Modern 2016 PS 23 Key

Q12D.4 In this problem, we will consider the covalent bond, which illustrates how "sharing" a quanton can lead to an attractive force that has no easy classical explanation. Consider an H_2^+ molecule, where a pair of protons share a single electron. In order to make the problem tractable, we will ignore the repulsion between protons and model their interaction with the shared electron as if the protons were two square wells separated by a small distance, each about as wide as a hydrogen atom (0.1 nm). (This model may seem absurdly idealized, but more realistic models simply increase the complexity without adding any new insight.)

Run SchroSolver and choose the "Symmetric Well" potential energy function and a fixed well width of 0.5 nm. The ground state EEF *should* (by symmetry) predict that the electron is equally likely to be in either well, since the wells are identical. However, the eigenfunction might achieve this by having "bumps" in each well that have the same sign (a "symmetric" state) or opposite signs (an "antisymmetric" state). You can choose which is displayed by selecting the type from a pop-up menu in the window.

(a) Start with a center-to-center well separation of 0.75 nm. Show that the symmetric EEF has a slightly lower energy than the antisymmetric one (hand in a printout that provides supporting evidence).

(b) Explain qualitatively (physically) why this must be so. (*Hint:* Compare SchroSolver plots of the symmetric and antisymmetric functions, and explain why the wave-like "bump" in each well has gentler curvature in the symmetric case than in the antisymmetric case. How is that curvature linked to the energy of the state?)

(c) So the symmetric EEF is the true ground state for this system. Select this type of function and vary the wells' center-to-center separation (without changing anything else) from 0.55 nm in steps of 0.05 nm up to 1.10 nm, and make a chart of ground state energies (to at least 6 decimal places). You should see that the system's energy increases as we pull the wells apart.

(d) Explain why this must be. (*Hint:* Again, first explain why the "bump" in each well has gentler curvature if the wells are closer together.)

(e) Explain why this means that sharing the electron creates an attractive force between the wells. (*Hint:* Imagine pulling the wells apart. This will cause the system's energy to increase, as we have just seen. Then think about the *work* you must do on the system to do this.)

(f) Show that if the electron is in the *antisymmetric* state, sharing an electron leads to a *repulsive* force between the wells, and explain why this must be so.

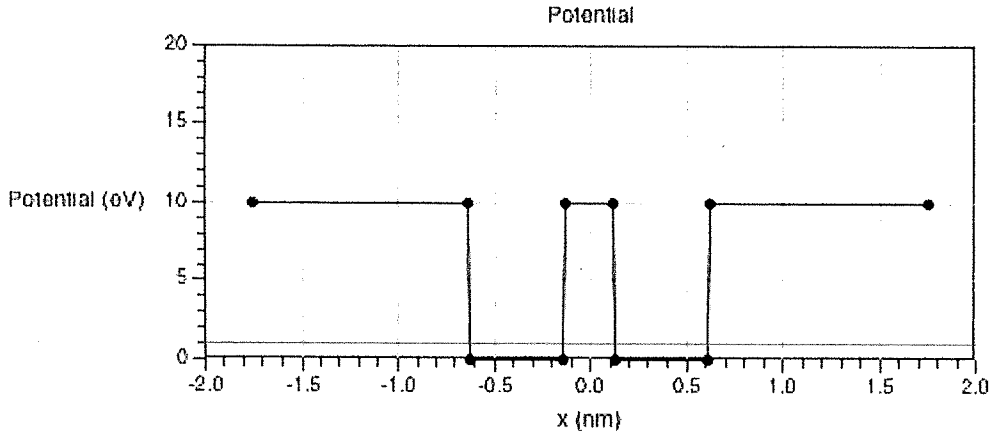
(a) I am running this on Schrosolver. We see the symmetric solution has lower energy than the antisymmetric solution.
$E_{sym} = 0.981$ eV $\quad E_{anti} = 0.999$ eV (see next page).

