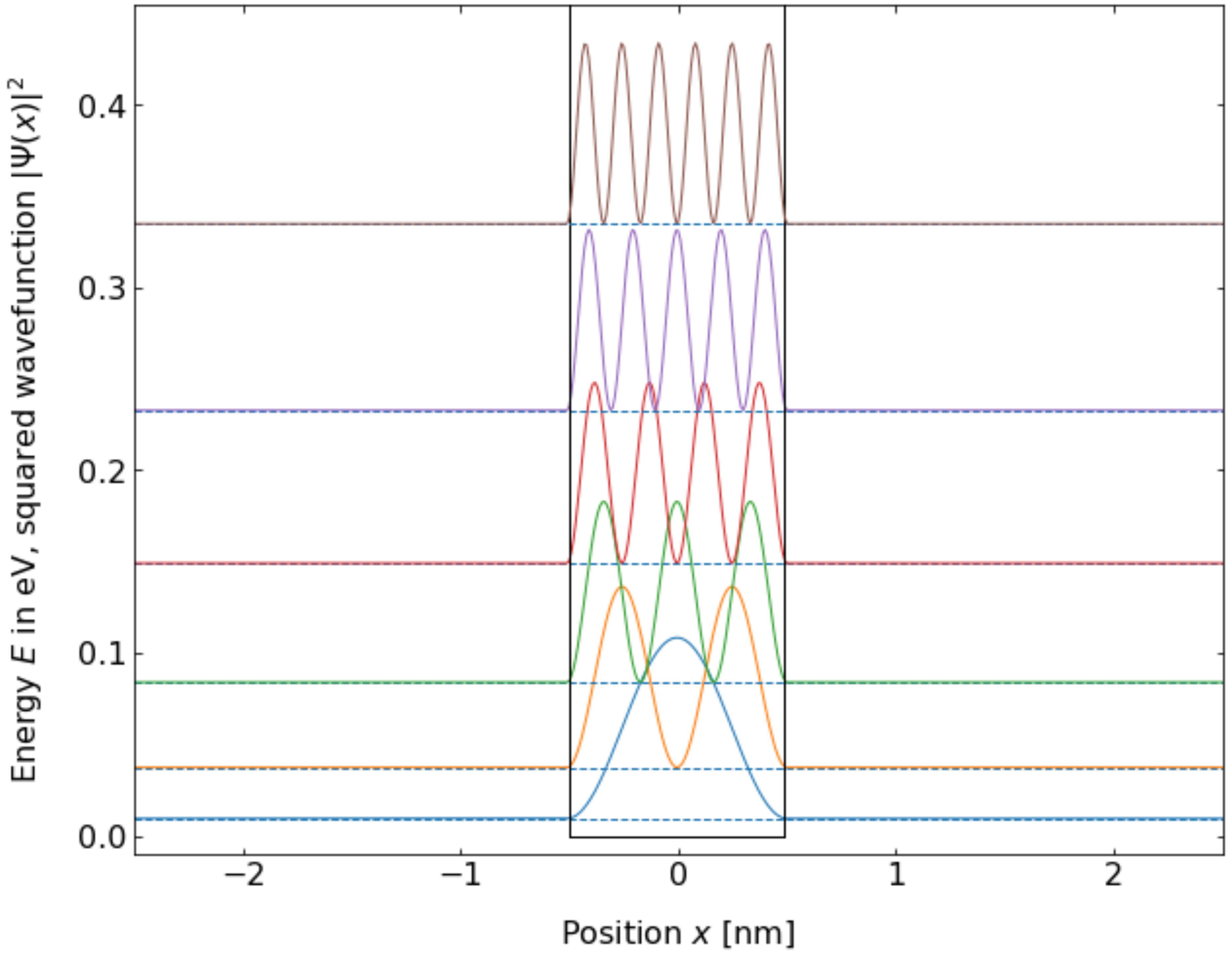
Recap - the potential well

Recap - infinite potential well



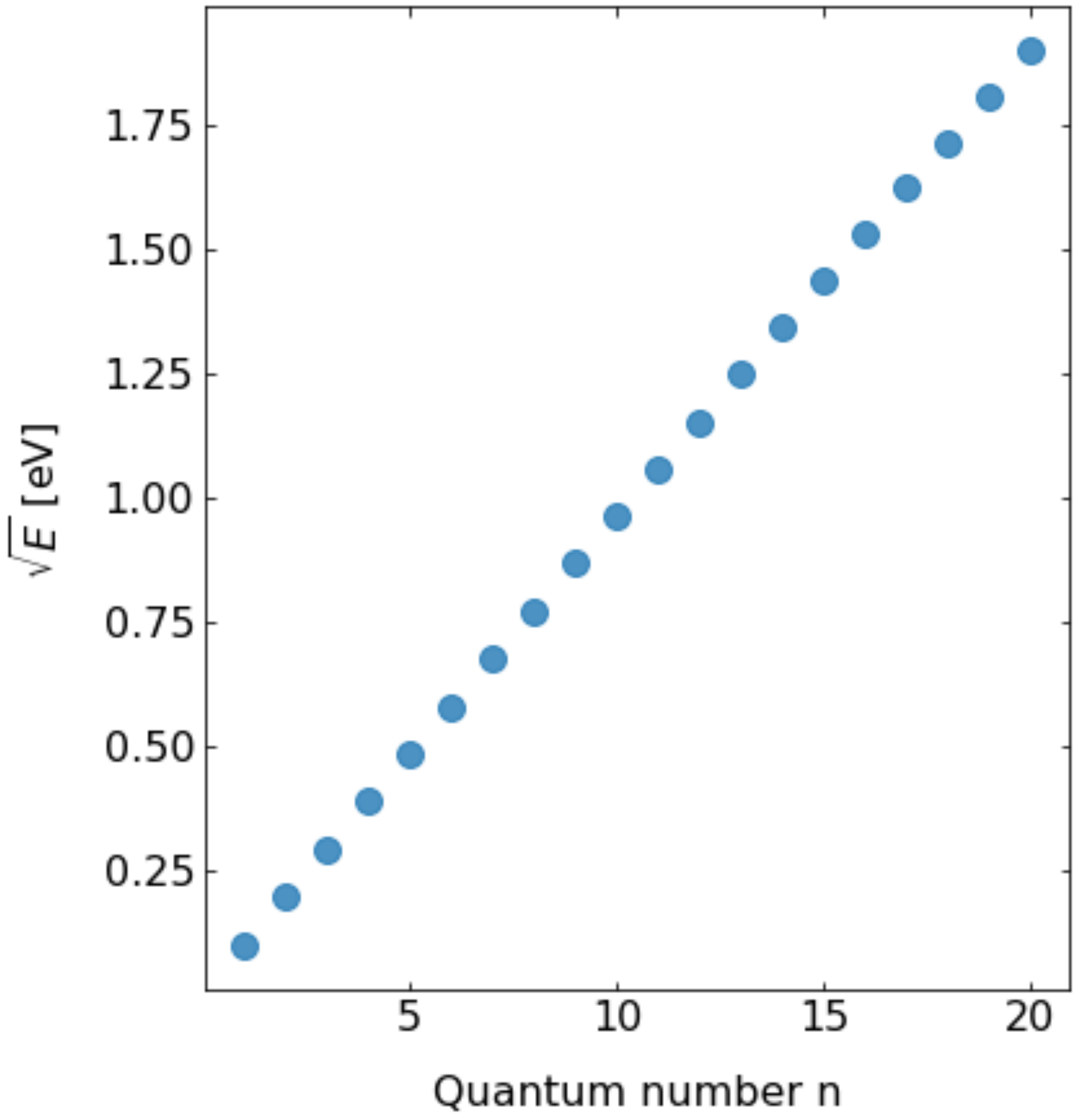
Recap - infinite potential well

$|\psi(x)|^2$

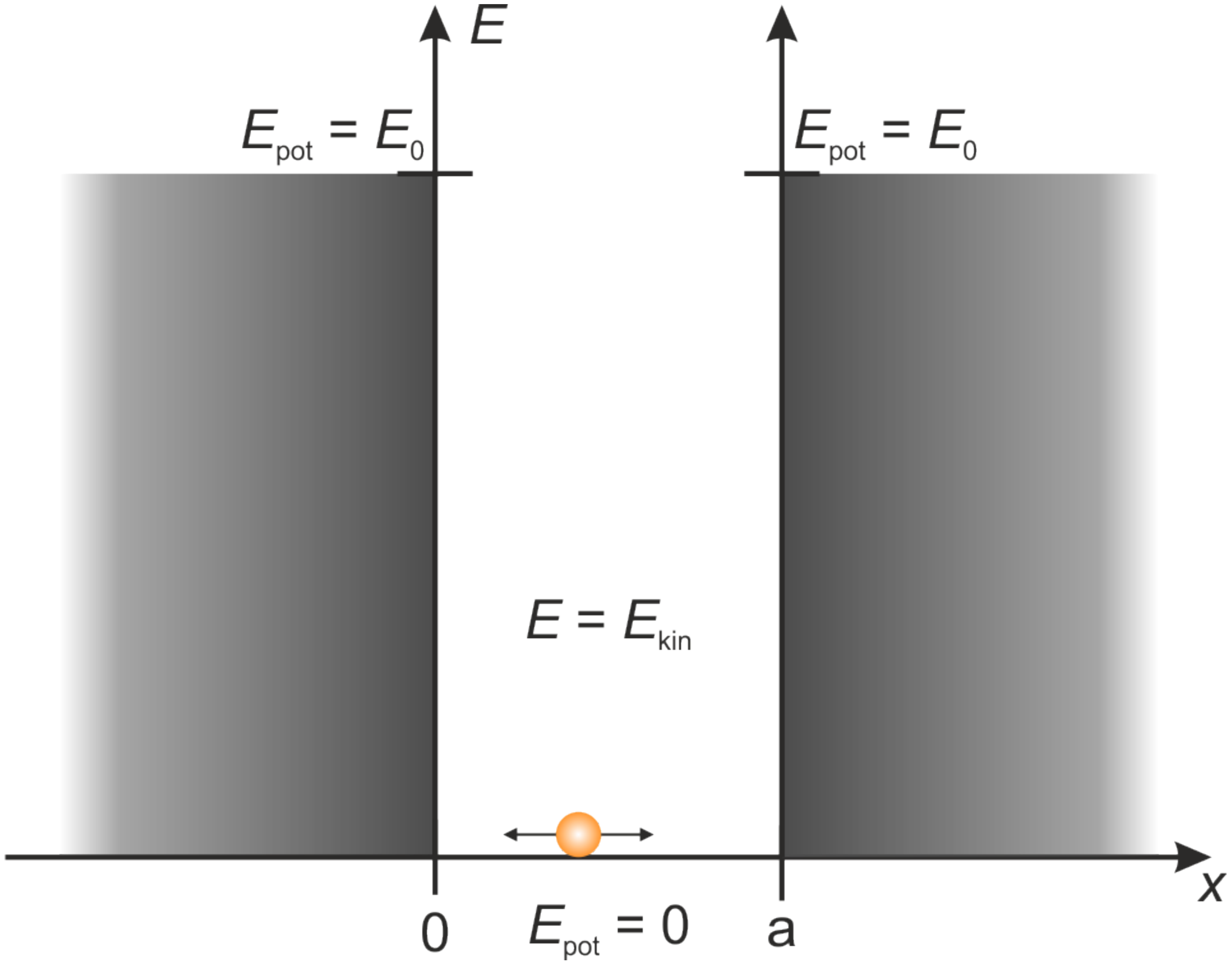


- No probability outside well
- $E_n \propto n^2$
- $E_n \propto a^{-2}$
- $E_1 > 0$

