Hi Ming-Hsien,

Yes, the Chat GPT piece that you sent is remarkable --- absolutely remarkable --- which I think allows a change in plan which *builds on it* and uses it for most of the text --- in fact for nearly all of the text.

In some places, it does not quite "hit the nail on the head" as one says in English (or New Zealand English). It shows how very difficult it is to express the nature of the bonding *precisely* correctly, and I would like to make some rewording.

Let me start by just expressing it as best I can in my own words, to you.

The most important issue is "covalent bonding". Yes, if we look in a metal *just between two neighbouring atoms*, then the electron system there does look just like a covalent bond --- in fact the basic nature of the bonding is the traditional two-atom two-electron type of bond, as pointed out in (refce I think Pauling around 1939???), and as one has for example in the traditional 'tight binding' form of Bloch functions as formulated by Bloch in his original paper (refce). In the sp-bonded metals it is a hybrid of s and p atomic electron orbitals, as it is in the traditional picture for metallic sodium whether based on 'tight binding' atomic orbitals or on the dominant cosine and sine parts of the Nearly Free Electron picture.

The difficulty comes in describing the electron bonding system as a whole. In the paper with Siyu we included a figure (maybe Fig. 3, from memory) showing for *aluminium* a region of about 20 atoms with a few full 2-electron bonds with up and down spins, and some other half-filled pair-bonding orbitals. Of course most of the interatomic nearest-neighbour regions are empty.

There are TWO aspects.

(1) metals are malleable, i.e. the atoms can move around each other, but the piece of metal does not break apart when hit with a hammer:

(2) there are so few bonds to hold onto all those 12 close neighbours. How can it? Why does the metal not just *fall apart* ?

Let us start with the second question. The first and most obvious aspect is that the figure referred to above is so empty, i.e. each aluminium atom has 12 close neighbours (in the fcc crystal structure), but only three electrons to form bonds with them. If instead of aluminium we envisage sodium with only *one* electron per atom, the picture gets even more extreme ---- more absurd one might say, with only one electron-per-atom for the atom to hold onto all those 12 close neighbours (actually 14 for the bcc structure of sodium). Why does the metal not just fall apart??? Yet metals are strong respectable (chemical) elements.

The answer lies in Quantum Mechanics, and the difficulty is to express the uniqueness and precision of quantum mechanics in simple language! In fact the answer lies in something unique to quantum mechanics with *no* analogue in classical physics. Let us return to the figure with a few bonds and half-bonds in aluminium. The half-bonds consist of an electron in a proper two-neighbours bonding orbital, but only filled with one electron of up or down spin. The intention of the figure was to convey how *all* the electrons are in fully bonding orbitals (so far, so good), but there are rather few of them to hold on to all those 12 neighbouring atoms (or 14 for the bcc crystal structure of sodium). The figure was supposed to catch the electron arrangement at *one* instant of time, while it fluctuates between *all* such pictures. But this is where we have strayed into a classical way of talking. The ground-state of the system in *quantum mechanics* is not a fluctuation between many states, but is *one* unique state that *includes* all the many components within it, as emphasised in the referenced article by Schroedinger. *Thus it has most of the characteristics of all the many components.*

The malleability of metals (the other property with which we characterised metals) is therefore easy to understand. If one hits a piece of metal with a hammer, the atoms are certainly a bit differently arranged, but the deformed state has practically the same volume as the basic crystal structure so that one has the same kind of picture for the quantum ground state of the deformed specimen. We might note that practically all metals when fully annealed have one of *three* crystal structures, with many of them having easy phase transitions between them at moderate temperatures and pressures. This already suggests that the detailed geometrical arrangement of the atoms is not so critical. The atomic core radius of a metal atom is typically about *half* the atomic radius, so that there is plenty of space for less regular structures to have much the same energy and properties as the ground state, i.e. for the metal to be malleable.

The electron quantum states have a spread of energies resulting from their bonding between atoms, and the total bonding energy
can be calculated rather easily to a first approximation (which will do for us). It comes to a typical pair-bond energy for each electron in one bond (which we shall call /h/),

multiplied by the **square root of the number C of neighbours that a typical atom can bond to.**

U(bonding) = (sq.rt C) /h/ per bonding electron.

This is the basic result which we have to apply. The surprising aspect is the square root, not common in discussion of electronic structure, but coming directly from a local atomic point of view.

Later

What does Chat GPT suggest?????

Can we describe where the square root comes from??? It is the width of the distribution. I don't feel like trying -- it will just come out garbled.

**************** Goodnight for now. What do you think???

Volker.