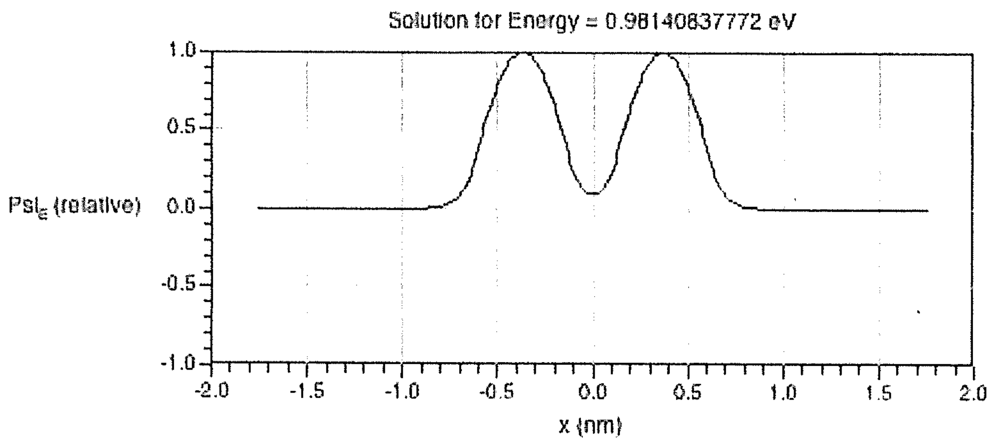
(b) This must be so because the antisymmetric solution has a node (zero crossing) in the barrier. This requires ψ_{anti} to drop a bit lower in value near the barrier edge, meaning the λ is slightly shorter in the antisymmetric case.

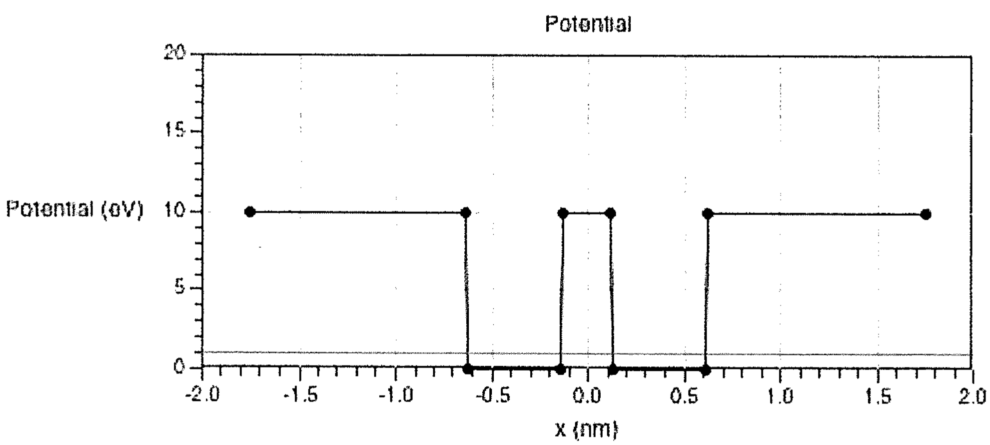
(c) I am systematically varying center-center separation and seeing the effect on ground state energy

