Physics B I

Answer the following questions regarding quantum mechanics.

Consider a particle of mass *m* moving in one dimension, confined within an infinite potential well. The potential $V(x)$ is given by

$$V(x) = \begin{cases} 0 \ (0 \leq x \leq L) \\ \infty \ (x < 0, x > L) \end{cases}$$

where *h* is the Planck constant and $\hbar = h/2\pi$.

I Write down the time-independent Schrödinger equation for the particle inside the well ($0 \leq x \leq L$). Let the wave function be ϕ and the energy be *E*.

II Using the equation from I and the boundary conditions $\phi(0) = \phi(L) = 0$, find the eigenfunctions $\phi_1(x), \phi_2(x)$ and corresponding eigenenergies $E_1^{(0)}, E_2^{(0)}$ for the ground state and the first excited state of this particle, respectively. The eigenfunctions should be real functions and normalized. You may use the following integral formula in your calculations:

$$\int_0^{n\pi} \sin^2 x \, dx = \frac{n\pi}{2}$$

III Determine the expectation value of the position for the ground state and the first excited state of the particle $\langle x_1 \rangle = \langle \phi_1 | \hat{x} | \phi_1 \rangle, \langle x_2 \rangle = \langle \phi_2 | \hat{x} | \phi_2 \rangle$. You may use the following integral formula in your calculations:

$$\int_0^{n\pi} x \sin^2 x \, dx = \left(\frac{n\pi}{2}\right)^2$$

Next, we investigate the effect of applying an electric field *E* in the *x*-direction to this system by using perturbation theory. The perturbation Hamiltonian is given by $\widehat{H}' = -qE\hat{x}$. Here *q* is the charge of the particle.

IV Calculate the first-order perturbation energy $\Delta E_1^{(1)} = \langle \phi_1 | \widehat{H}' | \phi_1 \rangle$ for the ground state $\phi_1(x)$.

V Due to the perturbation, the new ground state wave function can be expressed as a mixture of the original ground state ϕ_1 and the first excited state ϕ_2: ${\phi_1}' \approx \phi_1 + c\phi_2$. Find the mixing coefficient, *c*, using the following formula:

$$c \approx \frac{\langle \phi_2 | \hat{H}' | \phi_1 \rangle}{E_1^{(0)} - E_2^{(0)}}$$

You may use the integral formula below in your calculation.

$$\int_0^{\pi} x \sin x \sin 2x \, dx = -\frac{8}{9}$$

VI Calculate the expectation value of the particle's position $\langle x \rangle = \langle \phi_1{}' | \hat{x} | \phi_1{}' \rangle$, in this new ground state $\phi_1{}'$ to the first order in the electric field *E*.

(The end)

Answer the following questions about statistical mechanics.

Consider a model that describes the helix-coil transition of a polypeptide with N amino acids polymerized in a chain. Suppose that each of the N sites takes the two states, helix (H) or coil (C). Then, the polypeptide state can be described by a string of N characters such as CCH…HC. Suppose that the one-site energy of the C and H states is $E_C = 0$ and E_H, respectively. Suppose $s = e^{-\beta E_H}$, where $\beta = (k_B T)^{-1}$, k_B is Boltzmann constant, and T is temperature. This system is in thermal equilibrium at temperature T.

First, consider the case in which there is no interaction between sites.

I Find the partition function for one site. Then, based on the one-site partition function, find the partition function Z for the polypeptide using s and N.

II The polypeptide partition function Z can also be expressed using the number of times H appears in the polypeptide n_H, as the following equation.

$$Z = \sum_{n_H=0}^{N} g(n_H) s^{n_H}$$

$g(n_H)$ is the number of states. Find $g(n_H)$.

III The average helix fraction of the polypeptide is defined as $f_H = \frac{\langle n_H \rangle}{N}$, where $\langle n_H \rangle$ is the expected value of n_H. Show that the equation that calculates f_H from the polypeptide partition function Z is $f_H = \frac{s}{N}\frac{\partial \ln Z}{\partial s}$.

