Which state corresponds to a lower energy?

Which state corresponds to a lower <u>potential</u> energy?

∞   ∞

Potential

-a   a
    x

A $|\Psi|^2$

-a   a x

B $|\Psi|^2$
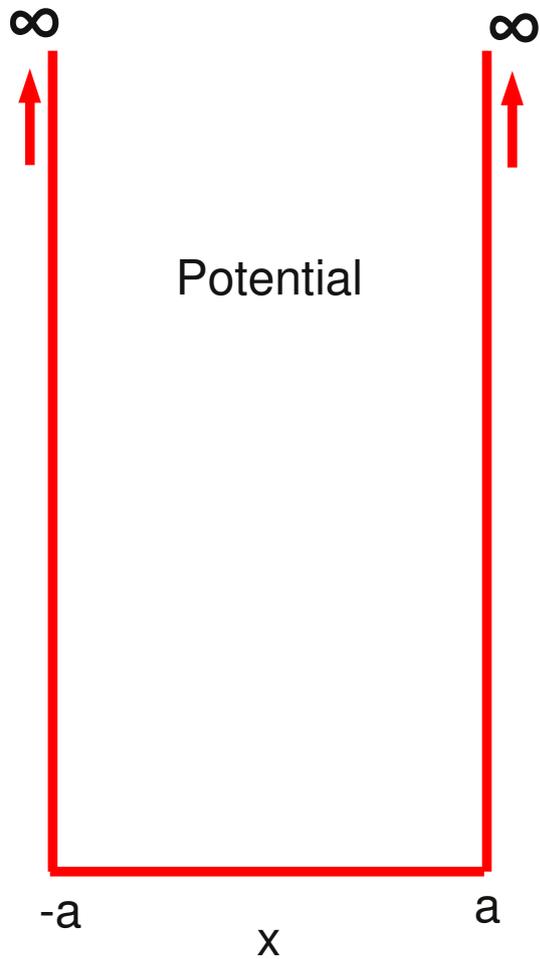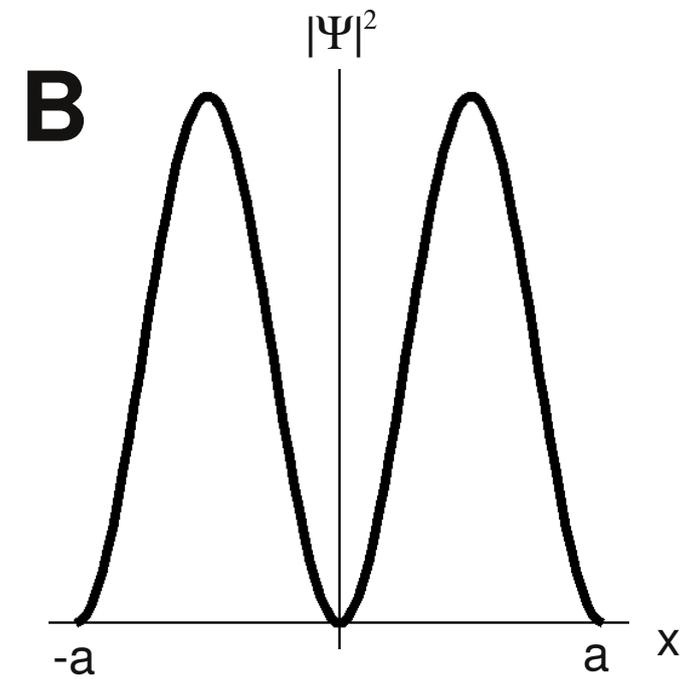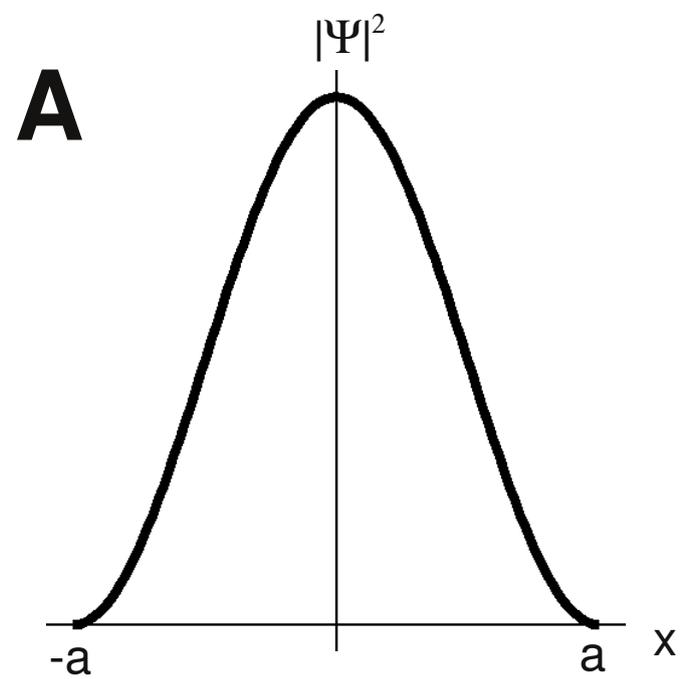
-a   a x

C Neither (potential energies are the same).