$\sqrt{E_n}$

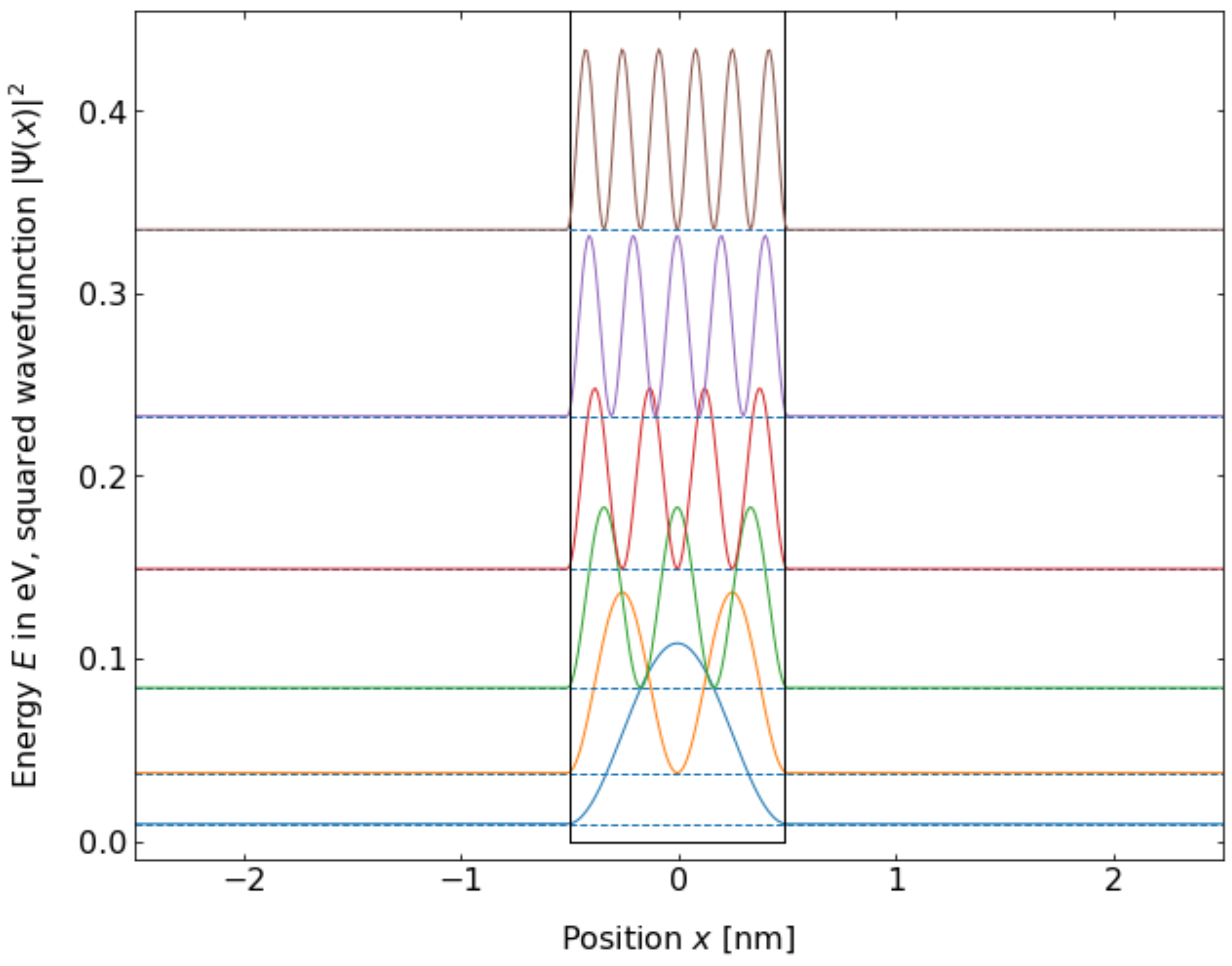


Recap - finite potential well

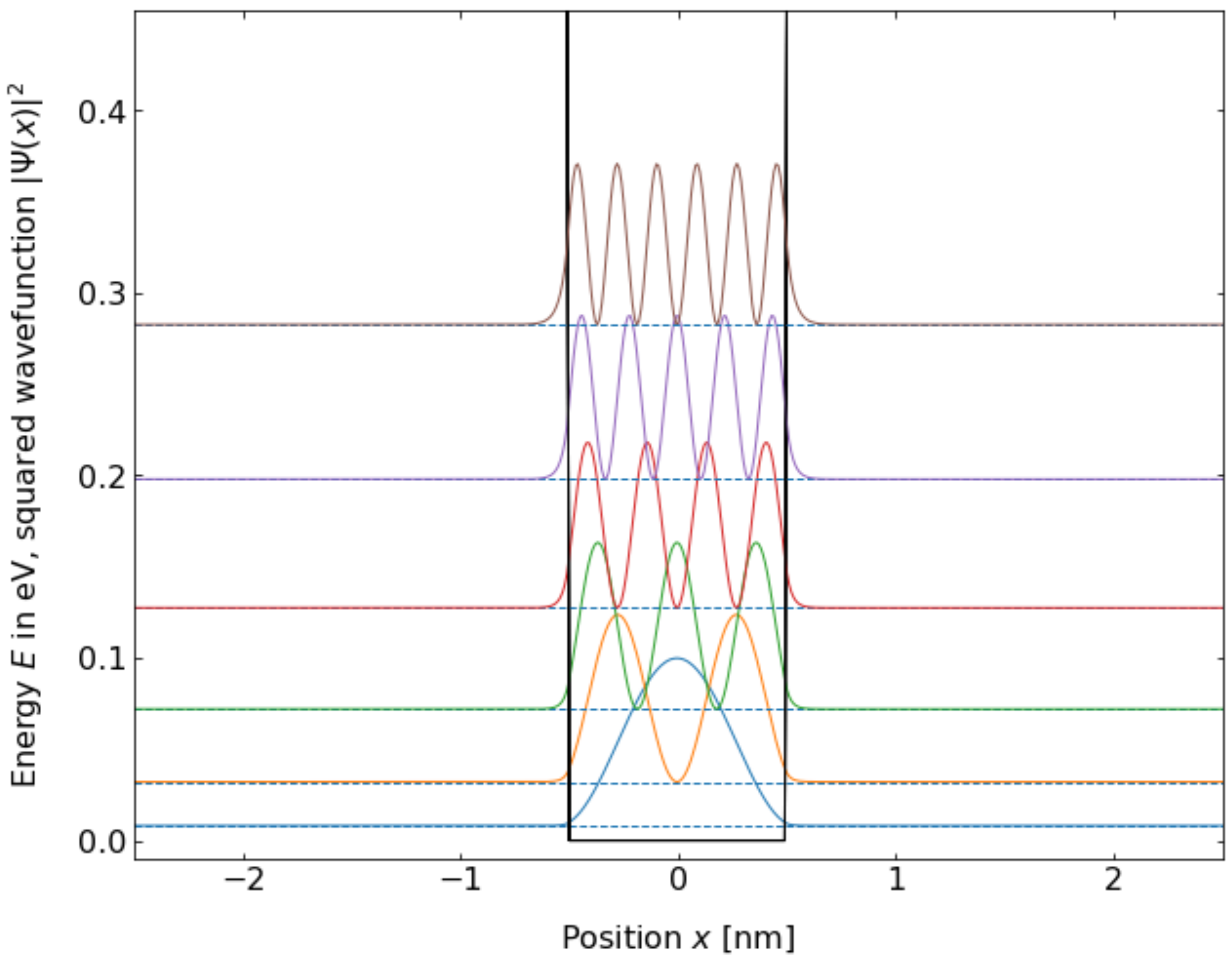


Recap - finite potential well

Infinite $\left|\psi(x)\right|^2$



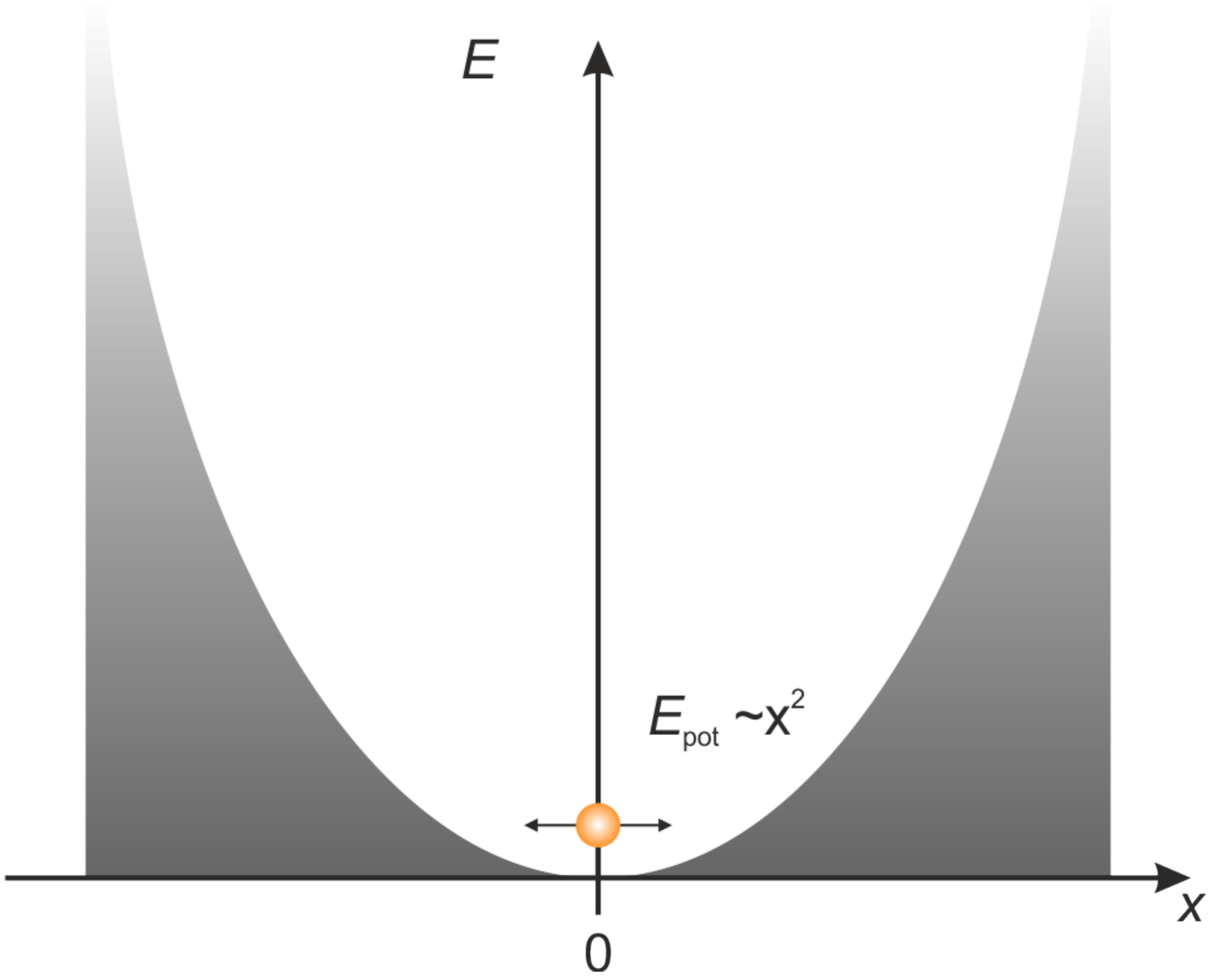
Finite $\left|\psi(x)\right|^2$



- Probability density decays exponentially inside potential wall
- Increased position uncertainty Δx
- Reduced momentum uncertainty Δp_x
- Thus, reduced energy E_n

