Physics B I

Solve the following problems.

The Hamiltonian of a harmonic oscillator of mass m and spring constant $m\omega^2$ is

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \frac{m\omega^2}{2}\hat{x}^2, \qquad \text{(I)}$$

where $\hat{x}$ and $\hat{p}$ are the operators for coordinate and momentum, respectively. The momentum operator is expressed as $\hat{p} = -i\hbar\frac{d}{dx}$ in terms of coordinate x. Here, $\hbar$ is given by $\hbar = h/(2\pi)$ in terms of the Planck's constant h. By using $\hat{x}$ and $\hat{p}$, a new set of operators can be defined as

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right), \qquad \text{(II)}$$

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right) \ . \qquad \text{(III)}$$

(1) Evaluate the commutator relation $[\hat{a}, \hat{a}^\dagger]$ between $\hat{a}$ and $\hat{a}^\dagger$ by using the commutator relation between $\hat{x}$ and $\hat{p}$, $[\hat{x}, \hat{p}] = i\hbar$.

(2) Show the Hamiltonian in equation (I) is expressed as $\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)$.

(3) Let $\hat{a}^\dagger\hat{a}$ be defined as $\hat{N}$. In addition, let the normalized eigenfunctions and eigenvalues of $\hat{N}$ be ϕ_n and n, respectively, so that

$$\hat{N}\phi_n = n\phi_n . \qquad \text{(IV)}$$

Show the following relation,

$$\hat{N}\hat{a}\phi_n = (n-1)\hat{a}\phi_n \ . \qquad \text{(V)}$$

(4) Equation (V) shows that $\hat{a}\phi_n$ is an eigenfunction of $\hat{N}$. The existence of the solutions to the Schrödinger equation of a harmonic oscillator requires that n must be an integer of 0 or more. For $n = 0$, we have

$$\hat{a}\phi_0 = 0 . \qquad \text{(VI)}$$

Show that ϕ_0 satisfying equation (VI) is a Gaussian function with respect to x.

(5) The following equations for $\hat{a}\phi_n$ and $\hat{a}^\dagger\phi_n$ can be derived as

$$\hat{a}\phi_n = \sqrt{n}\,\phi_{n-1}, \qquad \text{(VII)}$$

$$\hat{a}^\dagger\phi_n = \sqrt{n+1}\,\phi_{n+1} \ . \qquad \text{(VIII)}$$

Evaluate the following equations (IX) and (X), by using the orthonormal condition for ϕ_n,

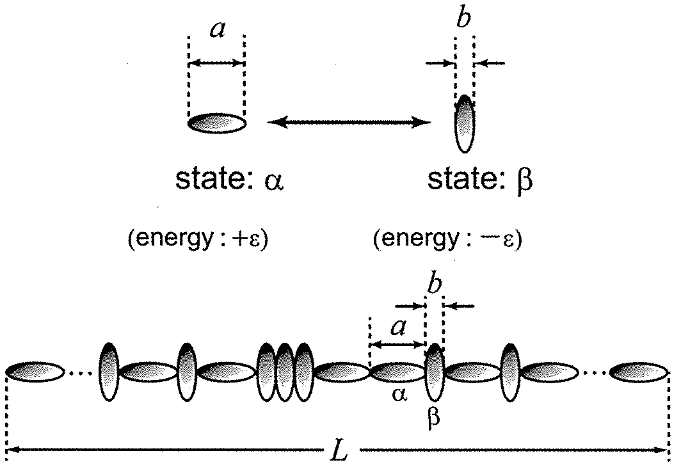
$$\langle x \rangle_n = \int_{-\infty}^{+\infty} \phi_n^*(x)\,\hat{x}\,\phi_n(x)dx, \qquad \text{(IX)}$$

$$\langle x^2 \rangle_n = \int_{-\infty}^{+\infty} \phi_n^*(x)\,\hat{x}^2\,\phi_n(x)dx \ . \qquad \text{(X)}$$

Physics B II

Solve the following problems.

As shown in the figure below, consider a one-dimensional chain consisting of N molecules which exist in two states (α and β), with correponding energies $+\varepsilon$, $-\varepsilon$, and lenghs a, b, respectively. There is no intermolecular interaction. Each molecule thus takes one of two states independently of surrounding molecular states. The molecular chain reaches a thermal equilibrium state (microcanonical ensemble). Note that k_B is the Boltzmann constant.



(1) Consider a state consisting of N_α molecules in α and N_β molecules in β, where $N = N_\alpha + N_\beta$. Then, evaluate the length L and the energy E_L of the molecular chain.

(2) Evaluate the thermodynamic weight $W(N_\alpha, N_\beta)$ in the state.

(3) Prove that the entropy S of the molecular chain is

$$S = -k_B \left\{ N_\alpha \log \frac{N_\alpha}{N} + N_\beta \log \frac{N_\beta}{N} \right\},$$

by using Stirling formula: $\log n! = n \log n - n \ (n \gg 1)$.

Consider the canonical distribution of the molecular chain contacting with the heat bath of constant temperature T. Generally, in the state of γ with corresponding the energy E_γ, the partition function Z of the canonical ensemble is described by the equation

$$Z = \sum_\gamma \exp\left(-\frac{E_\gamma}{k_B T}\right).$$

Continued to the next page.

(4) Evaluate the partition function Z_1 of one molecule and the partition function Z_N of the chain of N molecules.

(5) Using the result of Z_N, evaluate the Helmholtz free energy $F = -k_B T \log Z_N$, the entropy $S = -\partial F / \partial T$, and the internal energy $U = F + ST$.

(6) Evaluate the specific heat $C = \partial U / \partial T$, and draw the figure of C as a function of T. Note that the vertical and horizontal axes are expressed by C/Nk_B and $k_B T/\varepsilon$, respectively.