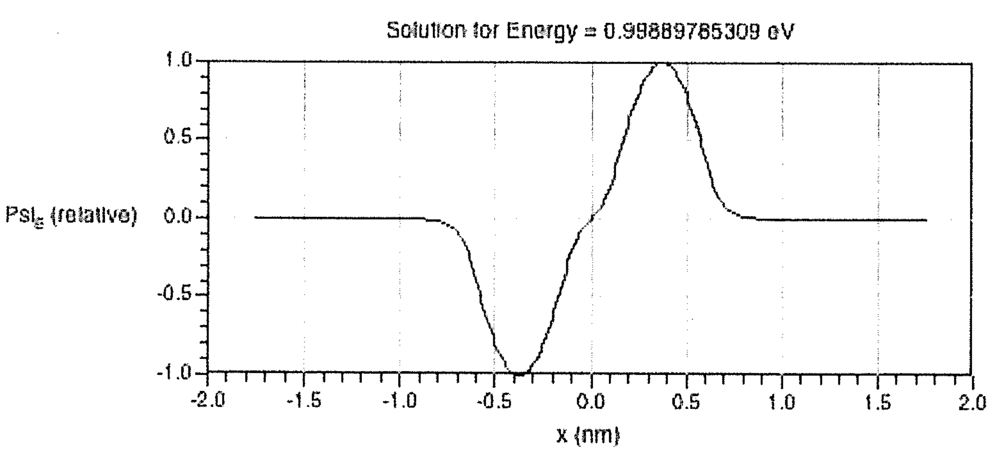
r_{cc}	E_{sym}
0.55	0.716308
0.60	0.900654
0.65	0.944628
0.70	0.973153
0.75	0.981408
0.80	0.987161

r_{cc}	E_{sym}
0.85	0.988889
0.90	0.990111
0.95	0.990481
1.00	0.990744
1.05	0.990823
1.10	0.990880


Potential
Potential (eV)
20
15
10
5
0
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0
x (nm)

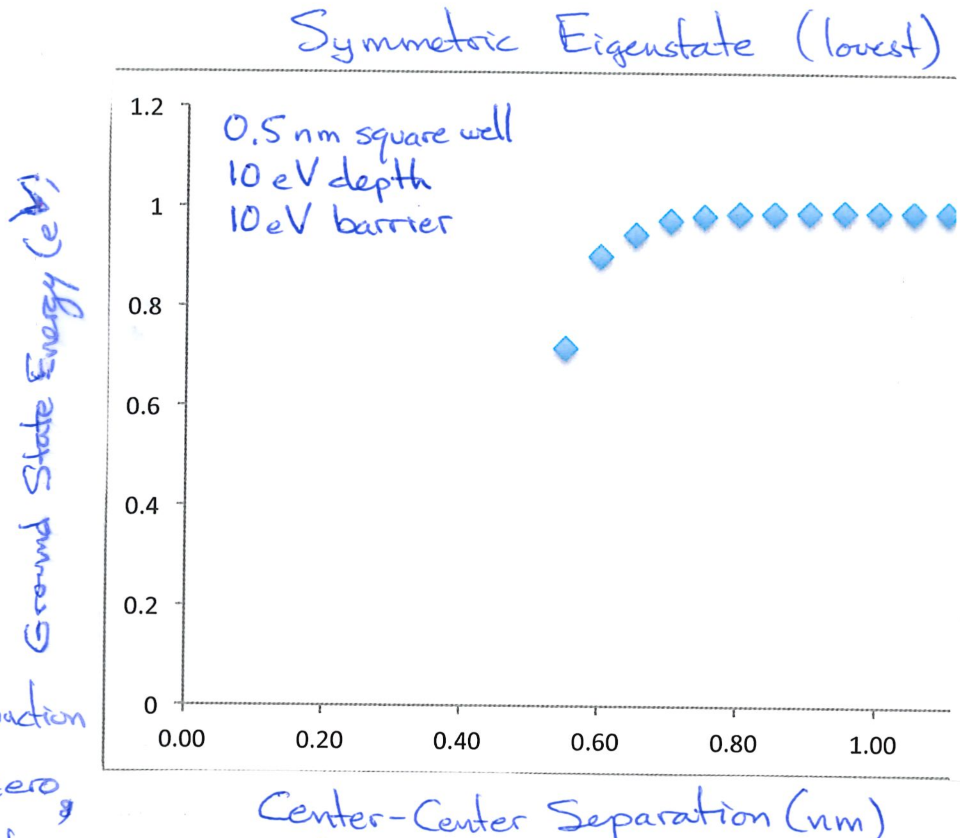

Solution for Energy = 0.98140837772 eV
Psi_E (relative)
1.0
0.5
0.0
-0.5
-1.0
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0
x (nm)


Potential
Potential (eV)
20
15
10
5
0
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0
x (nm)


Solution for Energy = 0.99889785309 eV
Psi_E (relative)
1.0
0.5
0.0
-0.5
-1.0
-2.0
-1.5
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0
x (nm)

We see that the system's energy does, indeed rise as the wells are pulled apart.