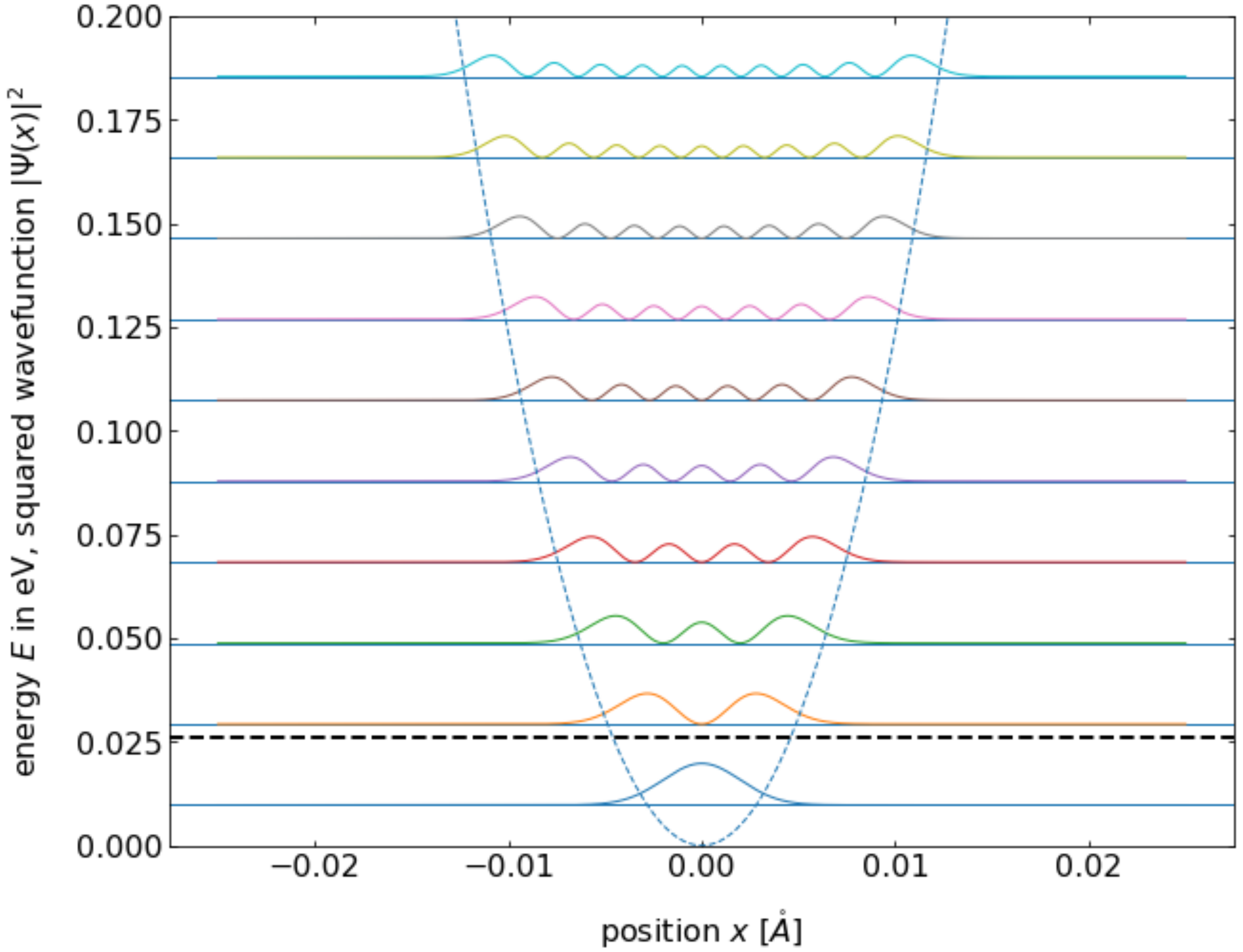
Recap - the harmonic oscillator

Recap - harmonic oscillator



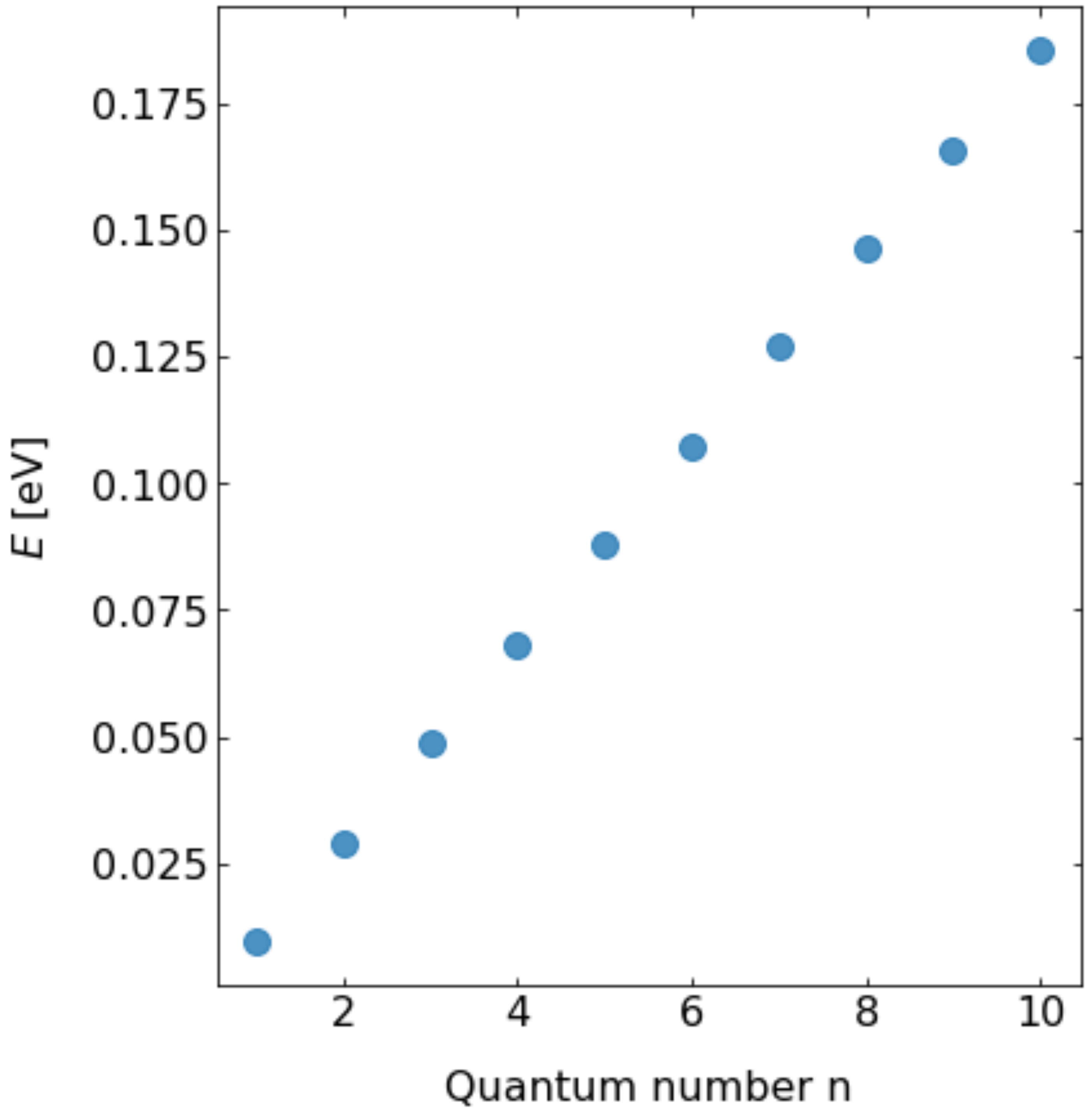
Recap - infinite potential well

$$|\psi(x)|^2$$



- $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$
- $E_n \propto n$
- $E_0 = \frac{1}{2}\hbar\omega$

$$E_n$$



The correspondence principle

The correspondence principle

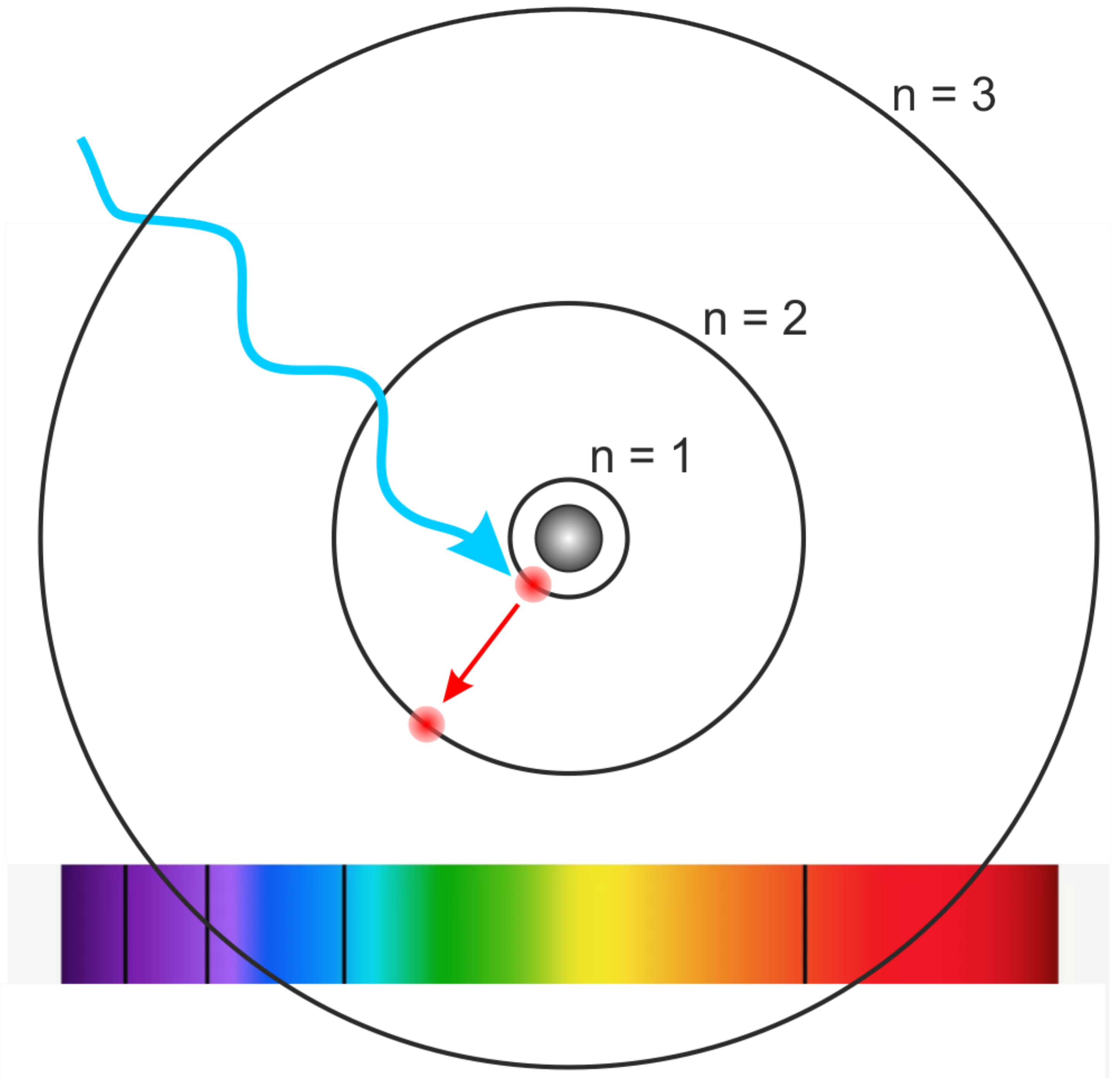
1st Bohr postulate (phase-integral condition):
Electrons propagate at particular orbits,
there they do not emit energy

$$\oint p\mathrm{d}q = nh \longleftrightarrow \mu v r_n = n\hbar \longleftrightarrow 2\pi r_n = nh/(\mu v)$$

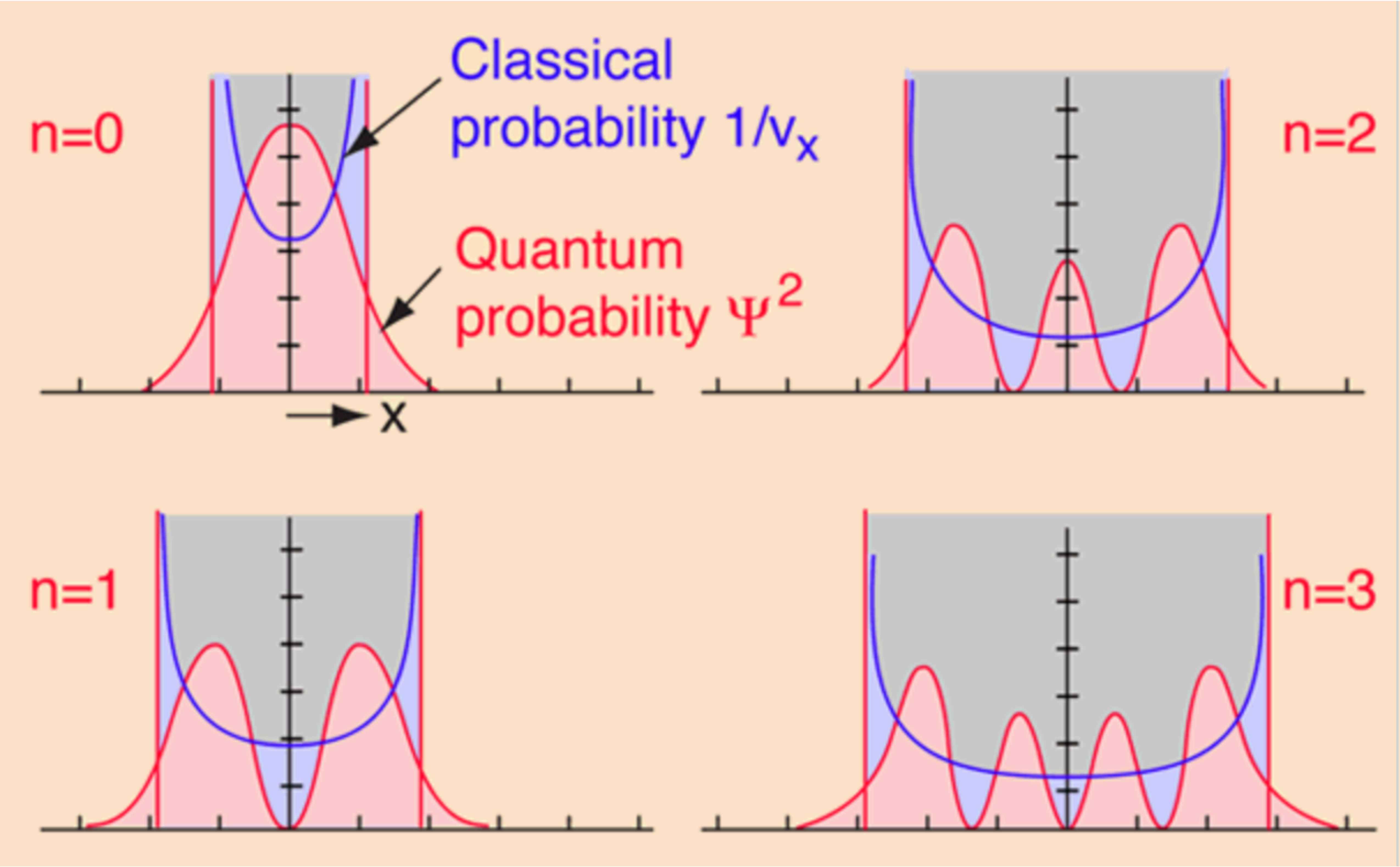
2nd Bohr postulate (frequency condition):
An atom can only change its energy through transition from one stationary state into another stationary state by absorption or emission of a photon

