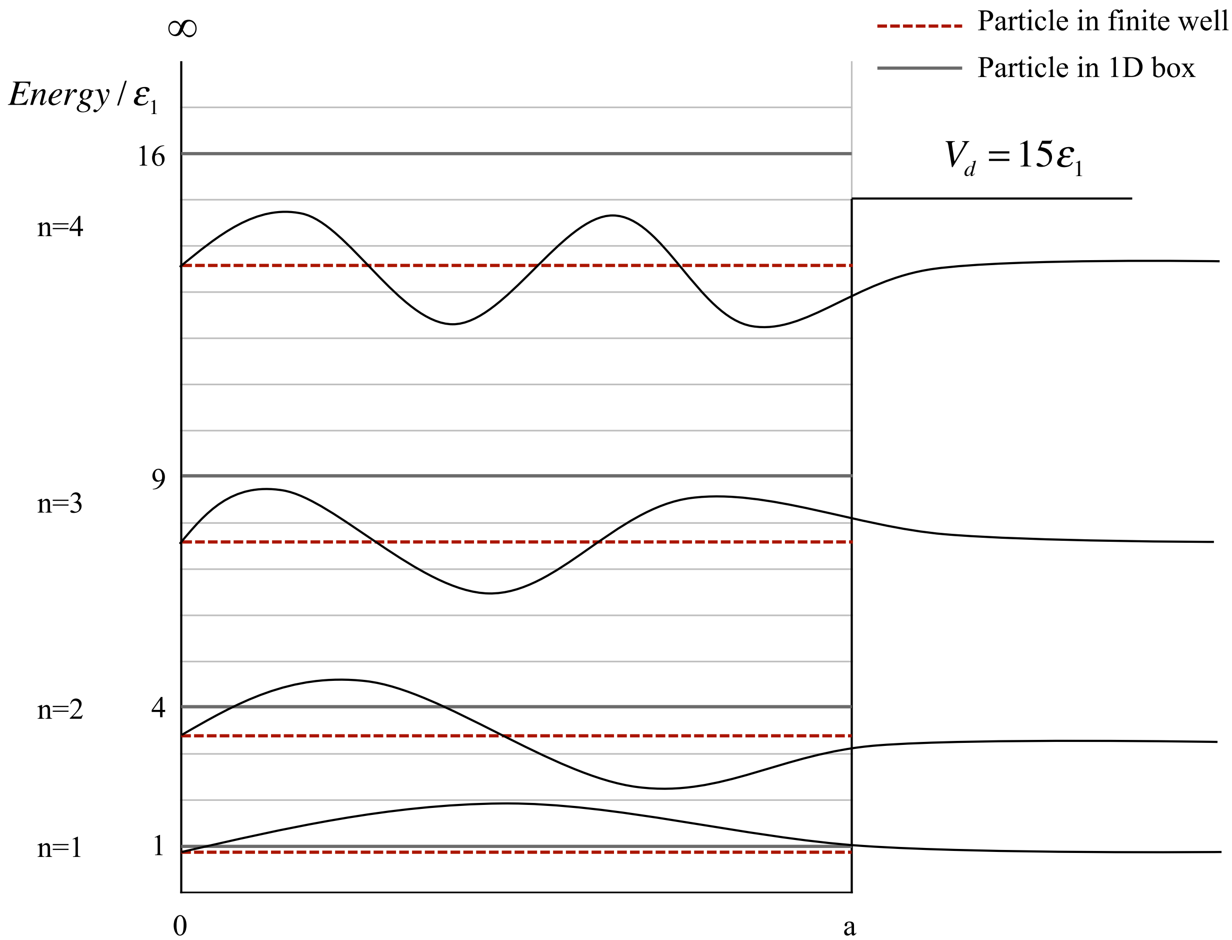
1.
(Textbook, pg. 69-70.)
Useful equations for particle in 1D finite depth well:

$$\eta_d = \frac{\sqrt{2mV_d}}{\pi\hbar}L$$

$$E_n = \eta_n^2\varepsilon_1 \cong \left(n-\delta_n\right)^2\varepsilon_1 = n^2\left(\frac{\eta_d}{\eta_d + 1/\pi}\right)^2\varepsilon_1$$

