

Clicker/Poll Question

Suppose we have a two-state system, where the energy of the ground state is 0 and the energy of the excited state is E_0 .

What is the partition function for this system? Note $\beta \equiv \frac{1}{kT}$.

A. $Z = 1 + e^{-\beta E_0}$

B. $Z = 1 + \beta E_0$

C. $Z = 1 - \beta E_0$

D. None of the above

E. ???

Clicker/Poll Question

Suppose we have a two-state system, where the energy of the ground state is 0 and the energy of the excited state is E_0 .

At what temperature is there a 50% probability that the system is in the ground state?

A. $kT = 0$

B. $kT = (\text{some value between } 0 \text{ and } E_0)$

C. $kT = E_0$

D. $kT = +\infty$

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A system has two states of energies $-\epsilon$ and 2ϵ . What is the probability of observing it in the higher energy state at temperature T ?

A. 0

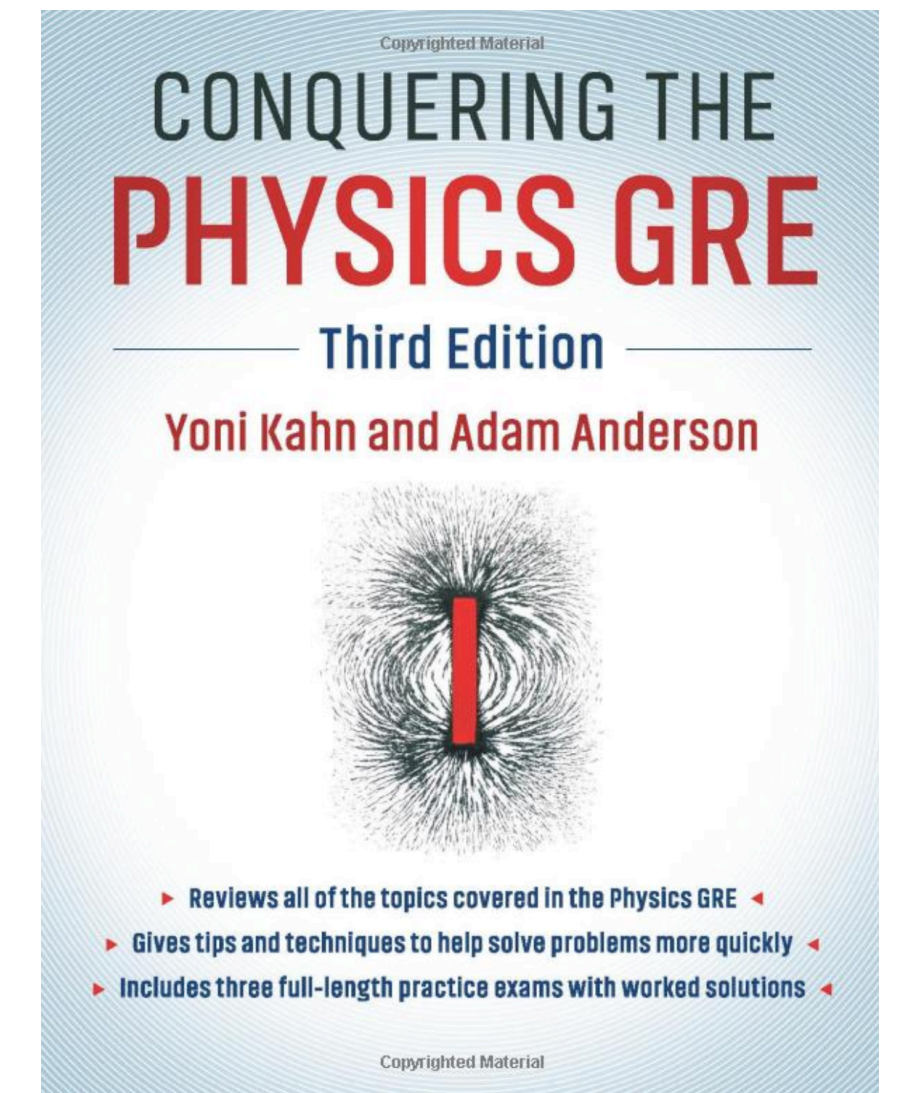
B. $\left[1 + \exp\left(\frac{3\epsilon}{kT}\right) \right]^{-1}$

C. $\left[1 - \exp\left(\frac{3\epsilon}{kT}\right) \right]^{-1}$

D. $\left[\exp\left(\frac{\epsilon}{kT}\right) + \exp\left(\frac{-2\epsilon}{kT}\right) \right]^{-1}$

E. 1

Problem is from



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What is the partition function of a one-dimensional quantum harmonic oscillator?

