

## Lecture 16 - Quantum oscillators

*What's Important:*

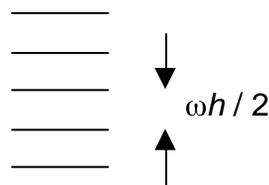
- quantum oscillator at  $T > 0$
- continuous quantum states

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**Quantum oscillators**

In the previous lecture we used the classical equipartition theorem to establish that the mean energy of a single oscillator in one dimension is equal to  $k_B T$ . But we know that the energy states of a quantum oscillator are discrete, not continuous. How does this affect its behavior at finite temperature?

The energy levels of a quantum oscillator are equally spaced, by an amount  $\omega h / 2$ , where  $\omega$  obeys the classical frequency formula  $\omega = (k/m)^{1/2}$ . That is



For quantum number  $n$ , the corresponding energy is

$$E_n = (n + 1/2) \omega h / 2 .$$

One route to obtain the mean energy for this system is to use the partition function, which now involves a sum over (nicely spaced) discrete states:

$$Z = \sum_{n=0} e^{-\beta(n+1/2)\omega h} \quad (16.1)$$

For notational convenience, define

$$x = \beta \omega h / 2 ,$$

so the sum becomes

$$\begin{aligned} Z &= e^{-x/2} \sum_{n=0} e^{-nx} \\ &= e^{-x/2} (1 + e^{-x} + e^{-2x} + \dots) \end{aligned}$$

The series in the brackets has the familiar geometrical series form

$$1 + a + a^2 + a^3 \dots$$

with

$$a = \exp(-x).$$

This series is solved in high school, but we repeat its proof. Let

$$S = 1 + a + a^2 + a^3 \dots$$

so that

$$aS = a + a^2 + a^3 \dots$$

Subtracting the second series from the first

$$S - aS = 1$$

or

$$S = 1 / (1-a).$$

Applying this formula to series in the partition function

$$e^{-nx} = \frac{1}{1 - e^{-x}}$$

and

$$Z = \frac{e^{-\beta\omega\hbar/2}}{1 - e^{-\beta\omega\hbar}} \quad (16.2)$$

To extract the mean energy, we use

$$\bar{E} = -\frac{\partial}{\partial\beta} \ln Z$$

so

$$\begin{aligned} \bar{E} &= -\frac{\partial}{\partial\beta} \ln \frac{e^{-\beta\omega\hbar/2}}{1 - e^{-\beta\omega\hbar}} \\ &= -\frac{\partial}{\partial\beta} \left[ -\frac{\beta\omega\hbar}{2} - \ln(1 - e^{-\beta\omega\hbar}) \right] \\ &= -\frac{\omega\hbar}{2} - \frac{(-1)(-\omega\hbar)e^{-\beta\omega\hbar}}{(1 - e^{-\beta\omega\hbar})} \\ &= \frac{\omega\hbar}{2} + \omega\hbar \frac{e^{-\beta\omega\hbar}}{(1 - e^{-\beta\omega\hbar})} \end{aligned}$$

Rearranging

$$\bar{E} = \omega\hbar \frac{1}{2} + \frac{1}{(e^{+\beta\omega\hbar} - 1)} \quad (16.3)$$

Let us examine two limits of this result:

### 1. $T \rightarrow \infty$ (or $\beta \rightarrow 0$ )

$$\begin{aligned} \bar{E} &= \omega\hbar \frac{1}{2} + \frac{1}{1 + \beta\omega\hbar - 1} = \omega\hbar \frac{1}{2} + \frac{1}{\beta\omega\hbar} \\ &= \omega\hbar \frac{1}{\beta\omega\hbar} \\ &= \frac{1}{\beta} \\ &= k_B T \end{aligned}$$

This is just the same result as we obtained classically: the quantum oscillator approaches the classical oscillator at high temperature.

## 2. $T \rightarrow 0$ (or $\beta \rightarrow \infty$ )

$$\bar{E} = \omega\hbar \frac{1}{2} + \frac{1}{(e^{+\beta\omega\hbar} - 1)}$$

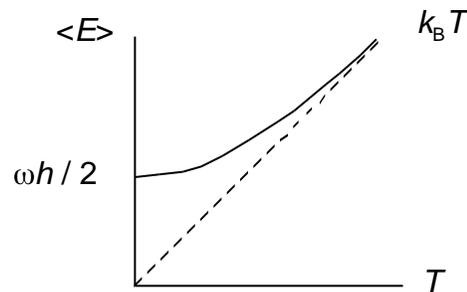
$$\omega\hbar \frac{1}{2} + \frac{1}{e^{+\beta\omega\hbar}}$$

$$\omega\hbar \frac{1}{2} + 0$$

$$= \frac{\omega\hbar}{2}$$

As expected, this is the ground state energy of the quantum oscillator.

Schematically, the general behavior of the quantum oscillator is



## Continuous quantum states

We have now treated a simple quantum problem where the partition function involves a sum over discrete states

$$Z = \sum_r e^{-\beta E_r}$$

What happens in the quantum mechanical situation with a continuum of states? When we discussed the partition function used in the equipartition theorem, we made the transcription

$$Z = \int e^{-\beta E} \dots e^{-\beta E} dq_1 \dots dp_f$$

Now,  $Z$  is just a sum over Boltzmann weights and is therefore dimensionless. What about  $\dots dq_1 \dots dp_f$ ? This series of integrals has units of  $(qp)^f = [\text{angular momentum}]^f$ .

To make  $Z$  unitless, we need to include a density of states factor, giving the number of states per unit phase space. From quantum mechanics, the density of states is one state per  $h$  (Planck's constant) so

$$Z = \frac{1}{h^f} \dots e^{-\beta E} dq_1 \dots dp_f \quad (\text{distinguishable particles})$$

At first, the sight of Planck's constant is alarming - after all, we've been treating classical problems with  $Z$  and have been able to ignore  $h$ . Where does it go? It cancels in expressions like

$$\frac{1}{Z} \frac{\partial}{\partial \beta} Z$$

(or, alternatively, it disappears when derivatives are taken of  $\ln Z$ ).