SEOUL NATIONAL UNIVERSITY – SCHOOL OF PHYSICS

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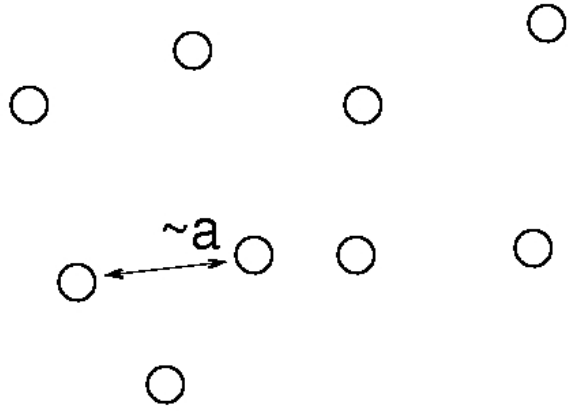
Solid State Physics II

Chapter 1 Hypothetical Hydrogen Solid

Jaejun Yu
jyu@snu.ac.kr
http://phya.snu.ac.kr/~jyu/

Hypothetical Hydrogen Solid

A solid, or, a condensed matter system in general, can be visualized as a mere collection of atoms. In this chapter, let us try to image what form of matter one can possibly get out of the collection of "hypothetical hydrogen" atoms as a function of temperature and density.



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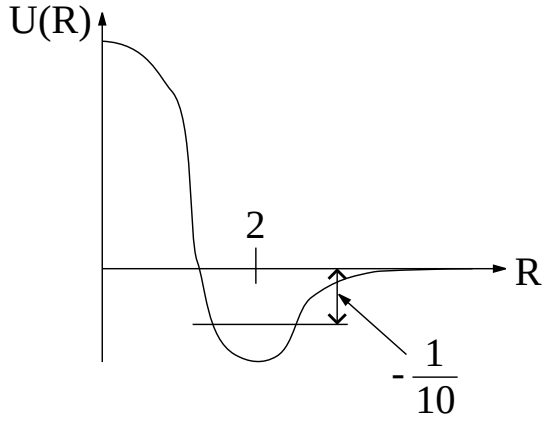
- Two hypothetical hydrogen atoms can also have a single bound state of an energy $-1/10$ a.u. and the mean separation between the atoms is about 3 a.u., leading to a H_2 hydrogen molecule.



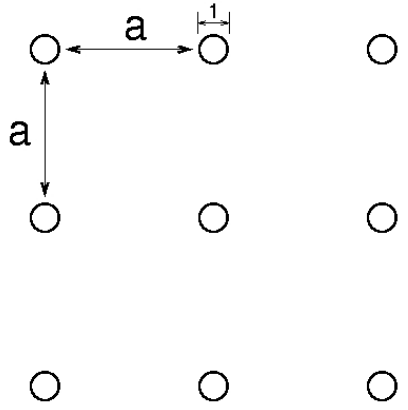
- The hypothetical H_2 molecules, interacting with each other through the van der Waals interaction, are assumed to have a single bound state of energy $-1/10^2$ a.u. and the mean distance between the atoms is about ~ 10.

In the limit of low density and low temperature

First, consider a regular array of the hypothetical atoms, for an example, in a cubic lattice. Suppose that the system is at $T = 0$ and the mean spacing between the atoms is relatively large, i.e., $a \gg 1$.

$$T = 0$$

$$a \gg 1 \quad \longrightarrow \quad n = \frac{1}{a^3} \ll 1$$



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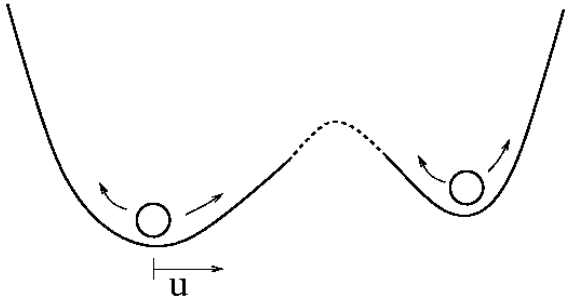
- What is a general criterion for the stability of a system?
  In classical mechanics, a particle in its equilibrium with restoring forces is called "stable". In other words, any displacement u from the equilibrium position has to be described by the equation of motion:

$$\frac{d^2u}{dt^2} = -\omega_o^2 u$$

  where ω_o^2 needs to be positive, i.e, $\omega_o^2 > 0$. If $\omega_o^2 < 0$, then it becomes unstable. In general, we can consider the energetics in its configuration space in order to identify the stability condition.