$$h\nu_{ik} = \left| E_i - E_k \right|$$

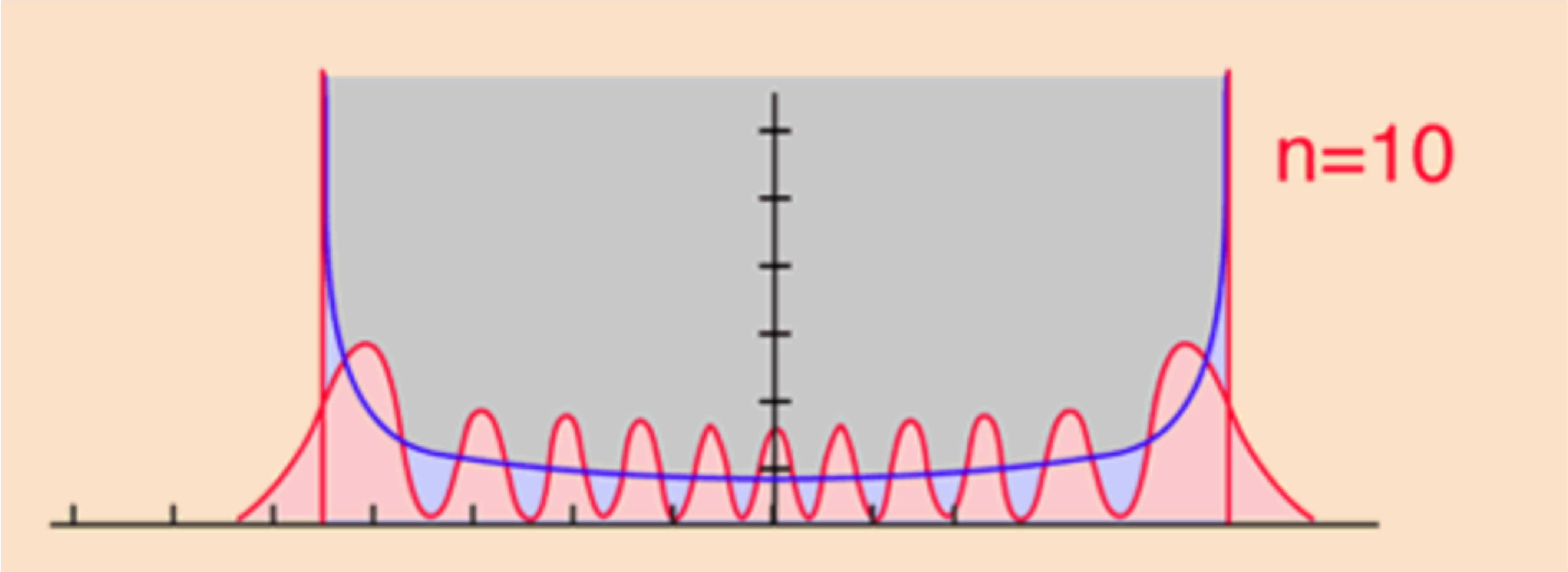
3rd Bohr postulate (correspondence principle):
The 1st and 2nd postulate have to correspond to the laws of classical physics for great n and big r_n



The correspondence principle - Bohr's 3rd postulate



- Example: harmonic oscillator
- For $n = 1$ qm. probability density contradicts classical probability
- For great n both approaches merge



http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/hosc6.html#c2

The correspondence principle - Heisenberg's refined version

- Every observable A (a macroscopic measurable value) is assigned to linear Hermitian operator $\hat{A}$ (real eigenvalues),
$\langle A \rangle = \iiint \psi^* \hat{A} \psi \, \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}z$

- If the operator $\hat{A}$ applied to the function ψ replicates the function up to a constant factor
$\hat{A}\psi = A\psi$,
the constant A is an **eigenvalue** and
the function ψ is an **eigenfunction**
of the operator $\hat{A}$

- Mean square deviation of eigenvalue

$$
\begin{aligned}
\left\langle A^2 \right\rangle - \langle A \rangle^2 &= \int \psi^* \hat{A}^2 \psi \, \mathrm{d}\tau - \left(\int \psi^* \hat{A}^2 \psi \, \mathrm{d}\tau \right)^2 \\
&= \int \psi^* \hat{A} \cdot \hat{A} \psi \, \mathrm{d}\tau - A^2 \left(\int \psi^* \psi \, \mathrm{d}\tau \right)^2 \\
&= A^2 \int \psi^* \psi \, \mathrm{d}\tau - A^2 \left(\int \psi^* \psi \, \mathrm{d}\tau \right)^2 \\
&= 0
\end{aligned}
$$

- If ψ is eigenfunction of the operator $\hat{A}$,
then $\left\langle \Delta A^2 \right\rangle = \left\langle \left(A - \langle A \rangle \right)^2 \right\rangle = 0$ and
the system is a state in that A is constant over time

The correspondence principle - Heisenberg's refined version

Examples:

- Position operator $\hat{r} = r$
- Momentum operator $\hat{p} = -i\hbar\nabla$
- Kinetic energy op. $\frac{\hat{p}}{2m} = -\frac{\hbar^2}{2m}\Delta$
- Potential energy op. $\hat{E}_{\mathrm{pot}} = V$
- Energy operator $\hat{H} = -\frac{\hbar^2}{2m} + V$
- Angular momentum op.
  $\hat{L} = \hat{r} \times \hat{p} = -i\hbar\hat{r} \times \nabla$

Examples:

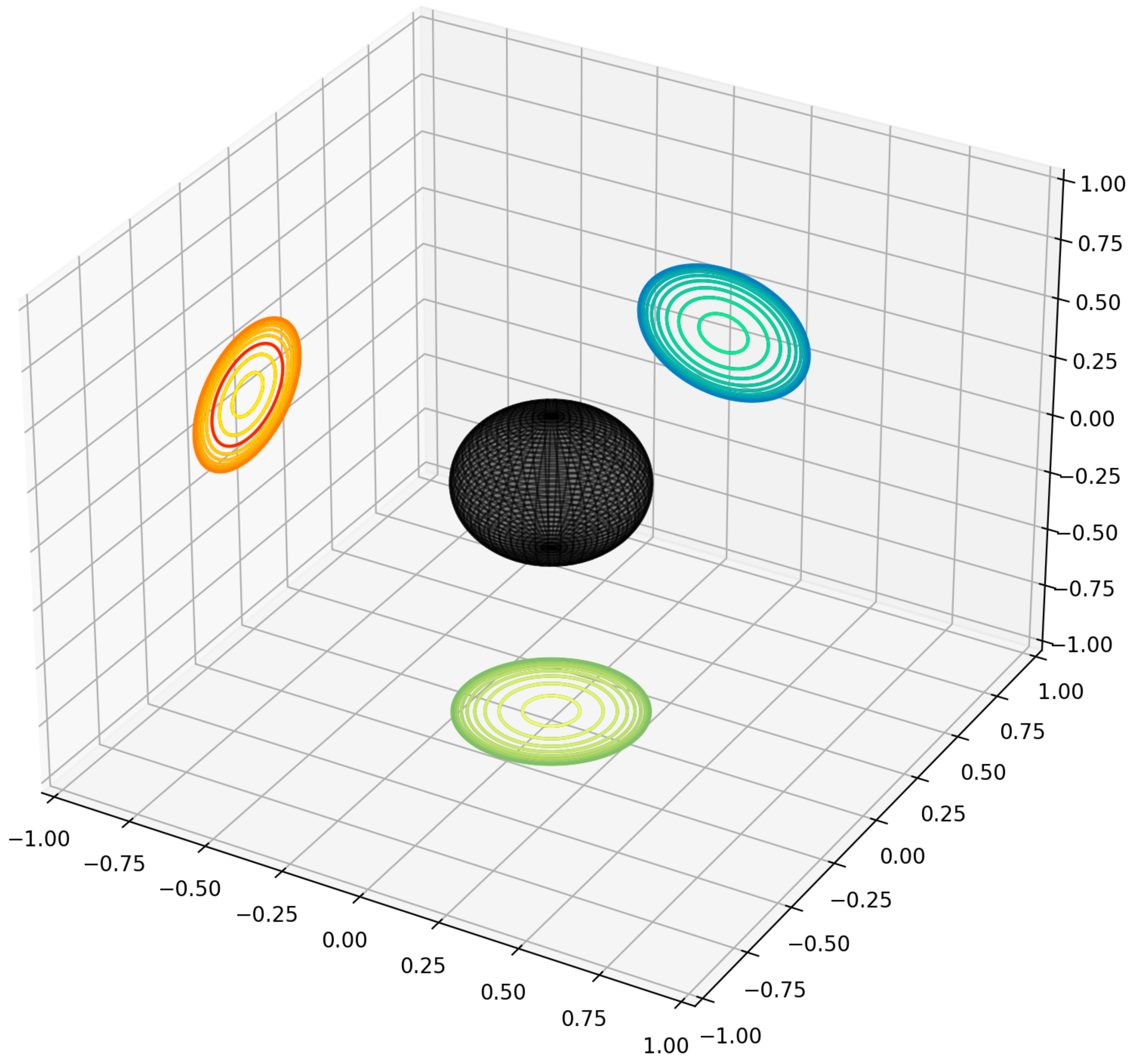
- $\hat{H}\psi = E\psi$
- $\langle p \rangle = -i\hbar \int \psi^* \nabla \psi \mathrm{d}\tau$

- The definitions for $\hat{r} = r$ and $\hat{p} = -i\hbar\nabla$ are only valid in position representation $\psi = \psi(r)$
- In momentum representation $\phi = \phi(p)$ the operators became
  $\hat{r}_p = i\hbar\nabla_p$ and $\hat{p}_p = p$