D None of the above.

Which state corresponds to a lower <u>kinetic</u> energy?

∞   ∞

Potential

-a   a

X

A

Ψ

-a   a   X

B

Ψ

-a

a   X

C   Neither (potential energies are the same).

D   None of the above.

For the previous three slides, the answers are A, C, and A.

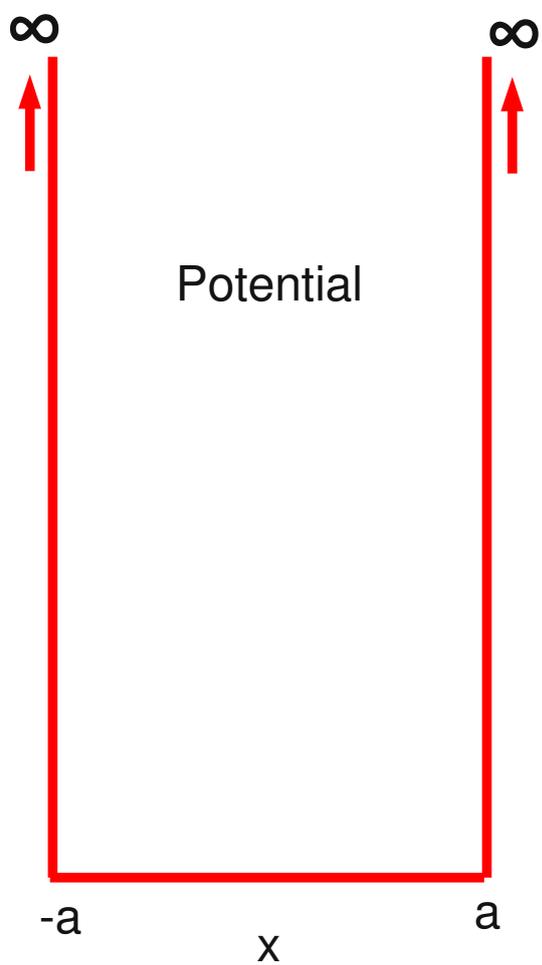The lower kinetic energy gives the nodeless wave function