(d) This must be the case because the wider the barrier, the more the wavefunction must decay toward zero. So with larger separation, the wavefunction is more confined in its square well, leading to shorter λ and higher energy.



(e) Pulling the wells apart raises the energy of the symmetric eigenstate. So it requires work to pull them apart. Since $dW = \vec{F} \cdot d\vec{r}$, this means there is a force pulling the wells together (an attractive force).

(f) Now for the energy trend in the lowest antisymmetric state

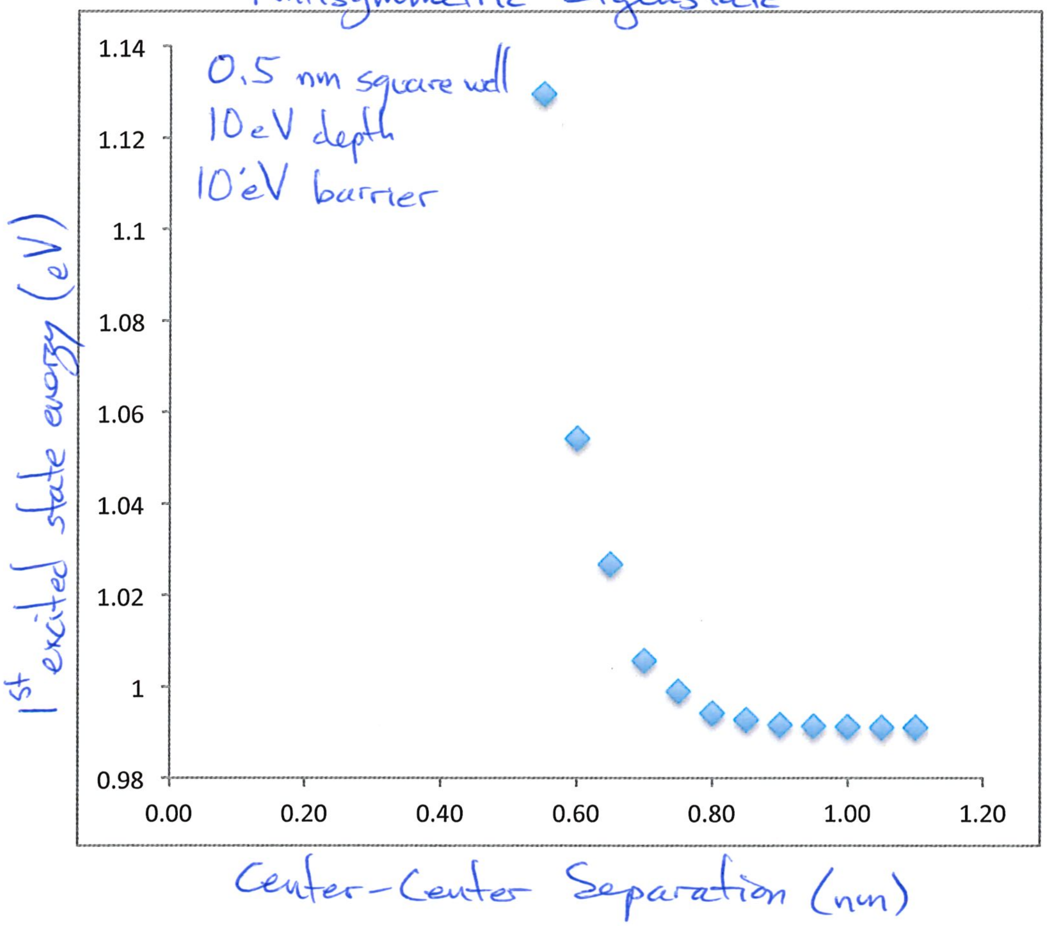
r_{cc}	E_{anti}
0.55	1.129566
0.60	1.054116
0.65	1.026591
0.70	1.005541
0.75	0.998898
0.80	0.994111