A particle in a specially symmetric potential

A particle in a specially symmetric potential - spherical harmonics

$Y_l^m = Y_0^0$



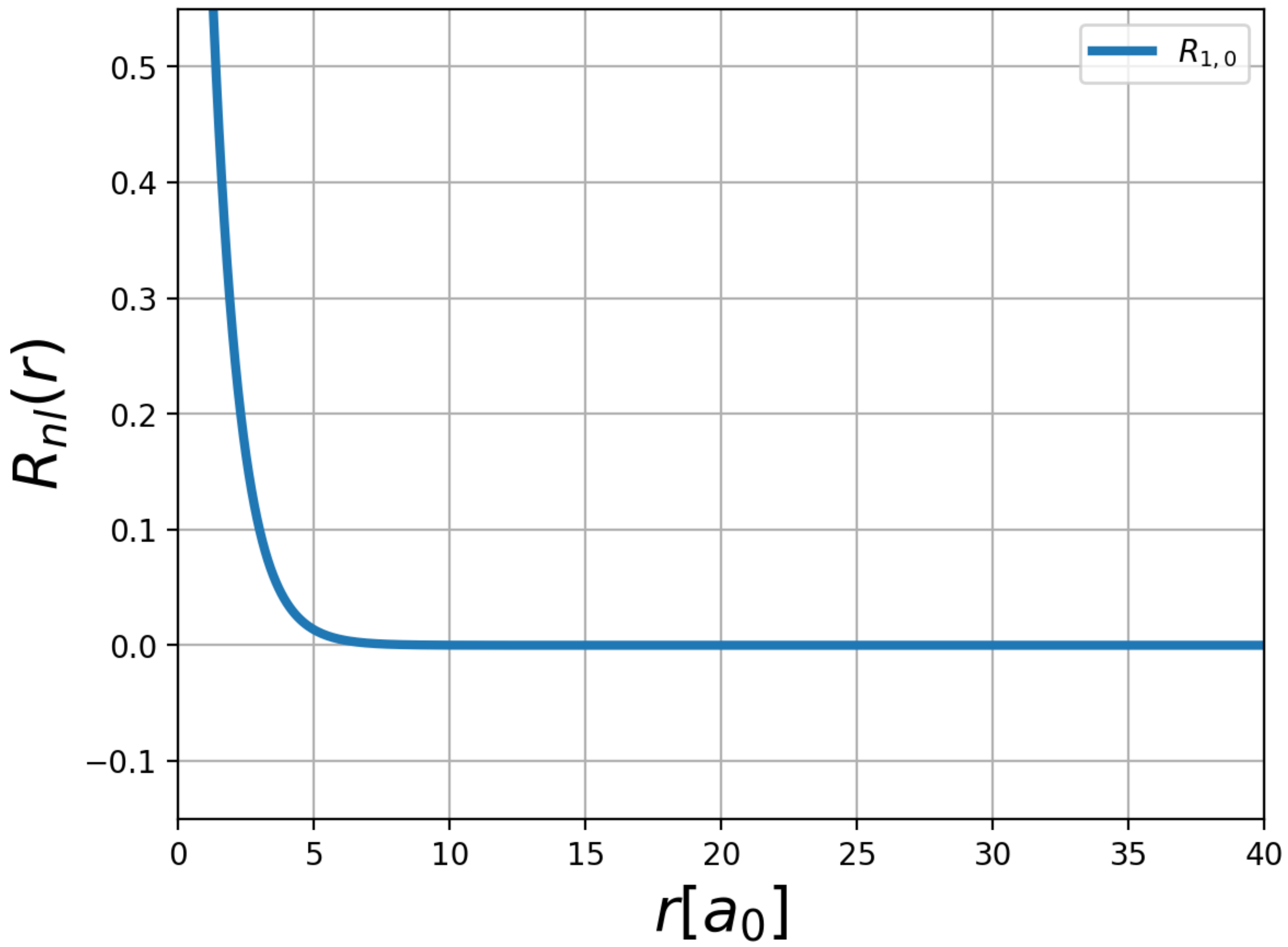
A particle in a specially symmetric potential - spherical harmonics