of A the lower total energy.
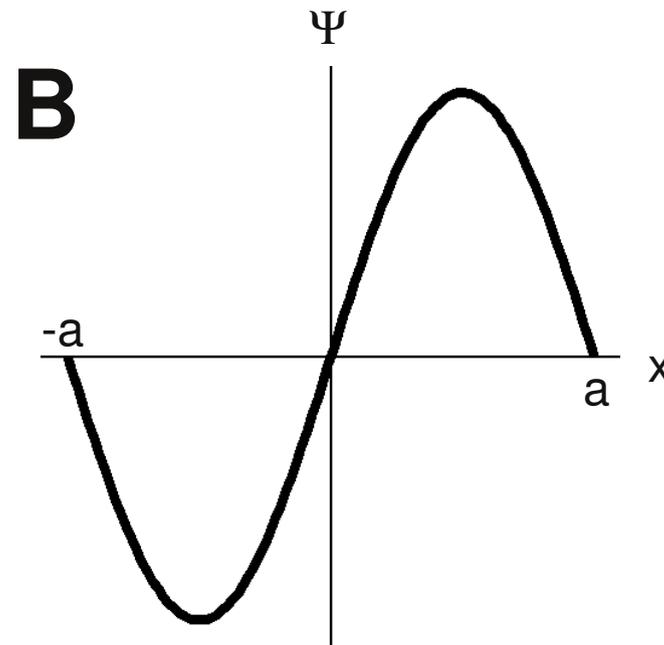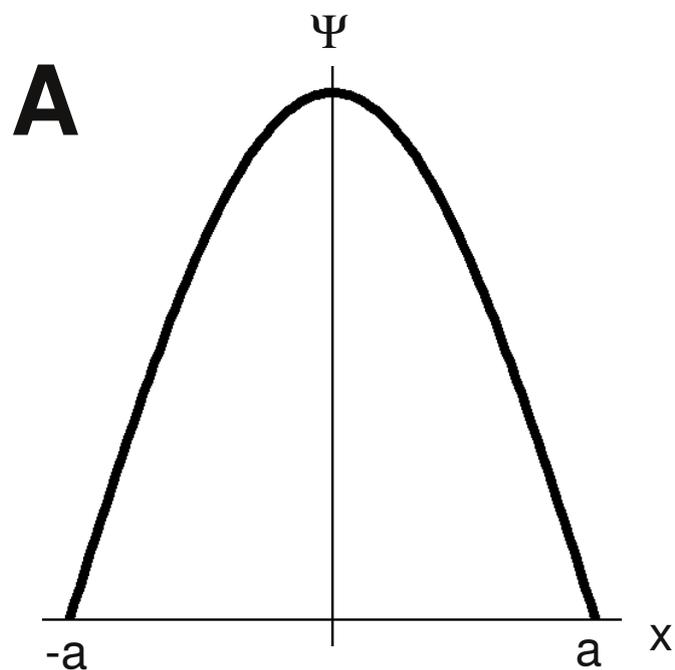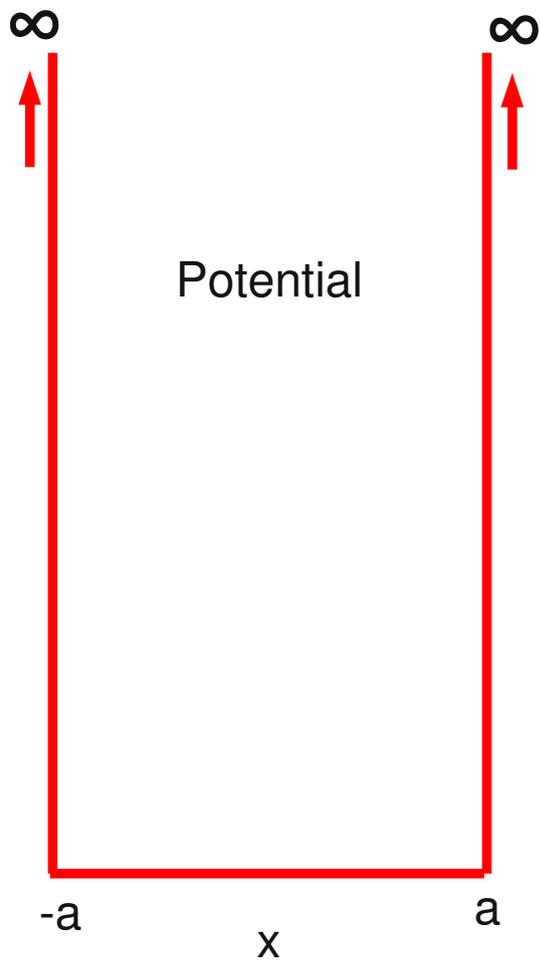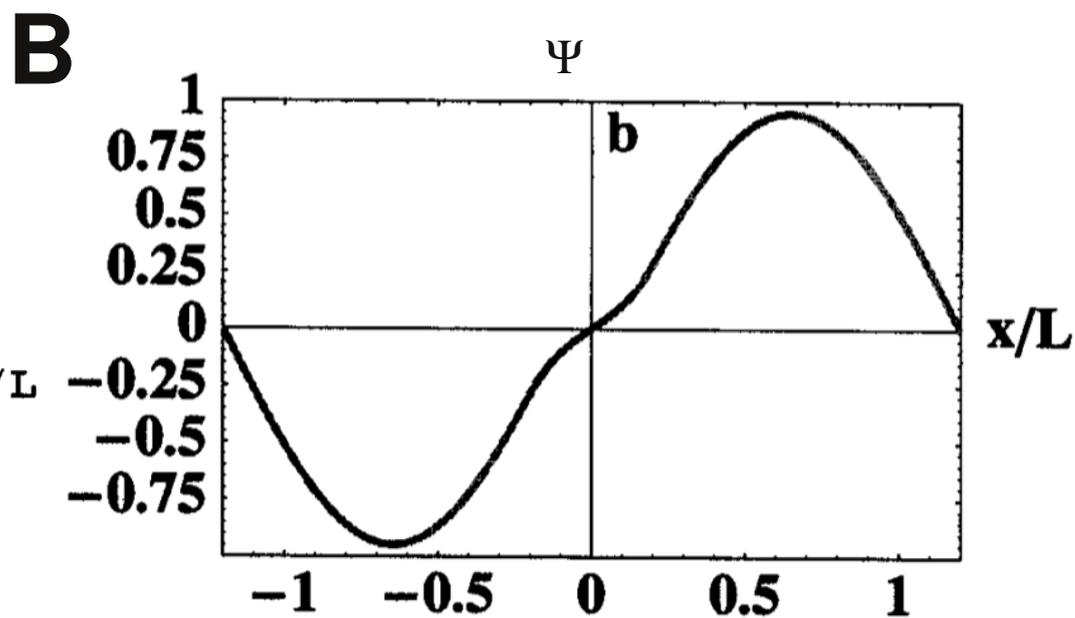