A. $\exp\left(\frac{-\hbar\omega}{kT}\right)$

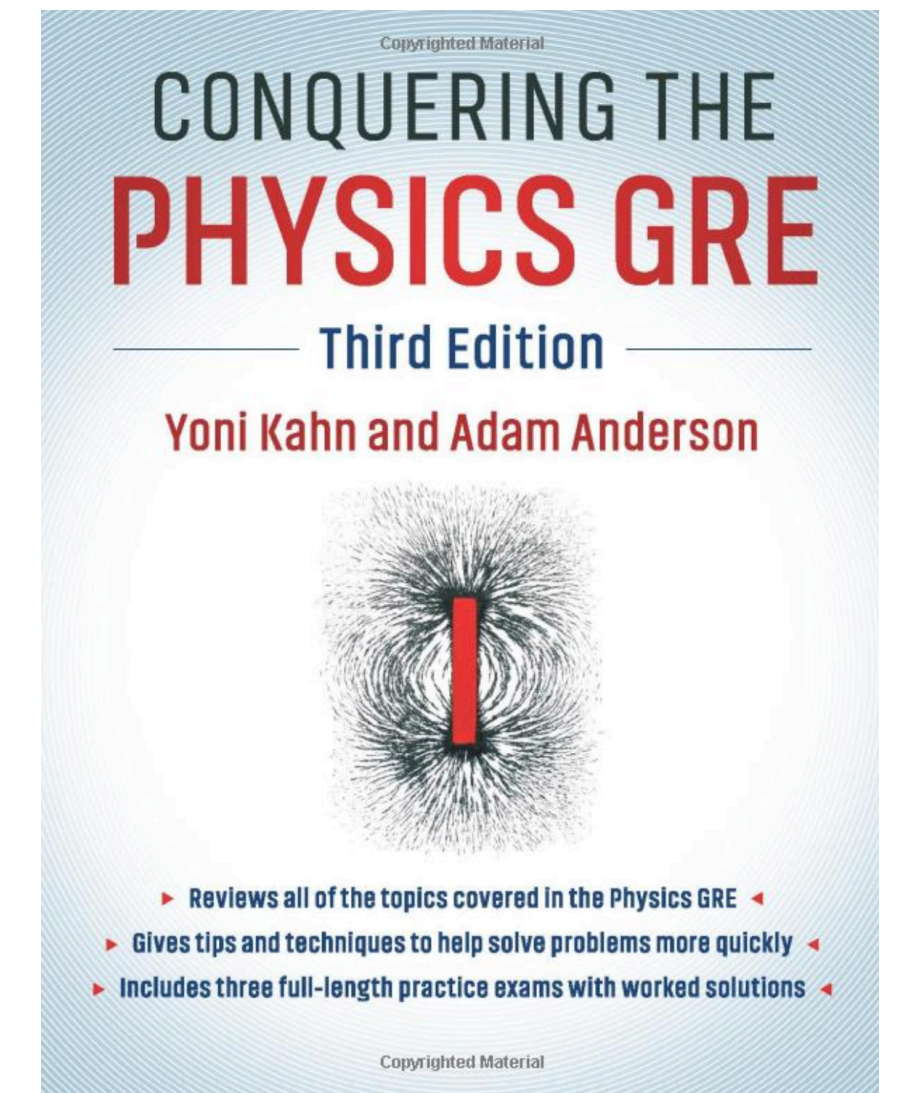
B. $1 - \exp\left(\frac{-\hbar\omega}{kT}\right)$

C. $\left[1 - \exp\left(\frac{-\hbar\omega}{kT}\right)\right]^{-1}$

D. $\left(2 \cosh \frac{\hbar\omega}{2kT}\right)^{-1}$

E. $\left(2 \sinh \frac{\hbar\omega}{2kT}\right)^{-1}$

Problem is from



Clicker/Poll Question

Suppose we have a two-state system, where the energy of the ground state is 0 and the energy of the excited state is E_0 .

What is the expected value of energy for this system at $kT = E_0$?

A. $(1/e)E_0$

B. $(1 - 1/e)E_0$

C. E_0

D. None of the above

E. ???

Try It Yourself

$$\bar{E} = \frac{\sum_i E_i e^{-\beta E_i}}{\sum_i e^{-\beta E_i}} = \frac{1}{Z} \sum_i E_i e^{-\beta E_i} = \frac{1}{Z} \left(-\frac{\partial Z}{\partial \beta} \right) = -\frac{\partial \ln Z}{\partial \beta}$$

Given the single-particle partition function

$$Z_1 = e^{-\beta\mu B} + e^{+\beta\mu B} = 2 \cosh(\beta\mu B)$$

- What is the expected value of energy for this particle?
- What is the total energy of the system of N dipoles?
- Redo part (A) with the partition function $Z_N = Z_1^N$, and show that you get the result that you got in part (B).
- I lied in part (C). Actually, the partition function is $Z_N = \frac{1}{N!} Z_1^N$ if spins are indistinguishable. Show that you get the same result as in both parts (B) & (C).