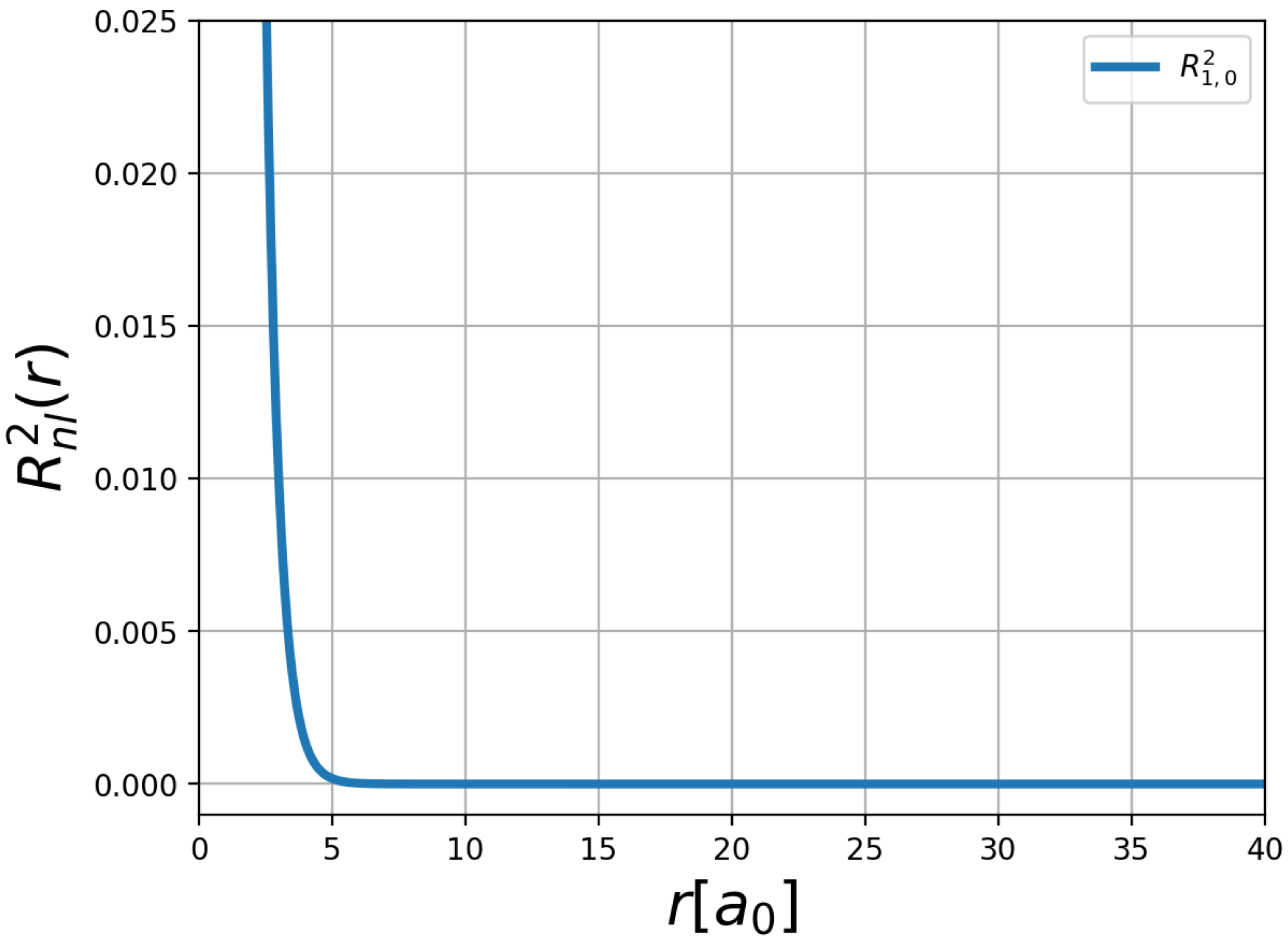
$Y_l^m = Y_1^{-1}, Y_1^0$ and Y_1^1

A particle in a specially symmetric potential - spherical harmonics

A particle in a specially symmetric potential - radial function

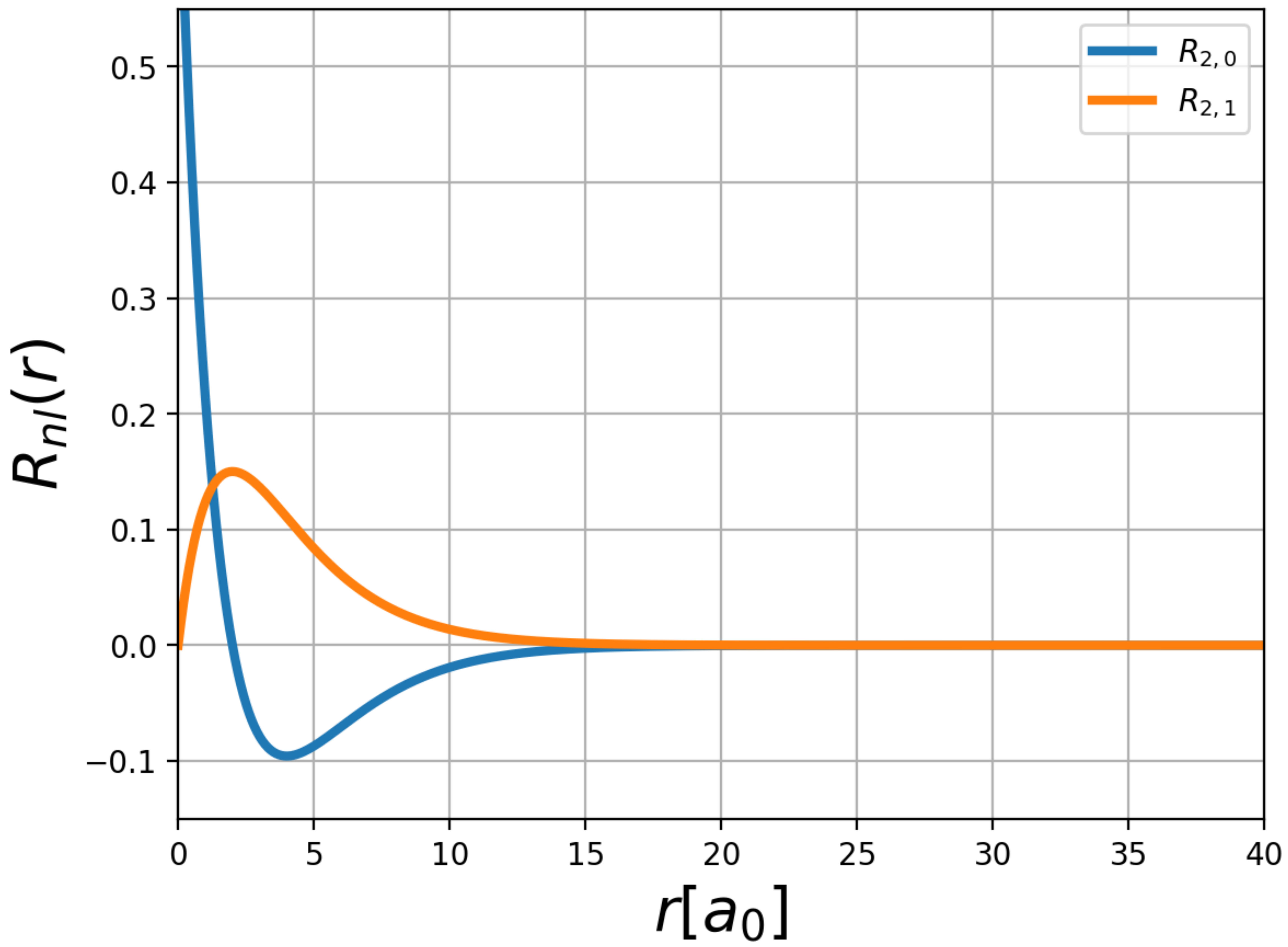
$R_{n,l} = R_{1,0}$

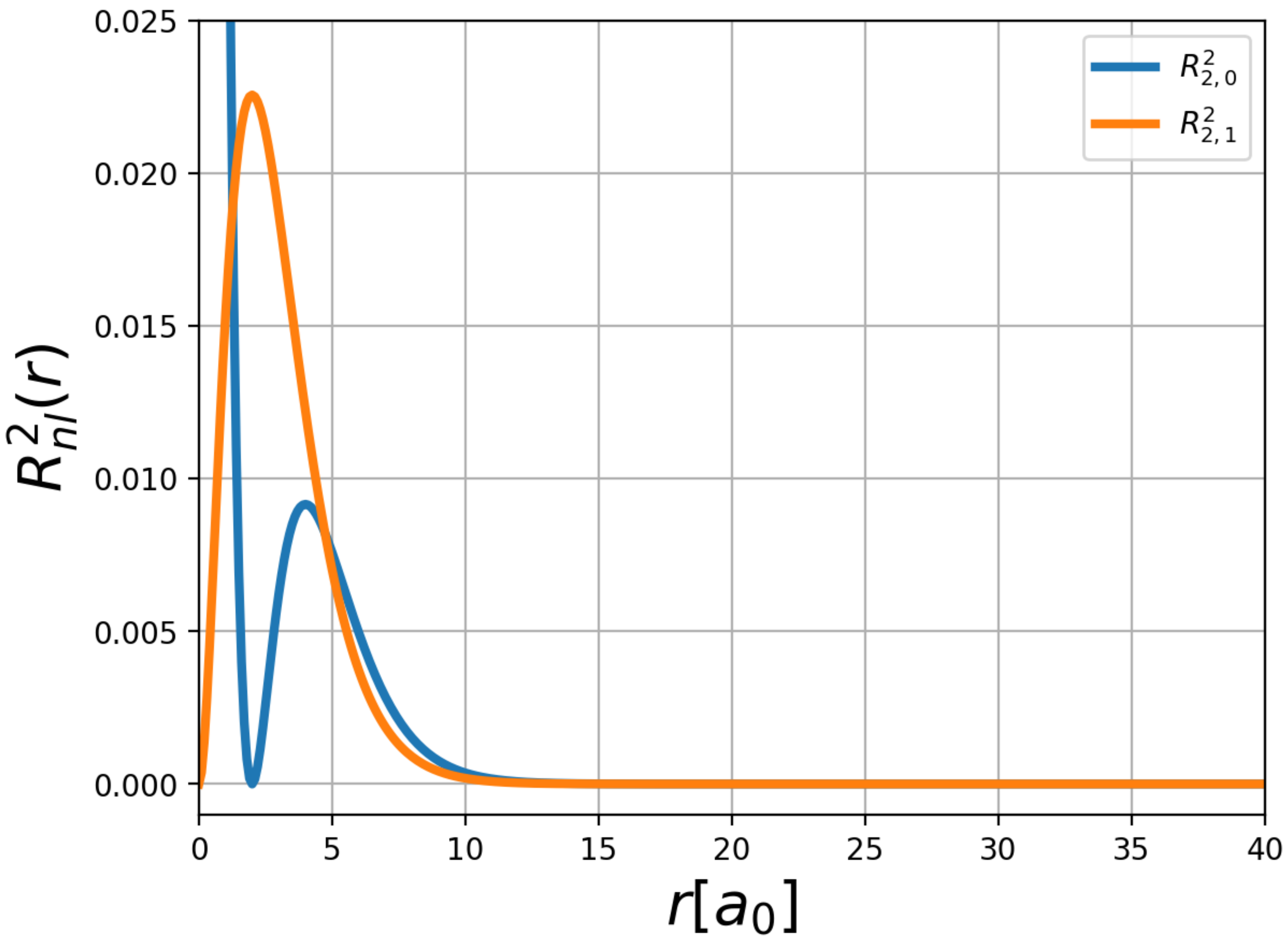




