Adsorption of O_2 in a magnetic field

Masatsugu Sei Suzuki

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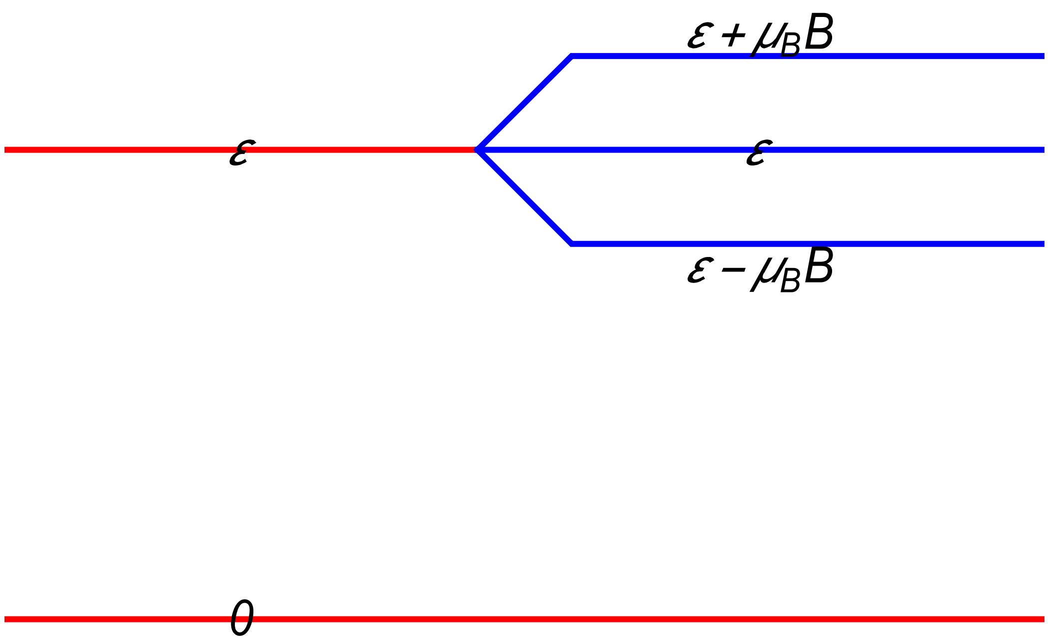
Suppose that at most one O_2 can be bound to a heme group, and that when $z(O_2) = 10^{-5}$ we have 90% of the hemes occupied by O_2. Consider O_2 as having a spin of 1 and a magnetic moment of 1 μ_B. How strong magnetic field is needed to change the adsorption by 1% at $T = 300$ K?



((Solution))

$$z(O_2) = 10^{-5}$$

There are four states:

1. State-1 Number of particle $N = 1$, energy $E = 0$.
2. State 2 $N = 1$, $E = \varepsilon - \mu_B B$
3. State 3 $N = 1$, $E = \varepsilon$
4. State 4 N = 1, $E = \varepsilon + \mu_B B$

The Gibbs sum:

$$Z_G = 1 + z(\mathrm{O}_2)e^{-\beta\varepsilon}(e^{\beta\mu_B B} + 1 + e^{-\beta\mu_B B})$$
$$= 1 + z(\mathrm{O}_2)e^{-\beta\varepsilon}K(B)$$

The probability:

$$P_1 = \frac{1}{1 + z(\mathrm{O}_2)e^{-\beta\varepsilon}K(B)}$$

$$P_2 = \frac{z(\mathrm{O}_2)e^{-\beta(\varepsilon-\mu_B B)}}{1 + z(\mathrm{O}_2)e^{-\beta\varepsilon}K(B)}$$

$$P_3 = \frac{z(\mathrm{O}_2)e^{-\beta\varepsilon}}{1 + z(\mathrm{O}_2)e^{-\beta\varepsilon}K(B)}$$

$$P_4 = \frac{z(\mathrm{O}_2)e^{-\beta(\varepsilon+\mu_B B)}}{1 + z(\mathrm{O}_2)e^{-\beta\varepsilon}K(B)}$$