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For a CO molecule, $\epsilon \approx 2 \times 10^{-4}$ eV. What is the expected energy in rotational mode(s) for an CO molecule at room temperature?

A. $(1/2)kT$

B. kT

C. $2kT$

D. None of the above

E. ???

$$\bar{E} = \frac{\sum_i E_i e^{-\beta E_i}}{\sum_i e^{-\beta E_i}} = \frac{1}{Z} \sum_i E_i e^{-\beta E_i} = \frac{1}{Z} \left(-\frac{\partial Z}{\partial \beta} \right) = -\frac{\partial \ln Z}{\partial \beta}$$

(last slide): $Z_{\text{rot}} \approx \frac{kT}{\epsilon}$

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The preceding proof of the equipartition theorem does not apply to quantum-mechanical systems. Why not?

- A. Quantum mechanical systems have discrete energy levels, which are not quadratic.
- B. Quantum mechanical systems have relatively big energy-level spacings (compared to kT), which make it a bad approximation to replace the sum with an integral in the proof.
- C. The proof only applies to particles which can be considered distinguishable. At low enough temperatures where we can't ignore QM, the fact that we have bosons vs. fermions becomes important.
- D. ???

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Suppose you are able to look down the z-axis and view particles that are either moving towards you or away from you. Of the following, which is the most likely speed that you would measure?

- A. 0
- B. The most probable speed, moving in the $\pm z$ direction.
- C. The rms speed, moving in the $\pm z$ direction.
- D. The average speed, moving in the $\pm z$ direction.
- E. ???

Clicker/Poll Question

Suppose we lived in 2 spatial dimensions. What would be the form of the distribution function (probability per unit speed interval)?

A. $\mathcal{D}(v) \propto e^{-\beta m v^2/2}$

B. $\mathcal{D}(v) \propto e^{-\beta m v}$

C. $\mathcal{D}(v) \propto v e^{-\beta m v^2/2}$

D. $\mathcal{D}(v) \propto v e^{-\beta m v}$

E. $\mathcal{D}(v) \propto v^2 e^{-\beta m v}$

Match the following with the required computation (the limits of the integrals are not specified since they depend on the particular quantity)

1. v_{rms}

2. $v_{\text{most probable}}$

3. v_{avg}

4. v_{median}

A. $\int v \mathcal{D}(v) dv$

B. $\int v^2 \mathcal{D}(v) dv$

C. $\int \mathcal{D}(v) dv$

D. $\frac{d}{dv} \mathcal{D}(v)$

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The previous slide wrote that $S = \frac{U}{T} + k \ln Z$ (for a system of N particles). Is this Z equal to Z_1 or Z_N ?

- A. Z_1
- B. Z_N
- C. ???

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From the thermodynamic identity for F ($dF = \dots$), find an expression for the pressure of a system in terms of the partition function.

A. $P = -kT \frac{\partial \ln Z}{\partial V}$

C. $P = -kT \frac{\partial Z}{\partial V}$

B. $P = +kT \frac{\partial \ln Z}{\partial V}$

D. $P = +kT \frac{\partial Z}{\partial V}$

E. None of the above (or not sure)

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For the nitrogen in this room ($V \sim 100\text{m}^3$), what is the correct order-of-magnitude of the quantum volume V_Q ?

- A. 10^{-15} m^3 .
- B. 10^{-23} m^3 .
- C. 10^{-31} m^3 .
- D. 10^{-38} m^3 .
- E. ???

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There was no degeneracy factor in the previous expression. Why is this?

- A. There is no degeneracy in a 3D particle-in-a-box.
- B. The degeneracy is in the energy, but since we're summing over triplets of n -values and not energy levels, there's no issue.
- C. The degeneracy is a small factor that won't matter for the partition function.
- D. ???

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Which of the following will help in the solution to Problem 6.47?

Problem 6.47. Estimate the temperature at which the translational motion of a nitrogen molecule would freeze out, in a box of width 1 cm.

- A. This is the temperature at which $V = V_Q$.
- B. This is the temperature where kT is equal to the ground-state energy of a particle-in-a-box.
- C. Both of the above are valid and will get the same answer (to the correct order-of-magnitude).
- D. Neither of the above is the right approach for this problem.