A particle in a specially symmetric potential - radial function

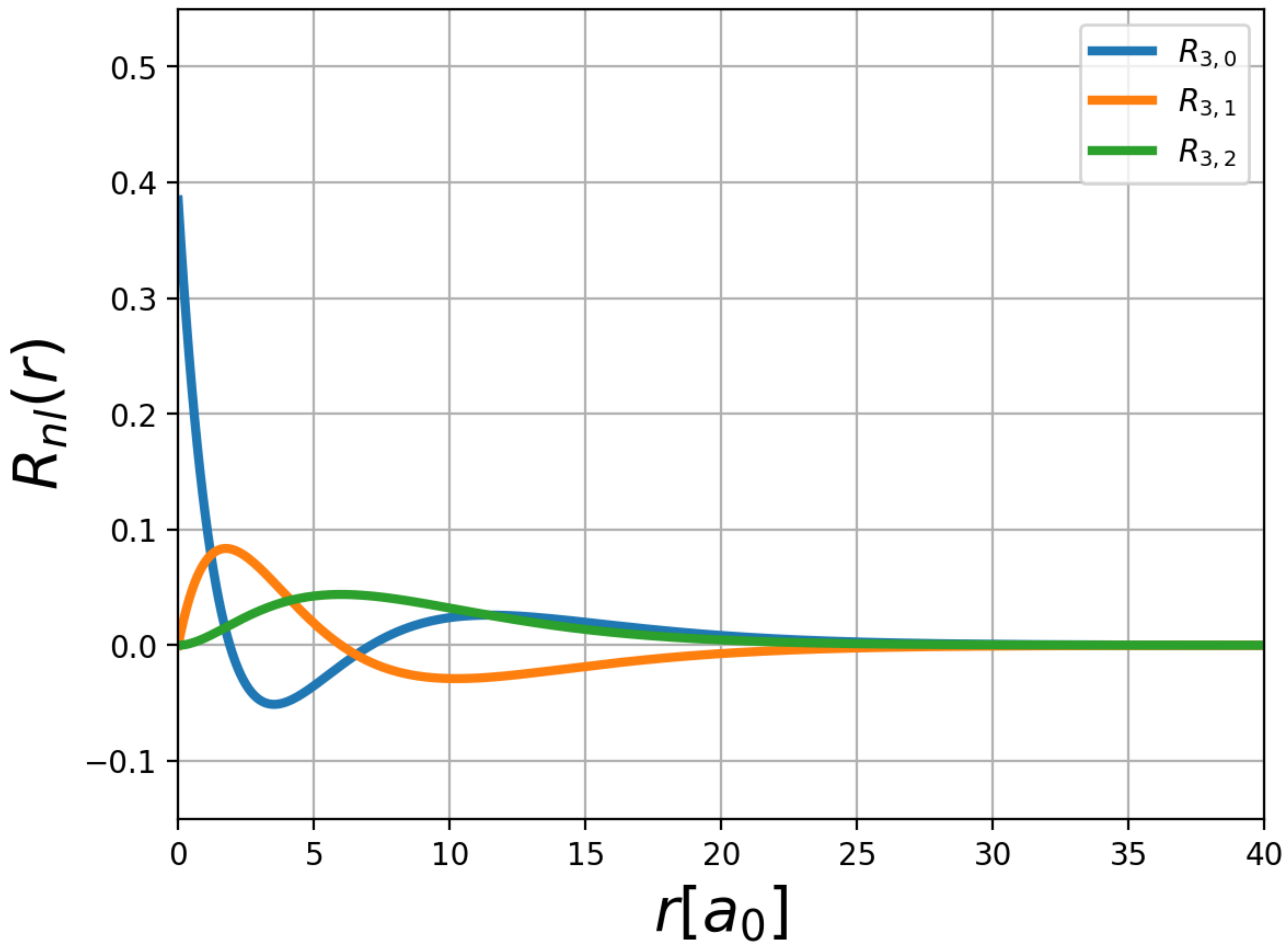
$R_{n,l} = R_{2,0}$ and $R_{2,1}$

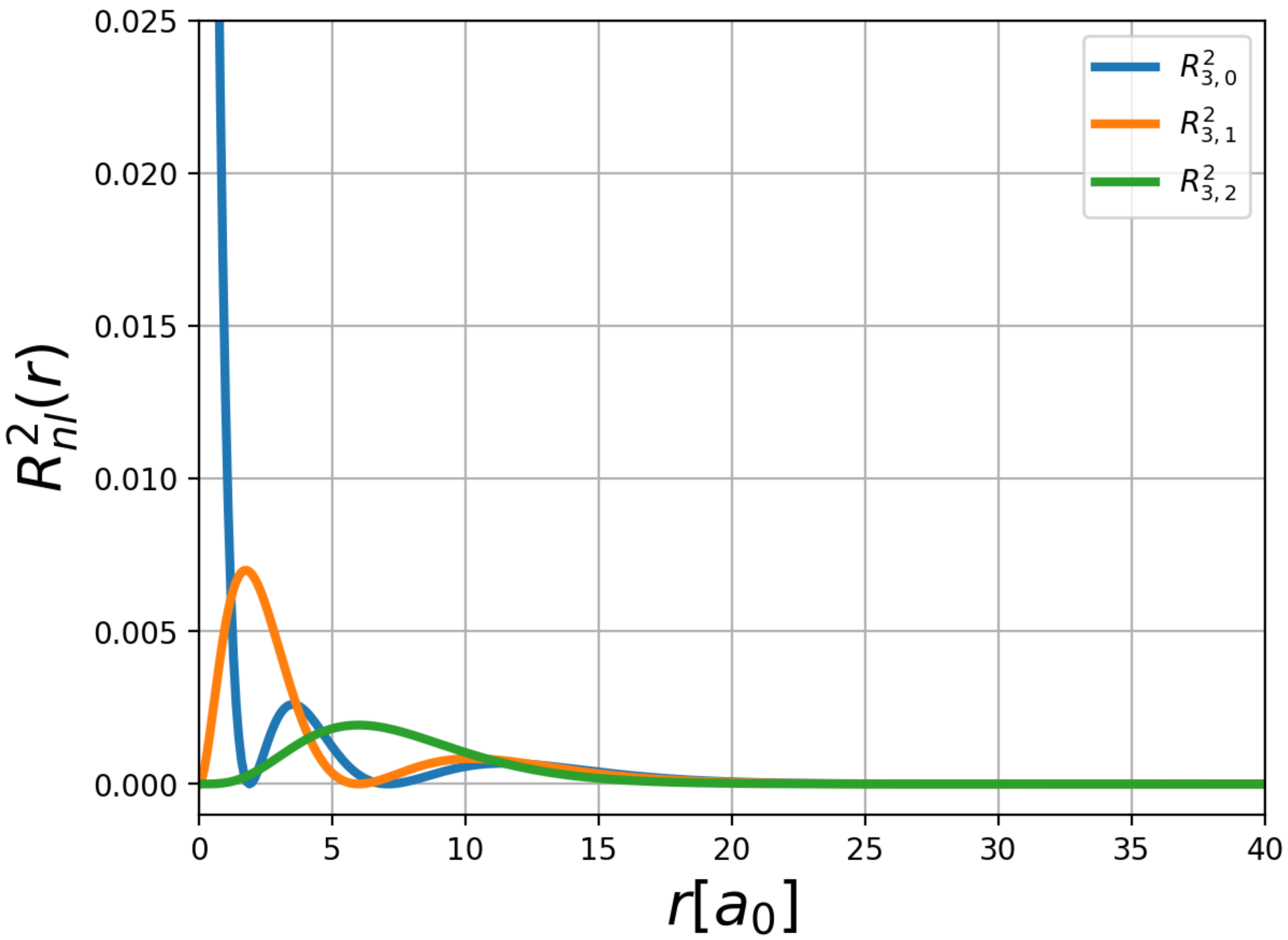




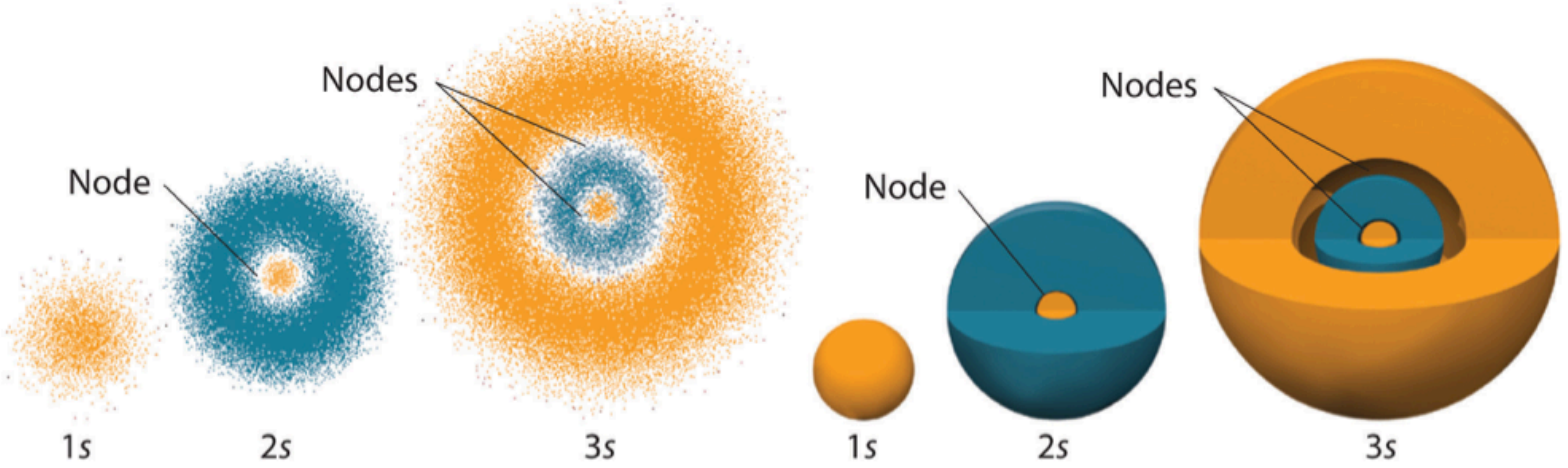
A particle in a specially symmetric potential - radial function

