Trapped Atoms in the Microcanonical Ensemble

Atoms can be trapped in a vacuum chamber with a restoring force that makes them oscillate about its center with angular frequency ω. The Hamiltonian for a single atom is

$$H = \frac{1}{2m}\vec{p}^2 + \frac{1}{2}m\omega^2\vec{r}^2.$$

A. Express H as the sum of 6 terms quadratic in the components of $\vec{r}$ and $\vec{p}$.

$$H = \frac{1}{2m}\left(p_x^2 + p_y^2 + p_z^2\right) + \frac{1}{2}m\omega^2\left(x^2+y^2+z^2\right)$$

It is convenient to change variables from the position vector $\vec{r}$ to a second momentum vector defined by $\vec{q} = m\omega\vec{r}$.

B. Express H as a function of $\vec{p}$ and $\vec{q}$.

$$H = \frac{1}{2m}\vec{p}^2 + \frac{1}{2}m\omega^2\left(\frac{\vec{q}}{m\omega}\right)^2 = \frac{1}{2m}\left(\vec{p}^2 + \vec{q}^2\right)$$

The differential phase space volume is $d\omega = d^3p\,d^3r$.

C. Express $d\omega$ in terms of differentials of p_x, p_y, p_z, q_x, q_y, and q_z.

$$d\omega = dp_x\,dp_y\,dp_z\,\frac{dq_x}{m\omega}\,\frac{dq_y}{m\omega}\,\frac{dq_z}{m\omega} = \frac{1}{(m\omega)^3}\,dp_x\,dp_y\,dp_z\,dq_x\,dq_y\,dq_z$$

The condition that the atom has energy ε is $H = \varepsilon$.

D. Express this condition in terms of the variables p_x, p_y, p_z, q_x, q_y, and q_z.

$$\varepsilon = \frac{1}{2m}\left(\vec{p}^2 + \vec{q}^2\right) \qquad p_x^2 + p_y^2 + p_z^2 + q_x^2 + q_y^2 + q_z^2 = 2m\varepsilon$$

The condition $H = \varepsilon$ implies that the components of $\vec{p}$ and $\vec{q}$ lie on a sphere in a 6-dimensional momentum space.

E. What is the radius of the sphere? $\sqrt{2m\varepsilon}$

The volume of a ball of radius R in n dimensions is $V_n = \pi^{n/2}R^n/(n/2)!$.

F. What is the phase-space volume of the 6-dimensional ball defined by $H < \varepsilon$.

$$\int d\omega = \frac{1}{(m\omega)^3}\int d^3p\,d^3q = \frac{1}{(m\omega)^3}\,\frac{\pi^3\left(\sqrt{2m\varepsilon}\right)^6}{3!} = \frac{1}{6}\left(\frac{2\pi\varepsilon}{\omega}\right)^3$$

G. What is the phase-space volume of the shell $\varepsilon - \delta/2 < H < \varepsilon + \delta/2$.

$$\frac{1}{6}\left[\frac{2\pi(\varepsilon+\delta/2)}{\omega}\right]^3 - \frac{1}{6}\left[\frac{2\pi(\varepsilon-\delta/2)}{\omega}\right]^3 \simeq \frac{1}{6}\cdot 3\left(\frac{2\pi\varepsilon}{\omega}\right)^2\frac{2\pi\delta}{\omega} = \frac{1}{2}\left(\frac{2\pi\varepsilon}{\omega}\right)^3\frac{\delta}{\varepsilon}$$

Compare your results with your neighbors.

Show your results to the instructor.

A large number N of atoms are trapped in the vacuum chamber.
The Hamiltonian is

$$H = \sum_{n=1}^{N} \left(\frac{1}{2m} \vec{p}_n^{\,2} + \frac{1}{2} m \omega^2 \vec{r}_n^{\,2} \right).$$

It is convenient to change variables from the position vectors $\vec{r}_n$ to additional momentum vectors defined by $\vec{p}_{N+n} = m\omega \vec{r}_n$, $n = 1, \ldots, N$.

H. Express H as a function of the $2N$ momentum vectors $\vec{p}_n$.

$$H = \sum_{n=1}^{2N} \frac{1}{2m} \vec{p}_n^{\,2}$$

The differential phase space volume is $d\omega = (d^3p_1 d^3r_1)\ldots(d^3p_N d^3r_N)$.

I. Express $d\omega$ in terms of differentials of the components of $\vec{p}_n$, $n = 1, \ldots, 2N$.

$$d\omega = \frac{1}{(m\omega)^{3N}} d^3p_1 \cdots d^3p_N$$

The condition $H = E$ implies that the components of $\vec{p}_n$, $n = 1, \ldots, 2N$ lie on a sphere in a $6N$-dimensional momentum space.

J. What is the radius of the sphere?

$$\sum_{n=1}^{2N} \frac{1}{2m} \vec{p}_n^{\,2} = E \qquad \sum_{n=1}^{2N} \vec{p}_n^{\,2} = 2mE \qquad \text{radius} = \sqrt{2mE}$$

The volume of a ball of radius R in n dimensions is $V_n = \pi^{n/2} R^n / (n/2)!$. $\quad n = 6N$

K. What is the phase-space volume of the $6N$-dimensional ball defined by $H < E$.

$$\int d\omega = \frac{1}{(m\omega)^{3N}} \frac{\pi^{3N}}{(3N)!} \left(\sqrt{2mE}\right)^{6N} = \frac{\pi^{3N}}{(3N)!} \left(\frac{2E}{\omega}\right)^{3N}$$

L. What is the phase-space volume of the shell $E - \Delta/2 < H < E + \Delta/2$.

$$\frac{\pi^{3N}}{(3N)!}\left[\frac{2}{\omega}\left(E+\tfrac{1}{2}\Delta\right)\right]^{3N} - \frac{\pi^{3N}}{(3N)!}\left[\frac{2}{\omega}\left(E-\tfrac{1}{2}\Delta\right)\right]^{3N} \simeq \frac{\pi^{3N}}{(3N)!} 3N \left[\frac{2}{\omega}E\right]^{3N-1} \frac{2}{\omega}\Delta$$

M. What is the number of microstates $\Omega(E)$ with total energy within $\Delta/2$ of E.

$$\Omega(E) = \frac{1}{N!} \cdot \frac{1}{(2\pi\hbar)^{3N}} \cdot \frac{\pi^{3N}}{(3N)!} \left(\frac{2E}{\omega}\right)^{3N} \frac{3N\Delta}{E} = \frac{1}{N!\,(3N)!} \left(\frac{E}{\hbar\omega}\right)^{3N} \frac{3N\Delta}{E}$$

Stirling's approximation is $\log n! = n \log n - n$.

N. Simplify the entropy $S(E) = \log \Omega(E)$ by keeping only the terms that are extensive in N.

$$S(E) = \log \Omega(E) = 3N \log \frac{E}{\hbar\omega} - \log(N!) - \log(3N)! + \log \frac{3N\Delta}{E}$$

$$\simeq 3N \log \frac{E}{\hbar\omega} - (N\log N - N) - (3N \log(3N) - 3N) + 0$$

Compare your results with your neighbors. $\quad = N\left(3 \log \frac{E}{\hbar\omega} - 4 \log N + 4 - 3\log 3\right)$

Show your results to the instructor.