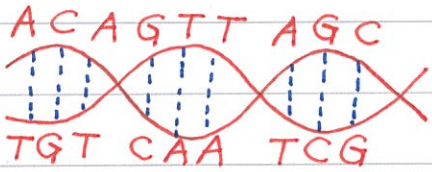
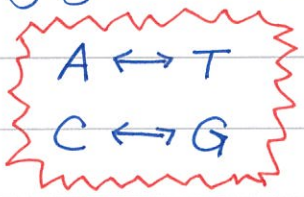
HH0138 How Is the Secret of Life Encoded?

In 1944, Schrödinger published a book entitled "What is life?" This is quite a big question to answer. In this book, Schrödinger proposed that the genetic information is carried by "aperiodic crystals"

↖ information in chemical bonds.

It turns out that the main idea is correct. In 1953, Watson and Crick proposed the double-helix model for DNA – the giant molecule carrying genetic information.





4 different nucleotides with the base pairing rules on the left.

To carry on genetic information from one generation to another, robustness is important. But, to make use of the genetic info, flexibility is necessary to produce various proteins. These two properties seem incompatible ... Can DNA somehow find optimal balance inbetween?

In modern perspective, the key of life is the interplay between information and energy. At room temperature (~300k) the thermal energy is about $k_B T_R$. Express it in eV,

$$k_B T_R \sim 0.025\,eV$$

← very important energy scale for living cells ☺

To understand DNA better, you may want to think how simple molecules form first ☺ We would like to derive the equation for molecular formation first and discuss covalent and ionic bonds. At the end, we come back to address the weak bonds in DNA ☺"

⑪ Schrödinger equation for molecular formation.

For simplicity, consider two atoms in 1D with mutual interaction $V(x_1-x_2)$. The total energy is

$$E = \frac{1}{2}m_1v_1^2 + \frac{1}{2}m_2v_2^2 + V(x_1-x_2)$$

← change variables!

Introduce the CM and relative coordinates,

$$X_c = \frac{1}{m_1+m_2}(m_1x_1+m_2x_2), \quad x = x_1-x_2$$

same relations for velocities V_c, v

It is straightforward to show that the total energy is

$$E = \frac{1}{2}Mv_c^2 + \frac{1}{2}\mu v^2 + V(x)$$

$M = m_1+m_2$ total mass

$\mu = \frac{m_1m_2}{m_1+m_2}$ reduced mass.

Rewrite the above expression in terms of momenta:

$$E = \frac{P_c^2}{2M} + \frac{p^2}{2\mu} + V(x)$$

In QM, $P_c \to -i\hbar\frac{\partial}{\partial x_c}$

$p \to -i\hbar\frac{\partial}{\partial x}$

Finally, one can write down the Schrödinger equation,

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2M}\frac{\partial^2\psi}{\partial x_c^2} - \frac{\hbar^2}{2\mu}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi$$

looking for stationary states

The t and X_c dependence can be solved easily,

$$\Psi(x_c,x,t) = \phi(x)\, e^{iP_cx/\hbar}\, e^{-iEt/\hbar}$$

← still need to solve for $\phi(x)$

Substitute into the Schrödinger equation to find the differential equation for $\phi(x)$,

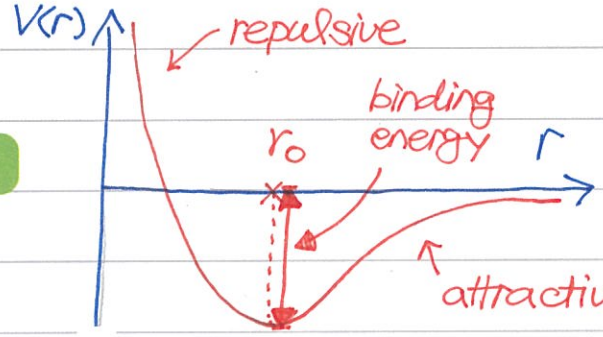
$$-\frac{\hbar^2}{2\mu}\frac{d^2\phi}{dx^2} + V(x)\phi = \varepsilon\phi$$

$$E = \frac{P_c^2}{2M} + \varepsilon$$

↖ CM motion.

