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Lecture Notes on Applications of the Heisenberg Uncertainty Principle

1 Statement of the Principle

The Heisenberg Uncertainty Principle States that the quantum probability amplitude associated with a particle (electron, photon, etc.) always has the property that the product of the spreads in the measured distributions of position ΔX and momentum ΔP exceed $\Delta X \, \Delta P \geq \hbar/2$.

2 Application to a particle in a Box: The Energy of Confinement

2.1 Analysis

If we have a particle of mass M confined to a box of length L centered on the origin $x = 0$, then repeated simultaneous measurements of the position X and momentum P of the particle will yield distributions about some mean values $< X >$ and $< P >$ with characteristic widths ΔX and ΔP, respectively. In this case, $< X >$ will be centered somewhere within the confines of the box and the width of this distribution in X will have a width no greater than $\Delta X \simeq L$. Additionally, we expect from symmetry that the distribution in momenta which we measure will also be centered about $< P >= 0$, and by the Uncertainty Principle, we know that there will be some width in the momentum distribution ΔP as well.

Now, technically, if we knew that that the distribution within the box were uniform, we could use the precise result from the lecture notes on statistics that $\Delta X = L/\sqrt{12}$. However, at this point we know very little about the shape of the probability distribution (later in the course we will see explicitly that this distribution is *not uniform*. One could argue that, still $\Delta X \simeq L$ is likely an overestimate. While this may be true, we will not concern ourselves with such precise factors here because we know that in the end, the results we generate at this point are just estimates of orders of magnitude.

With all this in mind, it is safe to say that $\Delta X \leq L$. The uncertainty principle states, however, that $\Delta X \, \Delta P \geq \hbar/2$. Thus we conclude that $\Delta P \geq \hbar/L$. Here again, we are being sloppy with the factor of two. We really don't trust our result to more than an order of magnitude, and so there no point carrying extra factors which take time to write down and to track. For instance, we could just as well write h/L instead of $\hbar/L$. At this level of analysis either starting point will lead to equally valid results.

If we now ask for the kinetic energy of the particle

$$T = \frac{P^2}{2M},$$

it too will have some distribution. On average,

$$< T >=< \frac{P^2}{2M} >,$$

and now we need to estimate $< P^2/2M >$. P typically has values in the range $(-\Delta P \longleftrightarrow \Delta P)$ and so in order of magnitude, typically, $P^2/2M \sim (\Delta P)^2/2M$ and so $< P^2/2M > \simeq (\Delta P)^2/2M$. This rough physical argument is all that is required in this discussion. If, however, you are uncomfortable with this, you can also use the precise statistical definition of ΔP from the supplemental notes on statistics, $(\Delta P)^2 \equiv < P^2 > - < P >^2$. Combining this with the fact that $< P >= 0$, precisely $< P^2 >= (\Delta P)^2$. Using either argument, we have

$$\begin{aligned} < T > &\sim \frac{1}{2M}(\Delta P)^2 \\ &\geq \frac{1}{2M}(\hbar/L)^2 \end{aligned}$$

There is thus an absolute minimum average energy which are particle may have,

$$< T >_{min} \simeq \frac{\hbar^2}{ML^2}$$

(Again, there is no point in tracking the factor of two which we have dropped.)

To get a feel for the importance of this result, we note that for an electron $M \sim 10^{-27} g$ confined inside of an atom $L \sim 1$Å, $< T >_{min} \sim 6\, eV$, which is nearly half of the binding energy of hydrogen and thus the energy of confinement is a significant and important effect in chemistry and atomic physics. The electron has a non-zero kinetic energy, just by virtue of its confinement to a finite region of space. This very general principle follows directly from the uncertainty principle, and just as the uncertainty principle holds regardless of the physical situation or apparatus, we will see that the energy of confinement arises in all situations regardless of the agent which causes the confinement. The confinement may arise explicitly from the presence of a rigid box or come about from the attractive interaction between of the electron to a particular region of space (to the vicinity of the proton in an atom, for instance).