$R_{n,l} = R_{3,0}, R_{3,1}$ and $R_{3,2}$

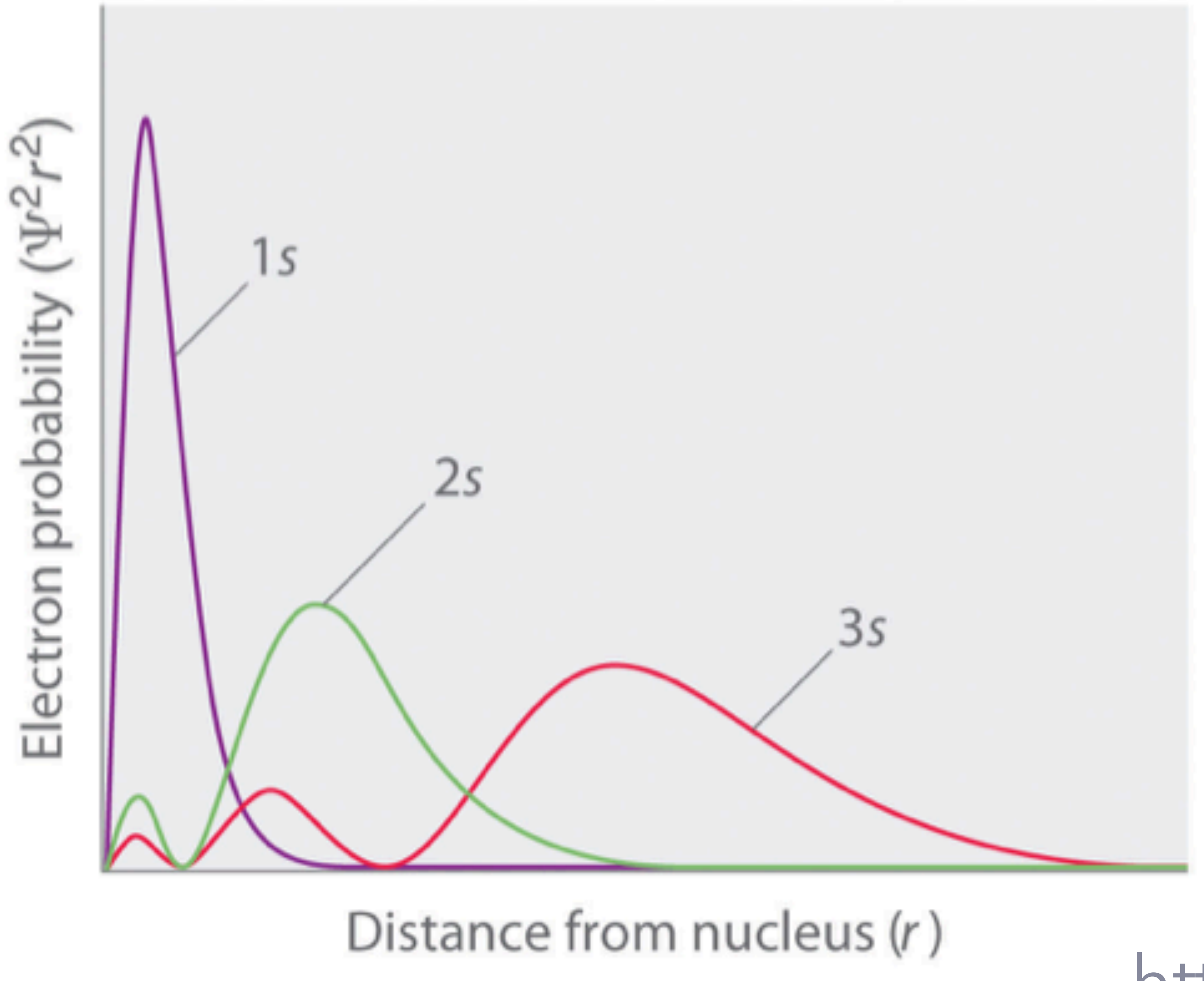




A particle in a specially symmetric potential - radial function



(a) Electron probability (b) Contour probability



(c) Radial probability

https://dpotoyan.github.io/Chem324/H-atom-wavef.html