Quantum Fluctuations

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A way to introduce quantum mechanics is through quantum fluctuations, i.e.: the fact that, even at zero temperature, you are in an unavoidably noisy environment. We're going to describe a formulation of quantum mechanics which allows us to find the ground state of a particle in a potential, or of many bosonic particles in interaction, putting the stress in the nature of fluctuations. All this story can be justified using Feynman's path integral formulation, but this is another story which will be told somewhere else...

Let us consider a classical particle in a 1D potential $V(x)$. The particle is simple, elementary. I know, I know that any particle is elementary as long as it is not hit strongly enough, so let's assume that we're not going to mistreat it too much... Our particle will have mass m. But we will assume it to be at a certain temperature T, measured in units of energy (really, $k_B T$). Then, the probability of it being at a certain point with a certain momentum p will be

$$\frac{1}{Z}\exp\left(-\beta\left(\frac{p^2}{2m}+V(x)\right)\right)$$

where Z is the partition function, i.e.: a given number in our problem (let's not worry about it) and $\beta = 1/T$.

Let's assume that nobody is going to make us any questions about the momentum of the particle. Therefore, we want a probability distribution only for x. Therefore, we integrate to all momenta.

$$P(x) = \int dp \frac{1}{Z}\exp\left(-\beta\left(\frac{p^2}{2m}+V(x)\right)\right) = \frac{1}{Z'}\exp\left(-\beta V(x)\right)$$

Hey, the integral on p can be done, it's just gaussian! We don't care for the result: we simply notice that it does not depend on x. Therefore, we got a nice probability distribution only for x, with a different normalization factor.

So far, so good, but let's move to the quantum world. A possibly entry is through the conversion of the particle into a ring, a closed chain, of P of new particles, which we will now call *beads* or *replicas*. All the beads have the same mass, m, and they are linked to their neighbours with springs of a certain coupling constant K, whose equilibrium length is zero. The elastic energy of the ring will be

$$W(x_1, \cdots x_P) = \frac{1}{2}K\sum(x_i - x_{i-1})^2$$

and it is understood that $x_0 = x_P$, so as to have a closed chain. See figure 1 to have an image...

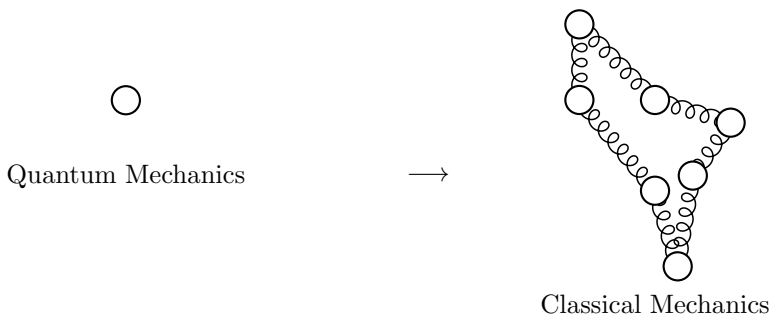

FIGURE 1. From quantum to classical mechanics.

But then, which is the "real" particle? Well, all of them are! It's quantum, remember? This is the famous *quantum cloud*. So, in order to know the probability of finding the particle at a position x we should compute the probability of *any* of the beads going there.

But, wait... why should this chain move? We will set it at a *finite temperature* T, same as we did with the classical particle. The case $T = 0$ can *not* be studied within this formalism, but we may make T very very small, as small as we want: $T \to 0$ instead of $T = 0$. Wait, then nothing will move, no? No, because the spring constant will be dependent on T. It will become softer as the temperature decreases, in such a way that the fluctuations will remain!! But let's not try to go too fast...

So, let's suppose that T is fixed. If K is very very high, $K \to \infty$, then the springs are very rigid and will be compressed to zero length. The particle becomes classical. If K decreases, the polymer opens up. In other terms: the quantum cloud spreads.

What about the mass of the particle? If the mass is high, the particle is very classical: K should be high too. Therefore, K should also depend on the mass.

Another point is: which number P to choose? In principle, the higher the better. But again, a problem seems to appear: if P increases then, for a fixed value of K and T, the polymer will extend, so the quantum cloud will be larger. What to do? Easy: we may make the strength of K depend on P too! Isn't it too many dependences for the same poor K? Perhaps, but it's going to work, you'll see!

So, summarizing: K should decrease as T decreases; K should increase as m increases; and K should increase as P does. Let's propose a form:

$$K \propto PT^2 m$$

Why the square on T? No proof for the moment, let's just say that otherwise fluctuations are inhibited as $T \to 0$. This form is almost OK. Only problem: units. It does not have units of a spring constant! If we measure (as we should) T in energy units (meaning that T is really $k_B T$), then the problem is corrected if we divide it all by $\hbar^2$. Check it! The final formula gets:

$$K = \frac{PT^2 m}{\hbar^2}$$

What's the meaning of this polymer? A physical picture may be provided this way. Each polymer is a "cyclic history" of a particle, i.e.: it repeats itself forever. The beads represent the same particle at different moments. The moments are separated by a certain fixed amount of time Δt, which didn't appear in the previous calculations.