- Energy curve:

$$E = E(\{x_i^o\}) + (x_i - x_i^o) \cdot \nabla_x E|_{x_i^o} + \frac{1}{2}(x_i - x_i^o)(x_i - x_i^o) \cdot \nabla_x^2 E\Big|_{x_i^o}$$



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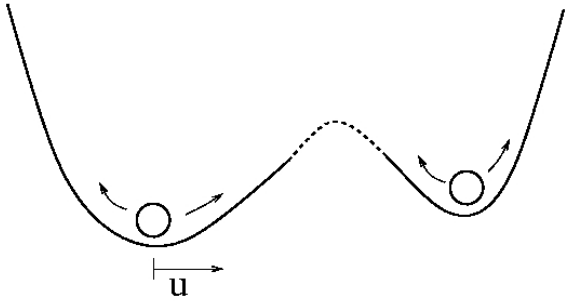

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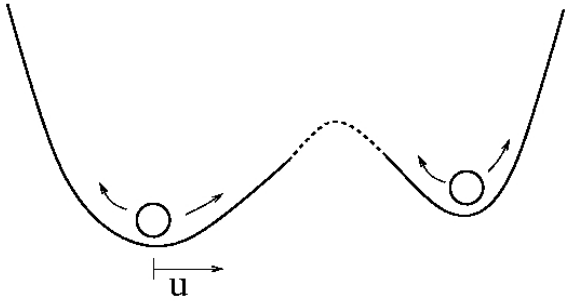

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  For examples, one can consider external perturbations, quantum fluctuations, etc.

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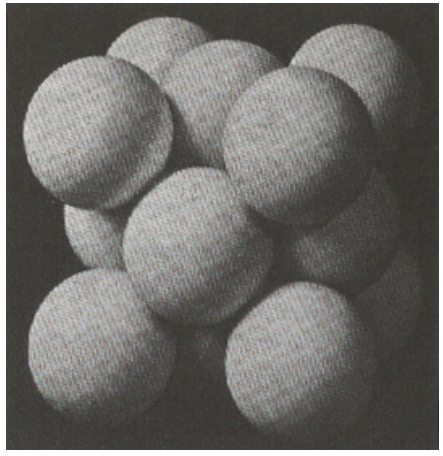

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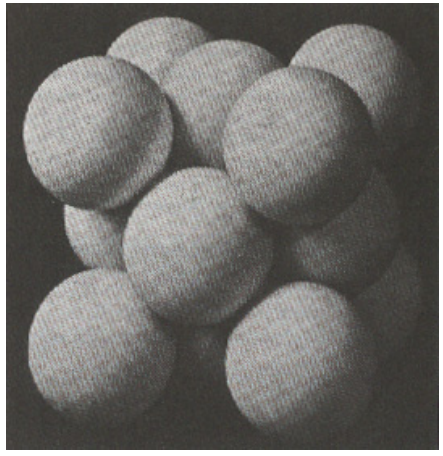
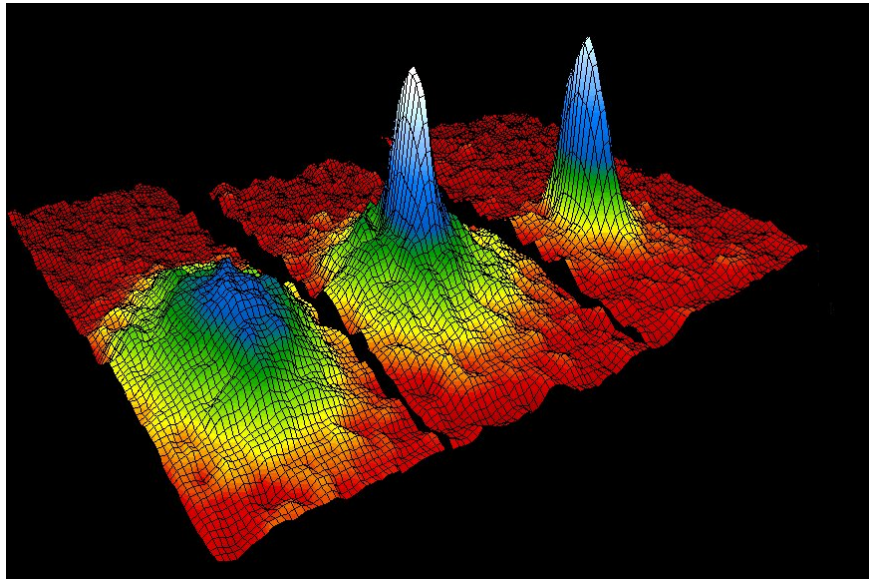


For an example, the inert gases form a close-packed lattice such as fcc or hcp structures. How does it apply for the case of hypothetical H_2 molecules? Could you also guess the density of such matter?

Question: In recent BEC (Bose-Einstein condensation) experiment, several researchers have succeeded in stabilizing the systems consisting of low density atoms. How could one make it possible? What forms of matter is it?



In the limit of high density and low temperature

Now, starting from the solid form of hypothetical hydrogen atoms, e.g., H_2 molecular solids, where the mean spacing between the atoms is about $a \sim 10$, let us apply an external pressure on the solid so that the mean spacing a becomes shorter and shorter as the pressure arises. Here we assume that the system is at $T = 0$.

