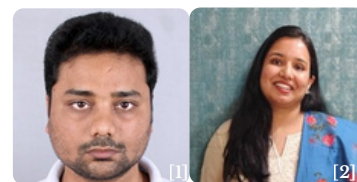


From learning to living: "Shh... what's happening deep in there"

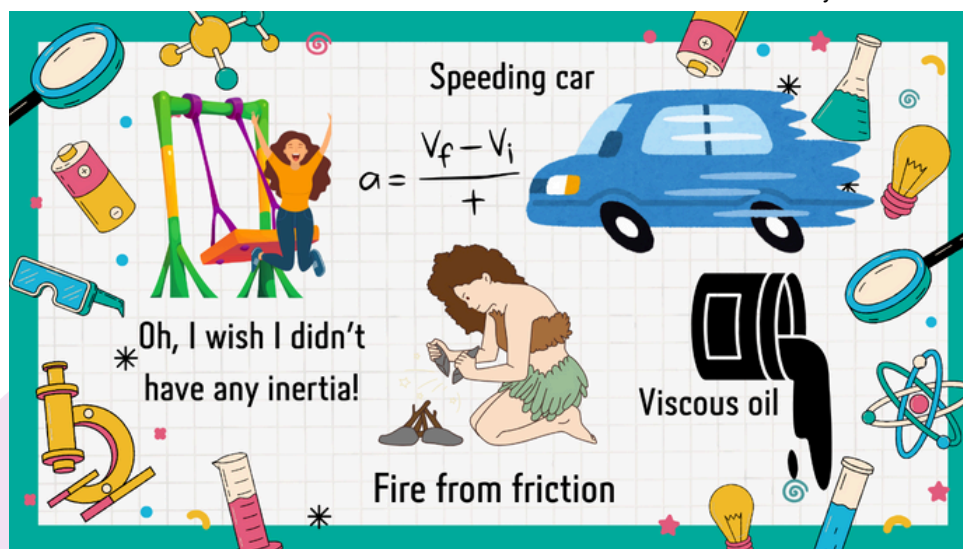
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We must have experienced “momentum”- when you collide with someone strong, “acceleration” – while driving, “inertia”- when falling from a swing, “friction”- applying brakes, “viscosity”- pouring oil. The physics we learn gives us an understanding of how things work around us, and how nature responds to any actions. However, building an intuition for anything is based on our past experiences. How do we relate to physical terms like “electric field”-unless we carry a strong presence, “drift current”-unless we have boarded a Mumbai local train, “energy structure” – unless you can see beyond the physical, “wave mechanics”- may be if you are a singing maestro, “quantum wavefunction”- unless you are a mystic (as physicist still don’t have an answer to it!).

Even in deterministic systems, practical constraints (e.g., imprecise instruments or chaotic dynamics) prevent exact predictions, necessitating probabilistic descriptions. Thus, this reminds us that probabilistic descriptions are not all that unknown to us, even in the classical domain, and are perceived as extrinsic limitations.

In quantum mechanics, probability is intrinsic to nature. The wavefunction $\psi(x)$ describes a system's state, where $|\psi(x)|^2$ gives the probability density of finding a particle at position x . This isn't due to measurement limitations but a core feature of reality. Now this is hard to logic with! And should we even bother about it? Well, for a material scientist it could be a threat to your “aims and objectives”.



Quantum mechanics phenomenon is quite sneaky; it may appear even if haven't planned for it (e.g., Raman scattering, Quantum capacitance, Tunnelling, plasmonic, diffraction contrast). Especially at smaller dimensions, we are more likely to find some quantum phenomenon either aiding or hindering what we set to achieve. But if we are stuck with quantum mechanics, it's better to make some acquaintance, or at least break some ice.

The point is that we use our daily life experiences to understand most of the classical mechanics physics. However, our perception is largely limited when we talk about physics at the atomic scale, and particularly, quantum mechanics. But this is not all that mind-boggling if approached with some help.

The resistance to accept arises when things do not fit into our logical framework, and it seems as if nature does not care about our logic. “Logic” is “deterministic” in nature; physical laws should give a measurable quantity. How do we know something exists if we cannot measure it? On the other hand, there are probabilistic and indeterministic things, and interestingly, they are important even to derive classical physics. Even to get a simple geometric area, we rely on an irrational number

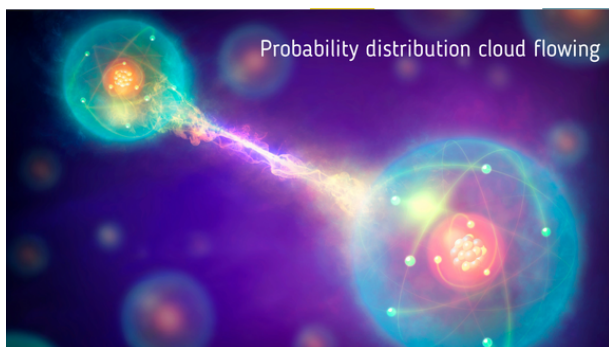
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If we look into the derivations in classical physics (which we often ignore!), probability arises from incomplete information about a system (e.g., not knowing the exact position/momentum of every gas molecule in a container). Thus, probability is epistemic (reflecting ignorance).