2.2 The Classical Limit

The energy of confinement is a purely quantum effect. In classical physics the particle may sit at rest with zero kinetic energy. It is the Heisenberg Uncertainty Principle which forces the spread in momentum giving rise to the non-zero kinetic energy. As this effect is not seen in classical physics, we must conclude from the correspondence principle that the effect is tiny in a macroscopic situation. For instance, for a ball on a pool table ($M \sim 100\, g$, $L \sim 100\, cm$), we find $< T >_{min} \sim 10^{-60}\, erg$, a truly negligible effect. There is a more formal way to look at this that does not require inserting the tiny value of $\hbar$ into the expression and running the numbers. One may instead take the mathematical limit $\lim_{\hbar \longrightarrow 0} < T >_{min} = \lim_{\hbar \longrightarrow 0} \frac{\hbar^2}{ML^2} \longrightarrow 0$ to find that the effect "vanishes" in "the classical limit". In a sense, $\hbar$ controls the importance of quantum mechanics and taking the limit $\hbar \longrightarrow 0$ is a way of "turing off" quantum mechanics.

3 Simple Harmonic Oscillator: Ground State/Zero Point Energy

3.1 Analysis

Now we consider a particle of mass M "confined" to the vicinity of the origin $X = 0$ with a spring of spring constant k. The energy of the particle is then given by the usual energy for a simple harmonic oscillator (SHO)

$$E = \frac{P^2}{2M} + \frac{1}{2}kX^2.$$

Again, by the uncertainty principle, no matter how we prepare our individual oscillators, there will be some spread in the distributions of the position and momentum X and P of the particles. Again, by symmetry, we expect $< X >=< P >= 0$.

The average energy of our systems under the distributions set up by our preparation of them is given by

$$\begin{aligned} < E > &= < \frac{P^2}{2M} + \frac{1}{2}kX^2 > \\ &= < \frac{P^2}{2M} > + < \frac{1}{2}kX^2 > \\ &= \frac{1}{2M} < P^2 > + \frac{1}{2}k < X^2 > \\ &= \frac{1}{2M}(\Delta P)^2 + \frac{1}{2}k(\Delta X)^2 \qquad (1) \end{aligned}$$

Here we have used the facts that the average of a sum is always the sum of the averages that the average of a constant times a variable is always the constant times the average of the variable. (If you feel uncomfortable with any of these manipulations, you may read about them in the supplemental notes on statistics.) At the final step, we used the same trick as in our discussion of the confinement to a box to conclude $< P^2 >= (\Delta P)^2$ and $< X^2 >= (\Delta X)^2$. The uncertainty principle puts an absolute lower limit on this energy as well. We know that $\Delta X\,\Delta P \geq \hbar/2$ and so we must have $\Delta P \geq \hbar/2/DeltaX$.

Although we need not at this point, we will be precise in our analysis of the SHO because we will later revisit this result when we have a full, formal theory. Also note that we can give an exact analysis in this case because the SHO just happens to have an energy quadratic in both X and P so that we can make the *exact* replacements $< X^2 > \longleftarrow (\Delta X)^2$ and $< P^2 > \longleftarrow (\Delta P)^2$.

Now, because $\Delta P \geq \hbar/2\Delta X$, we know

$$\begin{aligned} < E > &= \frac{1}{2M}(\Delta P)^2 + \frac{1}{2}k(\Delta X)^2 \\ &\geq \frac{1}{2M}(\frac{\hbar}{2\,\Delta X})^2 + \frac{1}{2}k(\Delta X)^2 \\ &= \frac{\hbar^2}{8M\,\Delta X^2} + \frac{1}{2}k(\Delta X)^2 \end{aligned}$$

There is a strict lower bound on the value which $< E >$ may have. This lower bound is given by the minimum of the function $E(\Delta X) = \frac{\hbar^2}{8M\,\Delta X^2} + \frac{1}{2}k(\Delta X)^2$.