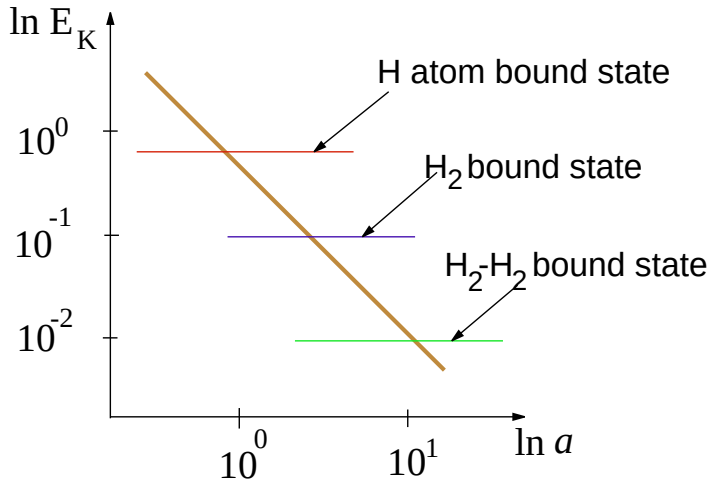
As the mean separation decreases and becomes less than the size of molecules, we can imagine that each electron attached to the *hydrogen atom* or *molecule* will be squeezed into a box of size a^3. As a result, the electrons will gain a kinetic energy

$$E_K \sim \alpha \frac{\hbar}{2ma^2} \sim \frac{\alpha}{2a^2}$$

Thus, if the kinetic energy of the electrons exceeds the binding energy of H_2 molecules due to the van der Waals interaction,

$$E_K > 1/10^2$$

the solid form of H_2 molecules will not be stable any more.



Question: As the density increases, i.e., $a \rightarrow 0$, we can guess that the electrons will gain more kinetic energy due to the spatial confinement. In terms of the electron's energy compared to the binding energies, can you guess what types of solids the *hypothetical* hydrogen atoms will form?

In the limit of high density and finite temperature

Question: Now suppose that the system is at a finite temperature, T, so that the electrons as well as protons can be excited. Depending on the scale of T, we may expect different configurations of atoms. Let us consider four different temperature ranges: (i) $T \ll 1/10^3$, (ii) $1/10^3 \ll T \ll 1/10$, (iii) $1/10 \ll T \ll 1$, and (iv) $1 \ll T$.

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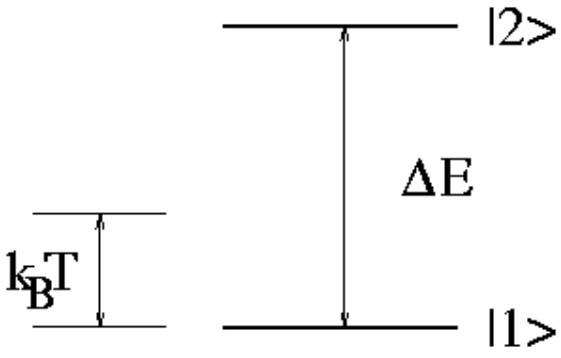
(i) $T \ll 1/10^3$

In this range of temperature, the thermal energy is far less than the binding energy due to the van der Waals interaction. In other words, the probability of the thermal excitation from the van der Waals bound state to the unbound molecular state is negligible.

$$P \sim \exp(-\Delta E/T) \ll 1$$

where $\Delta E = E_{unbound} - E_{bound} \sim 1/10^3 \gg T$.

Thus, all the electronic degree-of-freedom becomes frozen at this temperature range, and the remaining one is the translational motion of the H_2 molecule itself.



(i) (cont'd)

As we already discussed in the previous section, the H_2 molecules are likely to form a close-packed lattice with a lattice constant a. It means that the molecule will be confined in a space of length $\sim a$. At this point, we can explore more on the stability of the lattice in the high density limit, i.e., $a \ll 1$.

Although we have not discussed yet but will in the next chapter, the binding energy of the molecular lattice can be represented by a potential for the H_2 molecule at each lattice site:

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The quantum mechanical ground state of the H_2 molecule should have an energy of $\hbar\omega_o/2$. By applying the argument of the Quantum uncertainty principle, we can estimate the extension of the H_2 molecule as

$$K \sim \left\langle \frac{P^2}{2M} \sim \frac{1}{6000}(\Delta P)^2 \right\rangle \sim \frac{1}{6000(\Delta x)^2} \sim \omega_o$$

$$\Delta x \sim \frac{1}{\sqrt{6000\omega_o}}$$

In order to have this lattice stable, we may require

$$a_c = \frac{1}{\sqrt{6000\omega_o}} < a$$

Therefore, in the high density limit of $a < a_c \sim 1$ with $\omega_o \sim 1/600$, it can become a quantum liquid.

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Note: Once it becomes a quantum liquid, however, one need to reconsider the electronic configuration. Further, if $a \ll a_c$, one may have to consider the situation in which the H_2 molecule dissociate and the solids of hydrogen atoms, not the molecules, need be considered.

(ii) We can carry on similar discussions for the ranges of $1/10^3 \ll T \ll 1/10$, $1/10 \ll T \ll 1$, and $1 \ll T$. However, the situation becomes rather complicated because electrons will play an active role in various ways.