r_{cc}	E_{anti}
0.85	0.992648
0.90	0.991606
0.95	0.991290
1.00	0.991065
1.05	0.990997
1.10	0.990949

separation	Energy
0.55	1.129566
0.60	1.054116
0.65	1.026591
0.70	1.005541
0.75	0.998898
0.80	0.994111
0.85	0.992648
0.90	0.991606
0.95	0.99129
1.00	0.991065
1.05	0.990997
1.10	0.990949

(f) Because the energy decreases as the separation increases, having an electron in an antisymmetric eigenstate leads to a repulsive force between the potential wells. As barrier width decreases ψ must drop ever closer to zero at the barrier edge so it can reach zero mid-barrier. This results in greater confinement of particles in the wells as barrier width decreases, shortening λ and raising energy.

Antisymmetric Eigenstate



Q13D.3 (Requires integral calculus.) One can calculate the gravitational binding energy of a spherical object (such as the earth) as follows. Assume that the earth's density is a constant $\rho = M/[\frac{4}{3}\pi R^3]$, where M is the mass of the earth and R is its radius. Imagine disassembling the earth by removing a thin shell of material of thickness dr then another shell of thickness dr and so on.

(a) Show that the energy required to move a shell of thickness dr away from the earth when its radius has already been pared down to r is then

$$E = \frac{3GM^2 r^4\,dr}{R^6} \qquad \text{(Q13.23)}$$

(b) Do an appropriate integral to find the gravitational binding energy of the sphere.

(c) Use this to find the earth's gravitational mass deficit (in kilograms), assuming that the system's constituent parts are its atoms.

(a) The mass of the spherical shell is

$$dM = \rho A\,dr = \left(\frac{M}{\frac{4}{3}\pi R^3}\right)(4\pi r^2)\,dr = \frac{3Mr^2\,dr}{R^3}$$

The mass inside a radius r is

$$M(r) = \rho V = \left(\frac{M}{\frac{4}{3}\pi R^3}\right)\left(\frac{4}{3}\pi r^3\right) = \frac{Mr^3}{R^3}$$

The gravitational potential energy in place is then (relative to $U(\infty) \equiv 0$)

$$U = -\frac{GM(r)\,dM}{r} = -\left(\frac{G}{r}\right)\left(\frac{Mr^3}{R^3}\right)\left(\frac{3Mr^2}{R^3}\right)dr = -\frac{3GM^2r^4\,dr}{R^6}$$

So the energy required to take this mass to infinity is

$$E = 0 - U = \frac{3GM^2r^4\,dr}{R^6}$$

(b) To get the total gravitational binding energy we integrate

$$E_b = \int_0^R dr\,E(r) = \int_0^R \frac{3GM^2}{R^6} r^4\,dr = \frac{3GM^2}{R^6}\left.\frac{r^5}{5}\right|_0^R = \frac{3}{5}\frac{GM^2}{R}$$

(c) for earth $\Delta m = \dfrac{E_b}{c^2} = \dfrac{3(6.67\times10^{-11}\,\text{kg}^{-1}\text{m}^3\text{s}^{-2})(5.98\times10^{24}\,\text{kg})^2}{5(6.38\times10^6\,\text{m})(3.00\times10^8\,\text{m/s})^2} = 2.49\times10^{15}\,\text{kg}$

about 0.4 parts per billion of the earth's mass