The above result is very beautiful. The two-particle problem is simplified to one-particle problem! It is amazing that the concept of CM is still useful in the quantum world. Because the CM motion is simple, we will focus on $\phi(x)$.

Ⅶ Potential-energy diagrams. Consider two H atoms at distance r. The potential energy takes the shape,



When the atoms are too close, the nuclei are no longer screened by electrons – strong Coulomb repulsion due to the same positive charges. The attractive part is tricky. It arises from quantum fluctuations with a generic form $\frac{1}{r^6}$. The force is called van der Waals force. It can be reasoned in the following picture:

H atom H atom Q fluctuation! attraction ☺

Because the interaction between a pair of neutral atoms takes similar form, it is often approximated by Lennard-Jones potential,

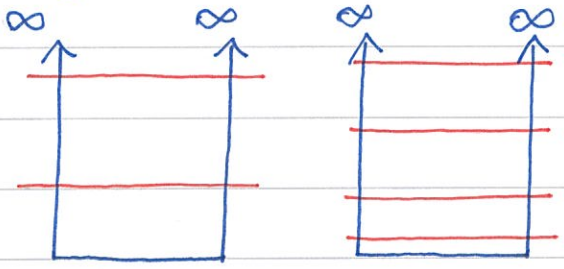
$$V_{LJ}(r) = \frac{A}{r^{12}} - \frac{B}{r^6}$$

Here A, B are positive constants. It is easy to find the minimum @ $r=r_0$.

$$\frac{dV_{LJ}}{dr} = 0 \rightarrow -12A r_0^{-13} + 6B r_0^{-6} = 0 \rightarrow r_0 = \sqrt[6]{\frac{2A}{B}}$$

Ignore the kinetic energy $P^2/2\mu$ momentarily – r_0 is the bond length and $|V(r_0)|$ is the binding energy. What about the effect caused by $P^2/2\mu$? In the infinite potential well, the lowest stationary state locates at

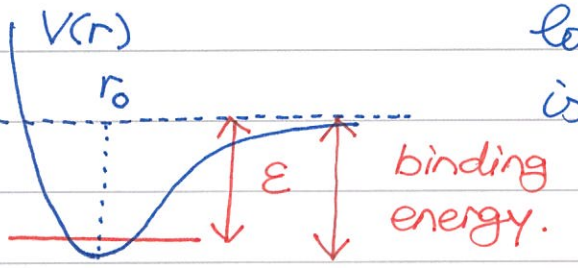
$$\varepsilon = \frac{\hbar^2 k^2}{2\mu} = \frac{\hbar^2 \pi^2}{2\mu L^2}$$



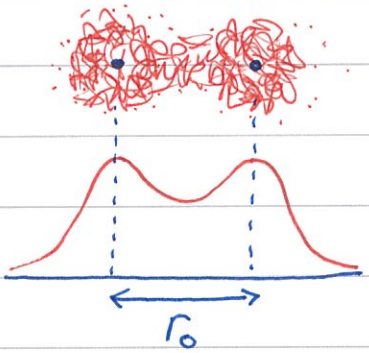
small μ large μ

The lowest energy $\varepsilon \approx 0$ as μ becomes heavy ☺

For general potential shape, the calculation is more complicated but the trend is similar. As long as the reduced mass is large, $|E| \approx$ binding energy. It is not so bad to view r_0 as the bond length and $|V(r_0)|$ as the binding energy ☺



⓫ Covalent and ionic bonds. The potential-energy diagram tells us why molecule is stable. Nice, but it doesn't tell us the whole story. For instance, where are the two electrons in H_2 molecule? To answer this question honestly, one needs to write down Schrödinger equation for 4 particles.... too tough. It turns out that the probability density for electrons is shared between two nuclei. Because electrons spend more time between nuclei, the two positively charged nuclei are attracted through the negatively charged electron cloud. This is the so-called covalent bond, explaining the formation of H_2 molecule ☺

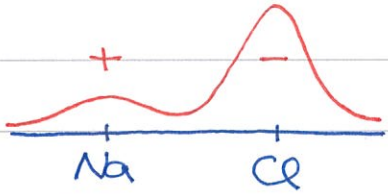


But in sodium chloride (NaCl), the electron sharing is NOT equal. The resulting bond is called ionic bond. Plot the probability density for the outermost electron of Na in NaCl.