We locate this minimum by setting the derivative equal to zero,

$$\begin{aligned} 0 = E'(\Delta X^*) \\ = -\frac{\hbar^2}{4M\,(\Delta X^*)^3} + k(\Delta X^*) \\ \Rightarrow (\Delta X^*)^4 = \frac{\hbar^2}{4Mk}. \\ \Rightarrow \Delta X^* = \left(\frac{\hbar^2}{4Mk}\right)^{1/4}. \qquad (2) \end{aligned}$$

(2) gives the localization for the particle in the SHO in its lowest energy state

One way to prepare this state would be to give the particles some mechanism to slowly loose energy (giving the particles charge so that they radiate electromagnetic energy as they oscillate, for example), and then waiting a long time. We now find the value of the energy in this this lowest energy state $E(\Delta X^*_)$,

$$< E >_{min} = E(\Delta X^*) = \frac{\hbar^2}{8M\,\Delta X^2} + \frac{1}{2}k(\Delta X)^2$$

$$
\begin{aligned}
&= \frac{\hbar^2}{8M}\left(\frac{\hbar^2}{4Mk}\right)^{-1/2} + \frac{1}{2}k\left(\frac{\hbar^2}{4Mk}\right)^{1/2} \\
&= \left(\frac{\hbar^2 k}{16M}\right)^{1/2} + \left(\frac{\hbar^2 k}{16M}\right)^{1/2} \\
&= \left(\frac{\hbar^2 k}{4M}\right)^{1/2} \\
&= \frac{1}{2}\hbar\sqrt{k/M} \\
< E >_{min} &= \frac{1}{2}\hbar\omega = \frac{1}{2}h\nu
\end{aligned} \tag{3}
$$

In the last step we used the familiar result that the angular frequency ω associated with the angular frequency of the SHO is $\sqrt{k}M$.

3.2 Ground State/Zero Point Energy

We thus see, that a system of harmonic oscillators cannot be made with zero average energy. The non-zero minimum average energy $< E >_{min}$ is known as the *ground state energy* or sometimes the *zero-point motion energy*. This is a purely quantum effect. A system of classical oscillators could all be left at rest $P = 0$ in their lowest energy configurations $X = 0$. But quantum mechanically, this would violate the uncertainty principle because then we would have $\Delta X\, \Delta P = 0 \cdot 0 = 0 < \hbar/2$.

We again verify that our result is in accord with the classical expectation in the limit $\hbar \longrightarrow 0$. One could plug "classical" values into (3) and find that an oscillator with frequency $\nu = 1\, s^{-1}$ has a minimum energy limit of $< E >_{min} \sim 3 \times 10^{-27}\, erg$, which is indeed a negligible energy on classical scales. Or, one could simply and efficiently take the formally limit $\lim_{\hbar \longrightarrow 0} \frac{1}{2}\hbar\omega \longrightarrow 0$.

Finally, in this case we found that at $< E >_{min}$ the particles are confined to a region $(\Delta X^*) = \left(\frac{\hbar^2 k}{4M}\right)^{1/4}$ and that for this configuration $T = \frac{\hbar^2}{8M\,(\Delta X^*)^2} \sim \frac{\hbar^2}{M\,(\Delta X^*)^2}$ in accord with our expectation for the energy of confinement, even when the confinement is the result of an attraction to the origin rather than from an explicit hard-box constraint.

4 Hydrogen Atom

Finally, we consider a system of Hydrogen atoms which have been left alone to radiate all of their excess energy. Classically, we would eventually (after about $10^{-9}\, s$) expect to find that all of the electrons have fallen into the nuclei at $R = 0$. According to the uncertainty principle, however, there must remain an uncertainty in the position $\vec{R}$ (measured from the proton) and momentum $\vec{P}$ of the electrons. Again, we expect $< \vec{R} >=< \vec{P} >= \vec{0}$. But that there will be some spread ΔR and ΔP in the distributions.

