

Listening to Molecular Quantum Mechanics

The mathematics that permits calculation of the electron energy density distribution in an orbital uses Schrodinger *wave equation* + *wave function* physics. The wave function calculations resemble the classical physics calculations of the resonant tones of musical instruments. The mathematical solutions are called eigenstates, and the system energies are called eigenvalues. The configuration that corresponds to the lowest system energy is the ground state orbital. A chart showing the separations between allowed quantum-state energies is called an energy level diagram. The energy level diagram for the hydrogen atom was first calculated by Niels Bohr.

As wave function physics advanced and more complicated atoms were modeled, it became evident that predictions based on calculated orbitals did not match the organization of elements based on chemical properties, as shown in the Periodic Table. But the results did agree if there could be two electrons per calculated orbital. The second atom in the Periodic Table is helium. The ground state helium atom has 2 electrons in hydrogen's *s*-orbital. The *s*-orbital is shown in Fig. 1.2,1. The number of atoms per orbital was doubled. The doubling of the number of atoms per orbital required introduction of the concept of electron spin. The existence of spin meant that there was an additional degree of freedom present in the electron. This additional degree of freedom is also present in other fundamental particles, like protons and neutrons.

The idea that fundamental particles are point objects is not consistent with Heisenberg's uncertainty principle, which says that if you precisely define a particle's momentum, you can't give it a zero size. You must give it a small sub-submicroscopic "size", which gives it a moment of inertia and an associated degree of freedom. The point physics of submicroscopic objects, like idealized electrons in atoms, distributes the particle density of each of the electrons over a 3-dimensional continuum of space. The physics of real electrons recognizes that the non-point nature of the electron adds another degree of freedom. Experiments show that the new degree of freedom is restricted to two discontinuous values. Mathematically, the two values are represented by two allowed spin angular momentum vectors (arrows). The electron has been arbitrarily assigned an allowed spin magnitude with index number = $1/2$, with a choice of two directions for the spin angular momentum axis. An electron with spin direction "up" is said to have spin $+1/2$, and an electron with spin direction "down" is said to have spin $-1/2$. In the helium atom the two electron spins have opposite directions. Their spin angular momentums cancel. The electron pair is a spin-zero pair.

The first orbital calculation that gave the known energy for the helium atom was achieved by Hylleraas. The physics requires that the modeler follow a second Pauli rule, which requires that a 2-particle spin-zero system obey a symmetry constraint called "coordinate exchange symmetry". A 2-particle system of point objects has 6 degrees-of-freedom, which can be taken as the x y z spatial location of the center-of-mass of the combined system, plus 3 degrees-of-freedom to describe the internal dynamics of the 2-particle system. If the internal geometric structure is that of a diatomic molecule like D_2 , the internal degrees-of-freedom express stretching vibrations along the system axis, plus two tumble modes about perpendicular axes. The Hylleraas solution has a different form. With the Hylleraas solution the energy minimizing solution has an internal structure with zero-separation between the 2 electrons, and no tumble or vibration motion. Instead, the two electrons of the helium atom overlap each other. If the electrons had the nuclear properties of deuterons, they would fuse.

The lesson for cold fusion is that if deuterons are going to be able to fuse at room temperature and pressure, they need to be subject to Pauli's requirement for coordinate exchange symmetry. This condition can be achieved under steady state conditions only if the energy-minimized solution of a 2-deuteron wave equation has the coordinate exchange symmetry form. Energy minimizing calculations show that this condition is satisfied if the deuterons have a quasiparticle geometry and the number of lobes in the quasiparticle wave function "orbital" exceeds about 1000.

As stated above, a two quasiparticle deuteron system has six degrees of x, y z freedom. One best thinks of the two deuterons as a single entity, and describes it in "center-of-mass, separation coordinates". One uses a position vector \mathbf{r}_{cm} to describe the density distribution of the 2-deuteron entity in the metal lattice, and a separation vector \mathbf{r}_{12} to describe the repeating internal structure that separates quasiparticle₂ from quasiparticle₁. The six degree-of-freedom wave function is written as the arithmetic product $\Psi(\mathbf{r}_{cm}) g(r_{12})$. In this math $\Psi(\mathbf{r}_{cm})$ is the orbital wave function described in Chapter 3.4, and $g(r_{12})$ expresses anticorrelation, instead of the vibration and tumbling dynamics of the D_2 molecule. Function $g(r_{12})$ modulates the amplitude of the composite 2-deuteron system. Approximate calculations show that $g(r_{12})$ has essentially the value 1.0 when the number of orbital lobes is much greater than 1000, and a lower value when the number of lobes is smaller, but above a threshold number.