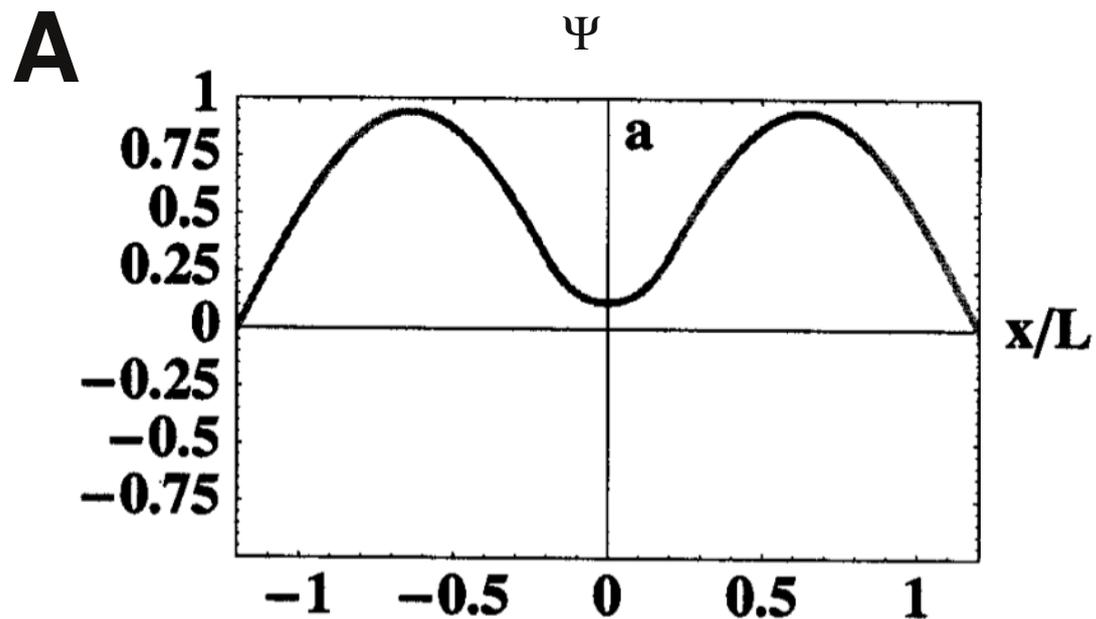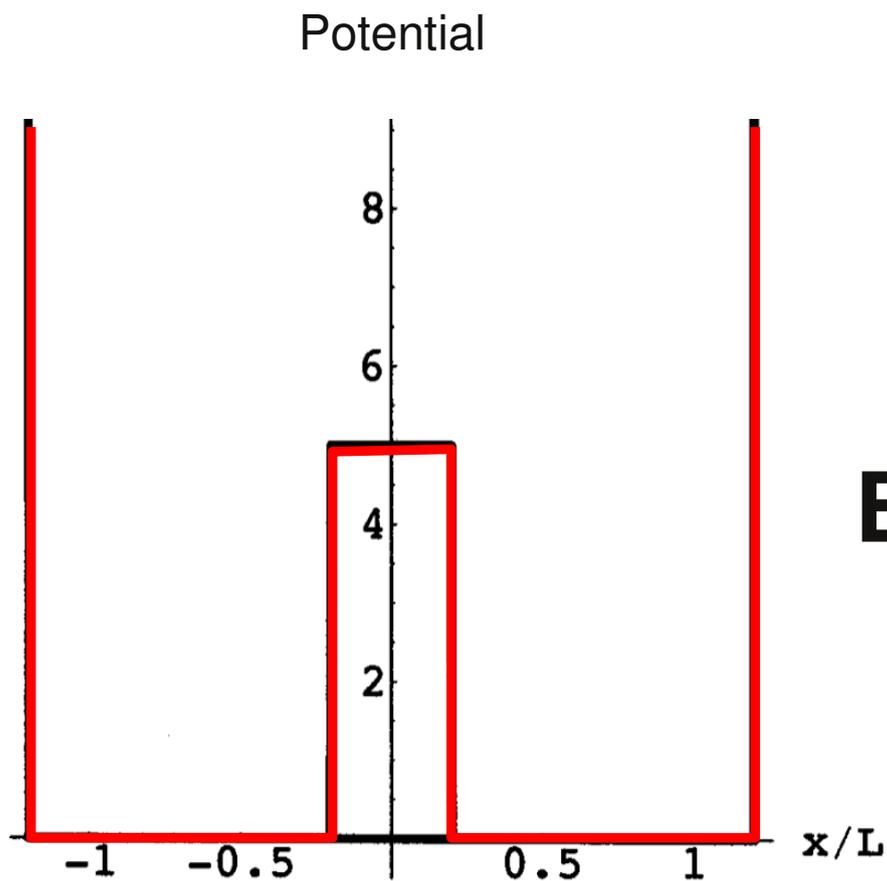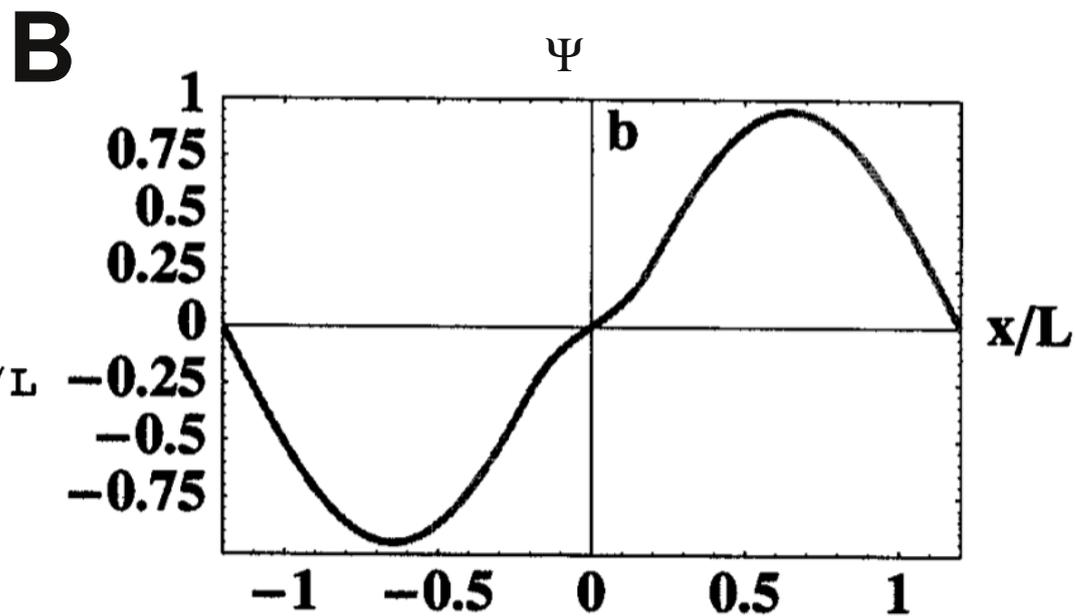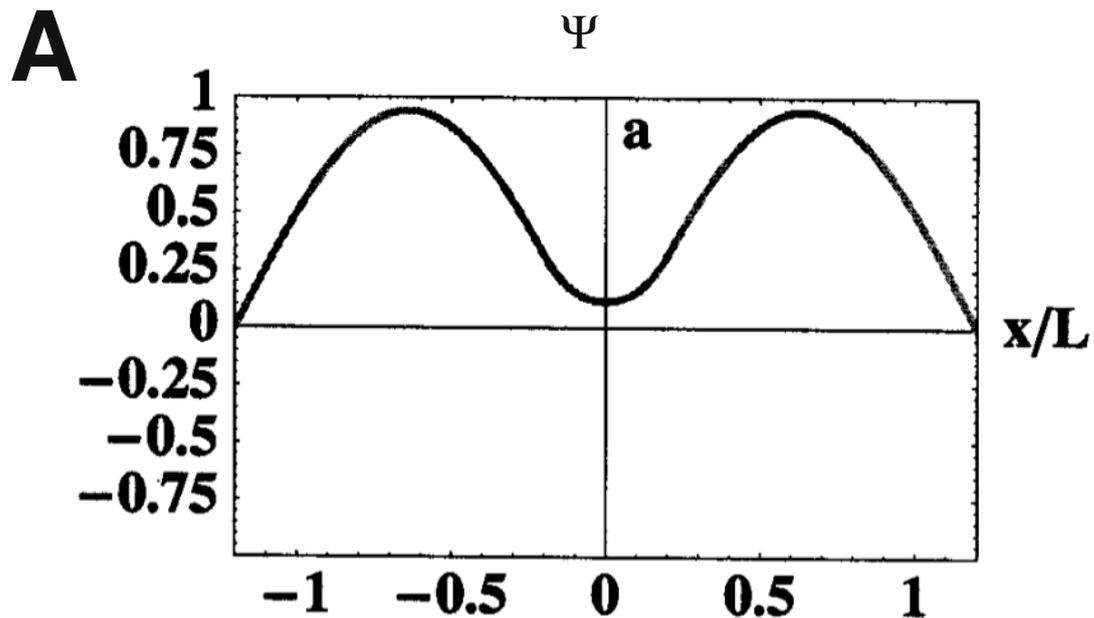