But then, what's the real meaning of this energy? Consider two consecutive beads. If they are separated a lot, it means that the particle has traveled a lot in that time Δt. Therefore, the separation between consecutive beads measures the velocity of the particle. But we have more: the energy depends on the square of this separation, therefore on the square of the velocity: it is a kinetic energy!!!

So we have a meaning for the polymer elastic energy: it is the average kinetic energy on the path. Wait, you may say. Then, we might be able to write it in this other way:

$$\frac{1}{P} \sum \frac{m}{2} \frac{(x_{i+1} - x_i)^2}{\Delta t^2}$$

right? Right. And if you compare this formula with the previous one you'll find:

$$T = \frac{\hbar}{P \Delta t}$$

But $P\Delta t$ is the total time of the history of the particle t_{max}. Therefore, $T = \hbar / t_{max}$. Don't forget this completely! That's why we can't take $T \to 0$: for that we should consider particle histories of infinite length... and our computers are too slow for that... :)

Now we understand this polymer energy as a kinetic term. What about the potential energy? It will be easier, don't worry. We'd like to put all the polymer in a potential such that, when computing

$$\sum_i V(x_i)$$

we got the average potential felt by the quantum particle along its history. Easy: get a new potential just dividing by the number of beads! The full energy of the polymer is:

$$\frac{1}{2}K\sum(x_{i+1}-x_i)^2+\frac{1}{P}\sum V(x_i)$$

The division by P is just in order to take the average potential, as we said.

Now comes the big assertion: doing classical Monte Carlo simulation of this polymer at finite T is equivalent to doing quantum simulation of the same particle at the same temperature. So, if you study the $T\to 0$ limit, you get the quantum ground state!!

Can we find out some basic facts about quantum mechanics from this formulation? Surely we can! We'll try a proof of Heisenberg's uncertainty relations. Let's forget by now about the potential. The energy of the system is the sum of terms of the form

$$\frac{1}{2}Kl_i^2$$

where l_i is the length of the "spring" between sites i and $i+1$ (cyclic). The theorem of equipartition tells us that each of these terms gets the same energy: $T/2$ (really $(1/2)k_BT$, but $k_B=1$, OK?). So we have:

$$\frac{1}{2}K\left\langle l_i^2\right\rangle = T/2$$

$$\left\langle l_i^2\right\rangle = \frac{T}{K}$$

Now we may ask what is the average "spread" of the quantum cloud, i.e.: the average value of $\left\langle R^2\right\rangle$. We may assume that we're taking a random walk with variable steps. If you take such a walk of P steps of (square) width $\left\langle l_i^2\right\rangle$, the average (square) width is:

$$\left\langle R^2\right\rangle = P\left\langle l_i^2\right\rangle = \frac{PT}{K}$$

But now, this distance is traversed in a time $P\Delta t$, right? So the average (squared) velocity is:

$$\left\langle V^2\right\rangle = \frac{PT/K}{P^2\Delta t^2} = \frac{T}{KP\Delta t^2}$$

We may assume that $\left\langle R^2\right\rangle$ is the variance in the position of the particle, Δx^2. The variance in the momentum may be computed as

$$\left\langle P^2\right\rangle = m^2\left\langle V^2\right\rangle = \frac{m^2T}{KP\Delta t^2} = \Delta p^2$$

Wait, we may have a try and check if these two expressions are according to Heisenberg's uncertainty principle:

$$\Delta x^2\Delta p^2 = \frac{PT}{K}\frac{m^2T}{KP\Delta t^2}$$

Now, operate! Use the definition of $K=PT^2m/\hbar^2$ and the expresion for $T=\hbar/P\Delta t \quad\to\quad \Delta t = \hbar/PT$:

$$\Delta x^2\Delta p^2 = \frac{T^2m^2}{K^2\Delta t^2} = \frac{T^2m^2}{\frac{P^2T^4m^2}{\hbar^4}\frac{\hbar^2}{P^2T^2}} = \frac{T^2m^2\hbar^4P^2T^2}{P^2m^2T^4\hbar^2} = \hbar^2$$

It was a very coarse-grained calculation, but it gives us Heisenberg's relation:

$$\Delta x\Delta p = \hbar$$

Remember some things that are important: the path is *not* a random walk, since it returns to its origin!

This formulation of quantum mechanics is especially useful for interacting bosons, such as the study of superfluid helium. This is developed in detail in the Reviews of Modern Physics of Ceperley in 1995. I'll tell you how this formulation allows an easy explanation of superfluidity, but this will be another day!