The form of $g(r_{12})$ is that of a "cusp function". Figure 3.5,1 pictures $\Psi(\mathbf{r}_{cm})$ and $g(r_{12})$ before fusion. The dips in the green $g(r_{12})$ function have sharp downward-facing points at their bottoms. One of these

sharp points occurs in each unit cell of a "2-deuteron internal structure mathematical lattice". Function $g(r_{12})$ modulates the amplitude of the 6-degree-of-freedom wave function at each point in the 3-dimensional deuteron quasiparticle-occupied lattice, as defined by $\Psi(\mathbf{r}_{cm})$. Figure 3.5,2 shows the change in $g(r_{12})$ geometry that occurs during the wave function collapse step in the fusion process. This collapse is Step 1 in the nuclear reaction process.

Another important discovery in molecular chemistry and physics has been a recognition that the geometry of a molecule can be made to change to a second geometric structure that has almost the same energy. The condition producing this change is called a Feshbach resonance. The change occurs during an energy scan process. If one can alter the environment in a manner that changes the energy of one of the configurations differently from the other, one can at some point make the two energies equal. The energy changing process is called a resonance scan. A scan across a resonance can switch the system's internal geometry, leaving the location of the center-of mass unaffected. The physics of molecular quantum mechanics shows that a back and forth scan across a resonance can lead to an energy transfer to the hosting environment. As applied to the quasiparticle nuclear states involved in quasiparticle deuteron fusion, the scan process can lead to a transition from a pre-scan paired deuteron state to a pre-scan near-resonance metastable initial nuclear state, accompanied by transfer of a small amount of energy and momentum to the hosting metal environment. The metastable nuclear state is a high-energy excited state, many MeV above the helium-4 ground state. However, the transfer of even a small amount of energy to the hosting lattice makes the nuclear reaction irreversible. The possible role of nuclear resonance was pointed out by Xing-Zhong Li, the head of the Chinese cold fusion effort. Physicist Scott Chubb identified momentum shocks as a means of transferring energy to the hosting environment. A subsequent energy cascade process completes the transfer of nuclear fusion energy to the hosting lattice.

Six Degree-of-Freedom Quasiparticle Wave Function

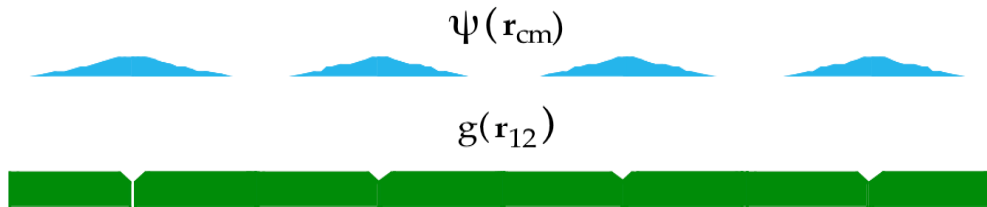


Fig. 3.5,1 Wave function amplitude in physical space $\Psi(\mathbf{r}_{cm})$ and wave function modulation factor in separation space $g(\mathbf{r}_{12})$ for a 2 quasiparticle deuteron entity.

$2\text{-D}_{\text{Bloch}}^+$ Coalescence to Nuclear Dimension

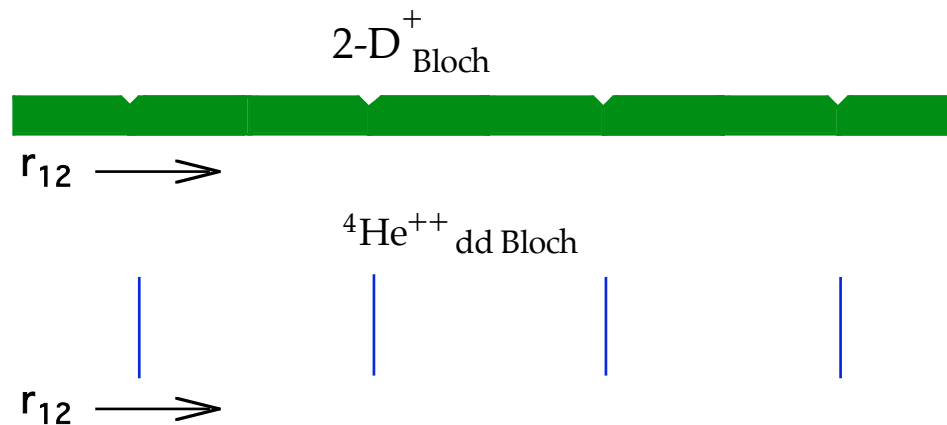


Fig. 3.5,2 Collapse transition of a quasiparticle 2-deuteron pair. The green image is the $g(\mathbf{r}_{12})$ internal geometry function before collapse to nuclear dimension. The four blue vertical lines is the $g(\mathbf{r}_{12})$ function after collapse to nuclear dimension.