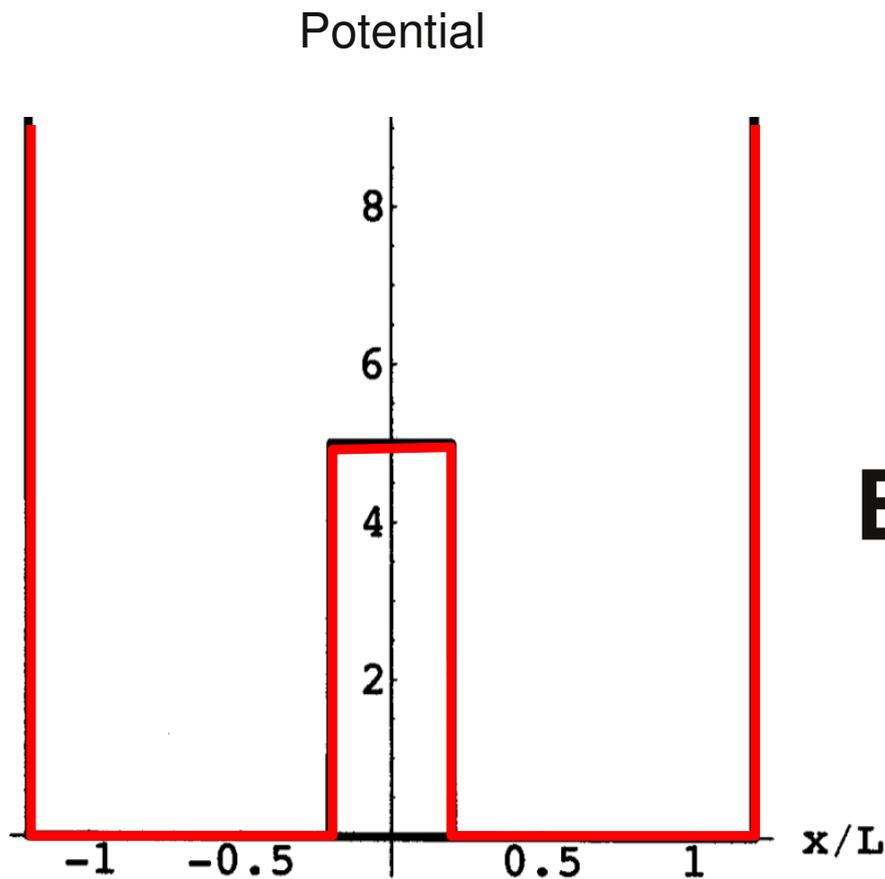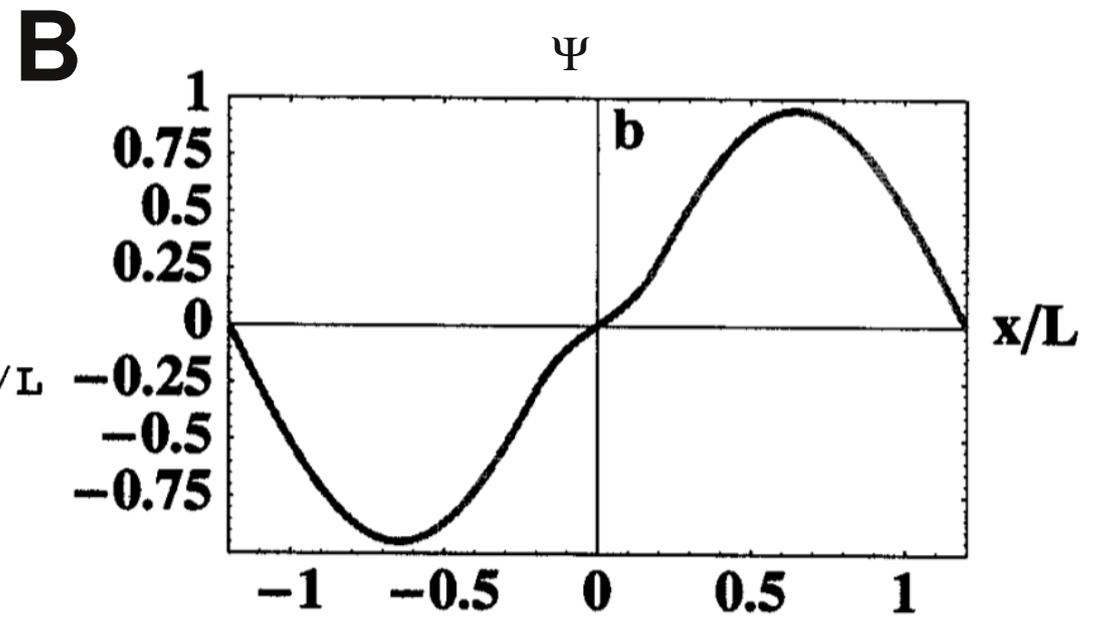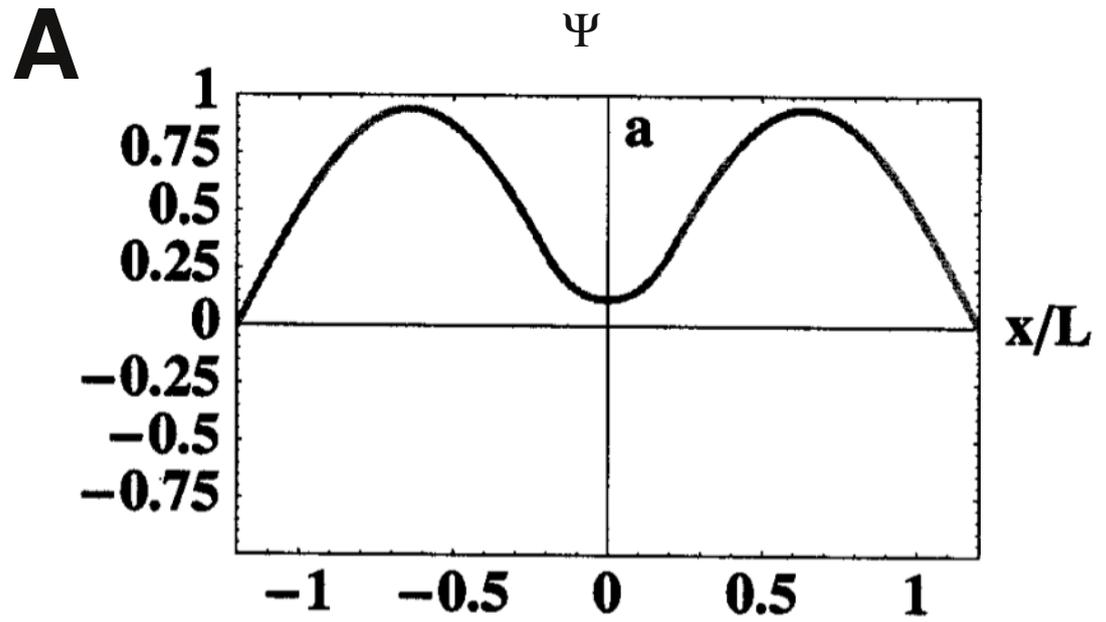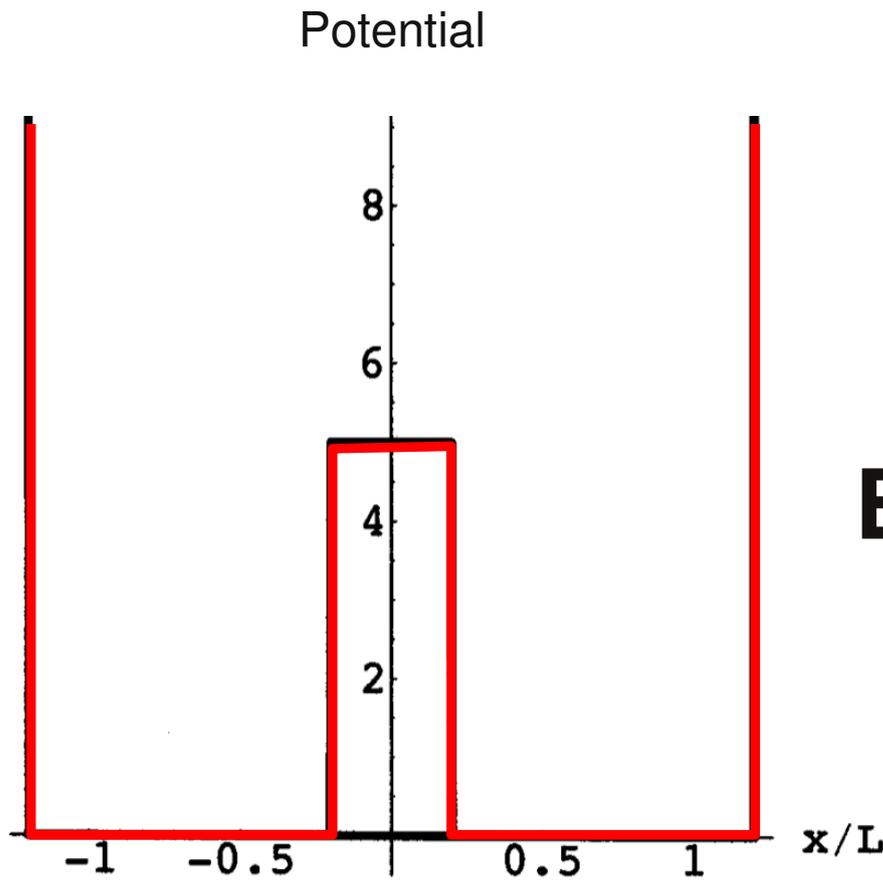
Which state corresponds to a lower energy?