In a hydrogen atom the energy of the electron is given by

$$E = \frac{P^2}{2M} - \frac{e^2}{|R|},$$

where M and e are the charge and mass of the electron respectively. The average energy we expect for our system of hydrogen atoms is then

$$
\begin{aligned}
< E > &= < \frac{P^2}{2M} - \frac{e^2}{|R|} > \\
< E > &= < \frac{P^2}{2M} > - < \frac{e^2}{|R|} > \\
< E > &= \frac{1}{2M} < P^2 > -e^2 < \frac{1}{|R|} >
\end{aligned}
$$

$$< E > \quad \simeq \quad \frac{1}{2M}(\Delta P)^2 - e^2 < \frac{1}{(\Delta R)} >$$

Here, as with the box, we are again being sloppy with precise values and are just making an order of magnitude estimate in order to gain qualitative understanding of the physics of the hydrogen atom.

We now apply the uncertainty principle, which tells us that $\Delta P \geq \hbar/\Delta R$ so that

$$\begin{aligned} < E > \quad &\geq \quad \frac{1}{2M}(\hbar/\Delta R)^2 - e^2 < \frac{1}{(\Delta R)} > \\ &\geq \quad E(\Delta R) \\ E(\Delta R) \quad &\equiv \quad \frac{\hbar^2}{2M(\Delta R)^2} - e^2 < \frac{1}{(\Delta R)} > \end{aligned}$$

Once again, we find a lower bound on $< E >$ by finding the minimum of $E(\Delta R) = \frac{\hbar^2}{2M(\Delta R)^2} - \frac{e^2}{(\Delta R)}$. Setting the derivative equal to zero,

$$\begin{aligned} 0 &= E'(\Delta R^*) \\ &= -\frac{\hbar^2}{M\,(\Delta R^*)^3} + \frac{e^2}{(\Delta R^*)^2} \\ \Rightarrow (\Delta R^*) &= \frac{\hbar^2}{Me^2} \equiv a_0 \simeq 0.5292\text{Å} \end{aligned}$$

The value we find for the width of the distribution of the electron about the proton is precisely the experimental size of the Hydrogen atom! The combination of constants which given this distance, $a_0 = \frac{\hbar^2}{Me^2}$, appears so often in atomic physics that is given a special name, the *Bohr radius.*

Finally, we have our estimate of the average energy of our systems in their ground state,

$$\begin{aligned} < E >_{min} \quad &\simeq \quad \frac{\hbar^2}{2M(\Delta R)^2} - \frac{e^2}{(\Delta R)} \\ &= \quad \frac{\hbar^2}{2M}\left(\frac{Me^2}{\hbar^2}\right)^2 - e^2\left(\frac{Me^2}{\hbar^2}\right) \\ < E >_{min} \quad &\simeq \quad -\frac{1}{2}\frac{Me^4}{\hbar^2} \simeq -13.6\,eV, \end{aligned} \tag{4}$$

which happens to be precisely the *ionization energy* of Hydrogen, the energy it takes to remove an electron from a hydrogen atom when it is in its ground state!

The exact agreement is accidental because this is only a semiquantitative argument. The fact that we got the correct order of magnitude is not an accident. It is a consequence of the fact that our argument contains all of the correct physics in this situations.

Note also the from this argument alone, we cannot understand why it is that all hydrogen atoms in their ground state have *precisely the same ionization energy.* This argument merely puts a limit on the lower bound the average ionization energy may have. There is no problem if all hydrogen atoms require the same energy for ionization, so long at that energy does not violate (4). The equality of the ionization energies for all hydrogen atoms in the ground state is an indication that there are strong *correlations* in the distributions for R and P. (See the notes on statistics for a discussion of correlation).

Finally, our results are in accord with the classical limit. As $\hbar \longrightarrow 0$ we find $(\Delta R^*) = \frac{\hbar^2}{Me^2} \longrightarrow 0$ and $< E >_{min} = -\frac{1}{2}\frac{Me^4}{\hbar^2} \longrightarrow -\infty$; the electron "falls" into the infinite well of the proton as expected classically.