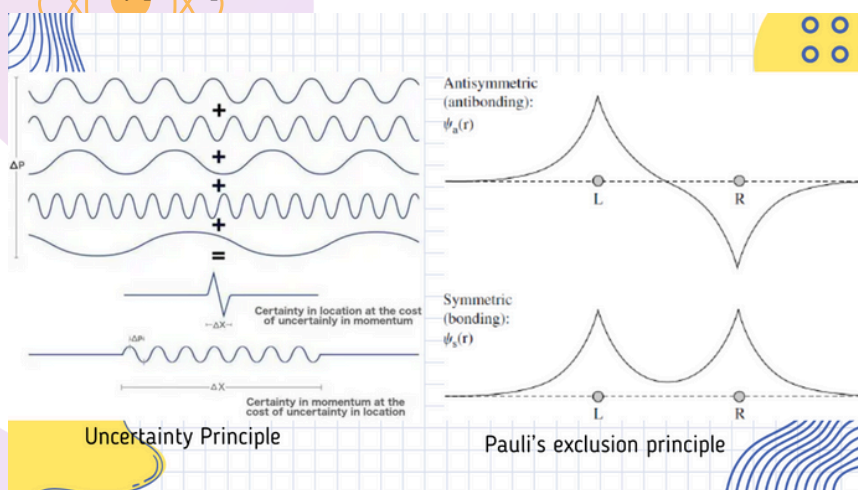
We may think that the material we work with is innate, but try telling that to an electron in that material which got no rest. An analogy would be you on a sail boat deep in an ocean. If you are a lucky electron, you may be in the Pacific (calm) or you can be in the Southern Ocean (Antarctica) struggling to survive. But we want to see this happening in a material, as it is important to solve the problem at hand and put the material to some application.

So, we disturb the already disturbed material and capture the difference when it goes down to its earlier state (Spectroscopy, XRD). Sometimes we disturb it so much that some of the electrons jump out of the material to tell us what was happening to them inside the material (Microscopy, XPS). Other times, we handle it more smartly by making use of “intelligence” about the subtle nature of the material's energy structure (NMR, EPR).

What is it exactly that we are disturbing? Delving further, energy levels or atomic orbitals are a cloud of probability distributions.



When we say a transition for an electron happened from ground state to excited state (e.g., optical transition), in reality, it is changing its probability distribution from a sphere (S-orbital) to maybe a dumbbell shape in space (P-orbital). When you do a UV-VIS spectroscopy of your sample, it would be interesting to visualise the clouds changing shape. What drives this change in shape? Well, the excitation we provided may be by changing the (potential) energies or some other induced interactions. Polarizability is the “squishiness” of these clouds. In Raman spectroscopy, these clouds are coupled with the vibrating nucleus, and they take on shapes (for an infinitesimal time, $\sim 10^{-15}$ sec) corresponding to a different energy level (virtual level). So next time you irradiate your samples with strong lasers, visualize the dynamically changing electron cloud because of the vibrations. A wave is essentially a distribution of any variation in space and time. So, the probability distribution and wave function exhibit wave nature. When we say wave nature, what we mean is that “nature or phenomenon” that any wave may exhibit. Thus, we can use waves on a string or water (for visualization) to build our intuition for quantum waves. What can we say about the position of a wave, which is a spread? At best, we can say a range, and a range leads to uncertainty or error (Heisenberg’s uncertainty principle).



A wave can be a superposition of other waves. If we superimpose waves to reduce uncertainty in position (i.e., narrow down the range), mathematically, we need to add infinite waves with fixed momentum (i.e., increasing the momentum uncertainty). We know what varies in acoustic, mechanical, or electromagnetic waves.

In quantum waves, from the definition, we know that instead of something physical, it is the probability that is varying with space and time. (Try plotting a probability distribution of yourself walking at different speeds: where are you most likely to be?) For example, let's think of a current flow. A current can be a flow of electrons, but electrons will flow to a changing probability distribution due to a change in energies (i.e., voltage).

An analogy would be you sitting in a sparsely filled classroom; the probability of you sitting in the class can be modulated based on your friends entering later. So, we say you moved to adjust to a new probability distribution. Anyway, of course, the probability will carry the object with it. A wave can spread, reflect, and interfere with another wave, which leads to a new wave that incorporates the interactions.

So, when we use a fundamental particle (i.e., single body wavefunction) to make molecules or solids (many-body wavefunction), wave interactions decide the overall wavefunction (The ocean analogy). Pauli's exclusion principle says electrons should have opposite spins to occupy the same orbital (probability distribution). This can be said in another way, that the wavefunction for fermions (electrons) is anti-symmetric. That is, if two fermions occupy the same quantum state (e.g., identical spatial and spin coordinates), swapping them leaves the wavefunction unchanged but also requires a sign change. The only solution is $\psi=0$, meaning such a state cannot exist.

Let us end with one more visualization: imagine yourself opening a refrigerator for a late-night ice cream that you didn't want to share or were not allowed to have, depending on your age. However, by mistake, you dropped your glass bowl (irreversible action), which fell and broke (sound wave).

No matter what you do, can you stop all the subsequent effects? (other than relying on your luck) Waves or quantum mechanics are like that! “A wavefunction collapses upon measurement.”

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