Which state corresponds to a lower potential energy?

Which state corresponds to a lower <u>kinetic</u> energy?

For the previous three slides, the answers are A, B, and A.

Again, the lower kinetic energy is the dominant mechanism. The kinetic energy density is given by the magnitude of the differential of the wave function, squared. So, if the slope of the wave function is greater *in magnitude*, then the kinetic energy is higher.
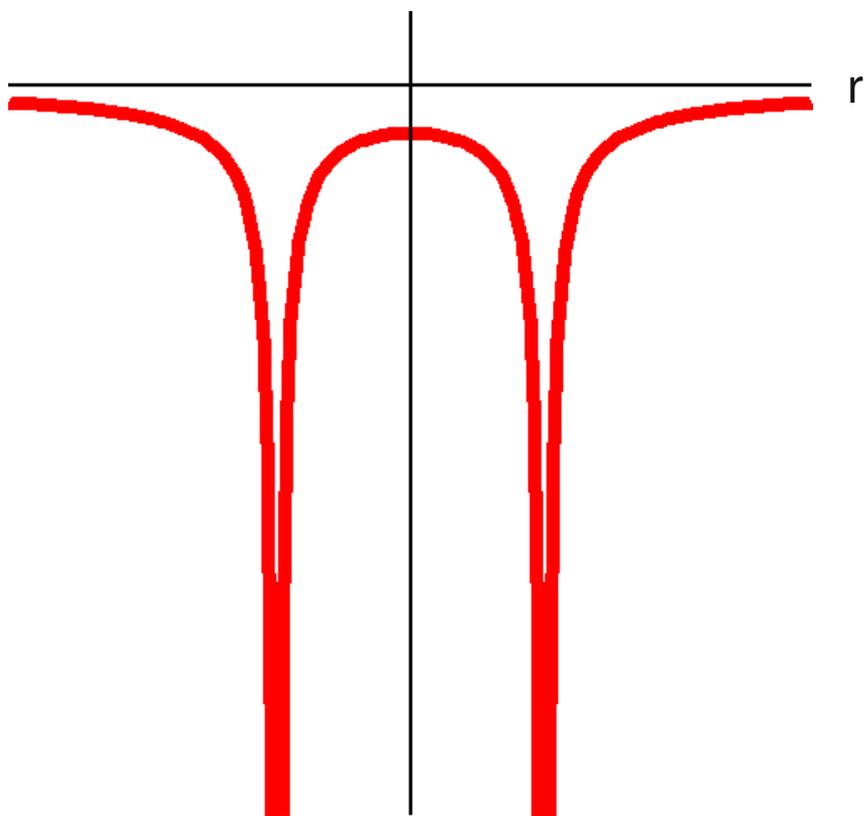
While it is not obvious without doing a real calculation, it turns out that the kinetic energy lowering for A is greater than the potential energy rise, and so that A is more stable.