IV Calculate f_H from the polypeptide partition function Z obtained in I using the equation in III. Then, illustrate the general shape of f_H along s. Note that s can be seen as the equilibrium constant between C and H, where C is more stable for $s < 1$ and H is more stable for $s > 1$.

Next, consider the case in which interactions between sites are introduced, making the model cooperative. In particular, consider that interaction is only introduced to the neighboring C and H (…CH… or …HC…) and its energy is $E_{CH} = \infty$. In this case, the polypeptide only takes all C state (C…C) or all H state (H…H).

V Find the polypeptide partition function Z for this case using s and N.

VI Calculate f_H from the polypeptide partition function Z obtained in V using the equation in III. Then, illustrate the general shape of f_H along s for sufficiently large N, and describe what is different from the case without the interaction.

(The end)

解答例

Example answers

Answer

I

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi(x) = E\,\phi(x)$$

II

The ground state at n=1:

$$\phi_1(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi}{L}x\right), E_1^{(0)} = \frac{\hbar^2\pi^2}{2mL^2}$$

The excited state at n=2:

$$\phi_2(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{2\pi}{L}x\right), E_2^{(0)} = \frac{2\hbar^2\pi^2}{mL^2}$$

III

$$\langle x_n\rangle = \frac{L}{2}$$

IV

$$\Delta E_1^{(1)} = -\frac{qEL}{2}$$

V

$$c = -\frac{32mL^3qE}{27\pi^4\hbar^2}$$

VI

$$\langle x\rangle = \frac{L}{2} + \frac{1024mL^4qE}{243\pi^6\hbar^2}$$

Physics BII Answer

I The partition function for one site is, $z_1 = e^{-\beta E_C} + e^{-\beta E_H} = 1 + s$

The partition function for the polypeptide is, $Z = (1+s)^N$

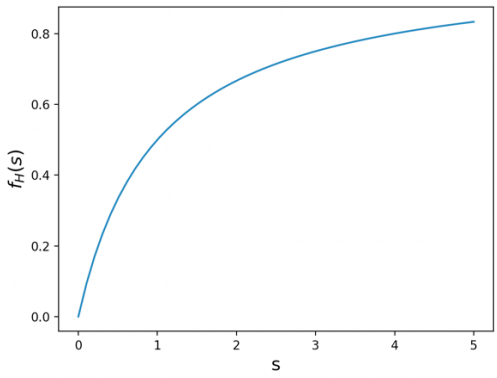
II $g(n_H) = \frac{N!}{n_H!(N-n_H)!}$

III

$$\frac{s}{N}\frac{\partial \ln Z}{\partial s} = \frac{s}{N}\frac{\sum_{n_H=0}^{N} n_H g(n_H) s^{n_H-1}}{Z} = \frac{1}{N}\frac{\sum_{n_H=0}^{N} n_H g(n_H) s^{n_H}}{Z} = \frac{\langle n_H \rangle}{N} = f_H$$

IV $f_H = \frac{s}{1+s}$

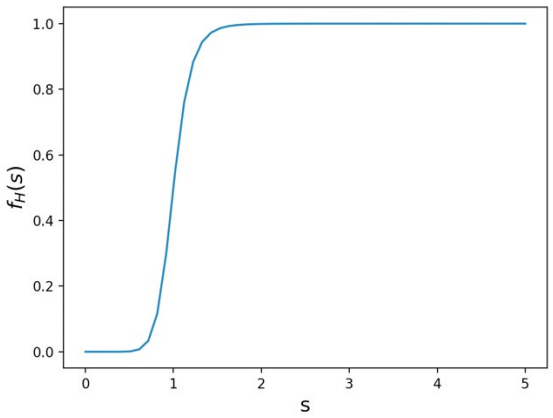
The general shape of f_H is,



V $Z = 1 + s^N$

VI $f_H = \frac{s^N}{1+s^N}$

The general shape of f_H is,



The difference from the case without the interaction is that f_H shows a sharp change around s=1.