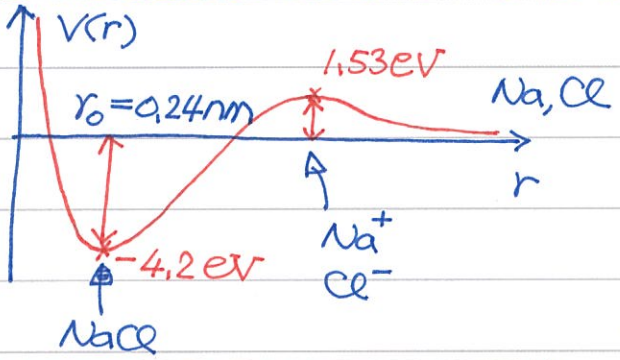
Na : $1s^2 2s^2 2p^6 3s^1$

Cl : $1s^2 2s^2 2p^6 3s^2 3p^5$

$\Rightarrow Na^+$, Cl^- closed shells.



⊘ Potential-energy diagram revisited. The potential energy diagram for NaCl is different from that for H_2 molecule due to the ionization barrier.



$$Na + 5.14\,eV \rightarrow Na^+ + e^-$$
$$Cl + e^- \rightarrow Cl^- + 3.61\,eV$$

Add up the ionization of Na and Cl :

$$Na + Cl + 1.53\,eV \rightarrow Na^+ + Cl^-$$

← needs energy to ionize Na, Cl 😊.

Thus, when Na, Cl atoms come closer, they need some energy to form ions Na^+, Cl^-. This creates an ionization barrier before the formation of NaCl.

Let us try a rough estimate for the binding energy ...

$$\mathcal{E}(NaCl) - \mathcal{E}(Na^+, Cl^-) \approx \frac{1}{4\pi\epsilon_0}\frac{(+e)(-e)}{r_0} \approx -6.0\,eV$$

Since $\mathcal{E}(Na^+, Cl^-) = 1.53\,eV$, $\mathcal{E}(NaCl) \approx -6.0\,eV + 1.53\,eV$,

$$\text{binding energy} = |\mathcal{E}(NaCl)| \approx 4.5\,eV$$

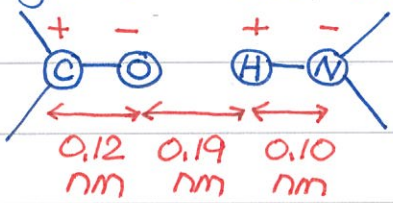
This rough estimate is very close to the measured value 4.2 eV.

⊘ Nucleotide binding energy. Either covalent or ionic bonds are strong, typically several eV as estimated before. However, the molecules still has residual interactions between them → often referred as weak bonds. Their strength is much weaker, typically in the range of 0.04 ~ 0.3 eV.

There are three types of weak bonds

dipole-dipole　　dipole-induced dipole　　van der Waals bond.

When one of the atoms in the dipole-dipole bond is hydrogen, the strength is strongest among weak bonds and thus acquires a special name — hydrogen bond. It is the bond holding DNA together. Let's estimate the binding energy between C & G.



$$U = \frac{1}{4\pi\varepsilon_0}\left(\frac{q_C q_H}{r_{CH}} + \frac{q_C q_N}{r_{CN}} + \frac{q_O q_H}{r_{OH}} + \frac{q_O q_N}{r_{ON}}\right)$$

The charges can be estimated from the measured dipole moment: $q_C = -q_O = 0.42e$, $q_H = -q_N = 0.19e$. Plug in all numerical values to obtain the potential energy

$$U \approx -1.86 \times 10^{-20}\,\mathrm{J} = -0.12\,\mathrm{eV}$$

This is comparable to the average kinetic energy at room temperature $\frac{3}{2}k_B T_R \approx 0.04\,\mathrm{eV}$. Because the energy scales are close, DNA can function in a living cell near room temperature. Amazing, isn't it?

清大東院

2014.0529