Note that

$$P_{234} = P_2 + P_3 + P_4 = \frac{z(\mathrm{O}_2)e^{-\beta\varepsilon}K(B)}{1 + z(\mathrm{O}_2)e^{-\beta\varepsilon}K(B)}$$

with

$$K(B) = 1 + e^{-\beta\mu_B B} + e^{\beta\mu_B B}$$

When $B = 0$, we have

$$\frac{z(\mathrm{O}_2)e^{-\beta\varepsilon}K(B=0)}{1 + z(\mathrm{O}_2)e^{-\beta\varepsilon}K(B=0)} = 0.90$$

or

$$\frac{3z(\mathrm{O}_2)e^{-\beta\varepsilon}}{1 + 3z(\mathrm{O}_2)e^{-\beta\varepsilon}} = 0.90$$

where $K(B=0)=3$

$$z(O_2)e^{-\beta\varepsilon}=3$$

Thus we have

$$P_{234}=\frac{3K(B)}{1+3K(B)}=0.91$$

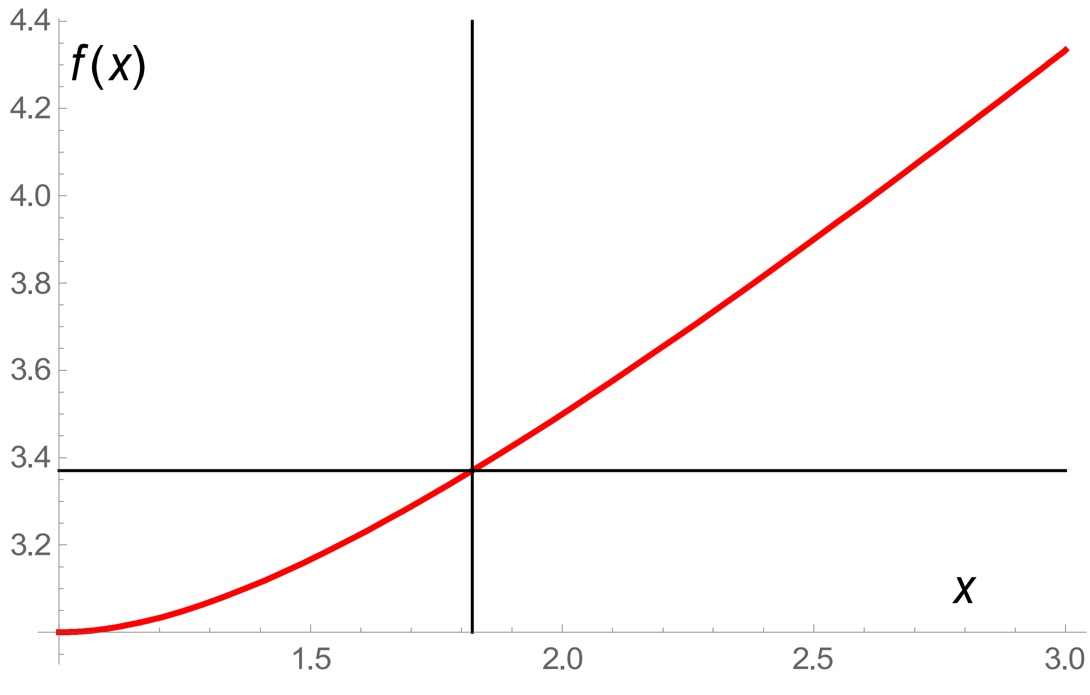
or

$$K(B)=3.37$$

We note that

$$f(x)=1+x+\frac{1}{x}$$

with $\quad x=e^{\beta\mu_B B}$.



We solve

$$f(x) = 3.37$$

leading to x = 1.821.

$$x = 1.821 = e^{\beta \mu_B B}$$

or

$$B = \frac{k_B T}{\mu_B} = 267.7 \text{ T}$$