A is the so-called "**bonding orbital**." B is the so-called "**anti-bonding orbital**."
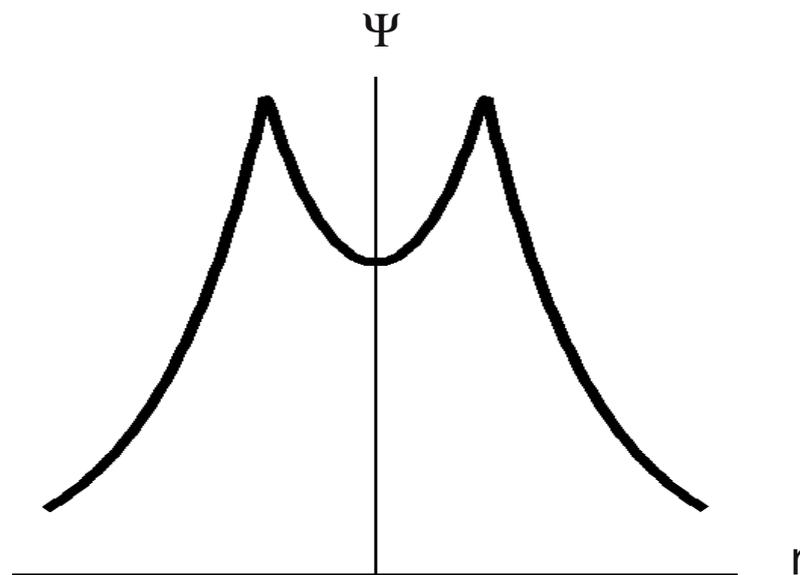
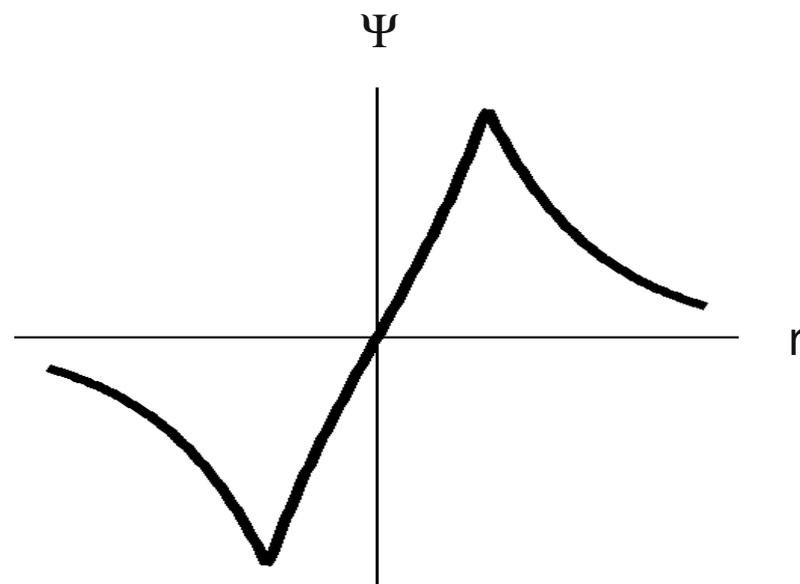# Which state corresponds to a lower energy?

Hydrogen Molecule

Potential

A

B

For the previous slide, the answer is A.

Again, a symmetric (and nodeless) wave function represents the lower energy bonding orbital, though.

However, the microscopic reason for the energy lowering is opposite to that of the double square well case.

In this case, it is the potential energy that drives the bonding. We will discuss it in lecture 04.