Based on the equations above, $\eta_d = 3.87$ and

$$E_n = n^2\left(\frac{\eta_d}{\eta_d + 1/\pi}\right)^2\varepsilon_1 = n^2\left(\frac{3.87}{3.87 + 1/\pi}\right)^2\varepsilon_1 \cong 0.85n^2\varepsilon_1$$



(Energy levels and wavefunctions are presented in the figure above.)

The energy levels of the particle in a box decrease when the well depth is finite (about 15% lower in this case). The energy level with large n changes the most, since the new energy level is still proportional to n^2.

When n=4, the particle is still bounded in this case (finite well). When x>a, the wavefunction decays exponentially (positive or negative). Among these four wavefunctions, n=4 decays the slowest and has the highest amplitude before decaying. Therefore, qualitatively speaking, n=4 has the greatest probability of finding the electron with x>a.

2. Four independent electrons system: electrons fill the energy levels from the lowest one, following the rule that 2 electrons fill 1 energy state.

	Energy in ε_1	Particle in a box (Estimation)	Particle in finite well
a	Σpopulation×energy	$2\times1+2\times4=10$	$(2\times1+2\times4)\times0.85=8.5$ Lower than estimated
b	I.E. = Final state – Initial state $= (E_{g.s.(+)} + V_d) - E_{g.s.}$	$(2\times1+4+15)-(2\times1+2\times4)=11$	$((2\times1+4)\times0.85+15)-(2\times1+2\times4)\times0.85=11.6$ Higher than estimated
c	E.A. = Final state – Initial state $= E_{g.s.(-)} - (V_d + E_{g.s.})$	$(2\times1+2\times4+9)-(2\times1+2\times4+15)=-6$	$(2\times1+2\times4+9)\times0.85-\left((2\times1+2\times4)\times0.85+15\right)=-7.35$ Lower than estimated, greater in magnitude
d	Particle in the box estimation: there are only 3 energy levels available. 4 energy levels available in the given finite well.	1→3: forbidden, weak intensity at 8 2→3: show up at 5	1→3: forbidden, weak intensity at 6.8 1→4: show up at 12.75 2→3: show up at 4.25 2→4: forbidden, weak intensity at 10.2

3. Five independent electrons system: electrons fill the energy levels from the lowest one, following the rule that 2 electrons fill 1 energy state.

	Energy in ε_1	Particle in a box (Estimation)	Particle in finite well
a	Σpopulation×energy	$2\times1 + 2\times4 + 9 = 19$	$(2\times1 + 2\times4 + 9)\times0.85 = 16.15$ Lower than estimated
b	I.E. = Final state – Initial state $= (E_{g.s.(+)} + V_d) - E_{g.s.}$	$(2\times1 + 2\times4 + 15) - (2\times1 + 2\times4 + 9) = 6$	$((2\times1 + 2\times4)\times0.85 + 15) - (2\times1 + 2\times4 + 9)\times0.85 = 7.35$ Higher than estimated
c	E.A. = Final state – Initial state $= E_{g.s.(-)} - (V_d + E_{g.s.})$	$(2\times1 + 2\times4 + 2\times9) - (2\times1 + 2\times4 + 9 + 15) = -6$	$(2\times1 + 2\times4 + 2\times9)\times0.85 - \big((2\times1 + 2\times4 + 9)\times0.85 + 15\big) = -7.35$ Lower than estimated, greater in magnitude
d	Particle in the box estimation: there are only 3 energy levels available. 4 energy levels available in the given finite well.	1→3: forbidden, weak intensity at 8 2→3: show up at 5	1→3: forbidden, weak intensity at 6.8 1→4: show up at 12.75 2→3: show up at 4.25 2→4: forbidden, weak intensity at 10.2 3→4: show up at 5.95