E0105: The functions $N(E)$ and $Z(T)$ for a particle in a double well

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The problem:

(a) Describe the possible trajectories of the particle in the double well.

(b) Calculate $N(E)$ and the energy levels in the semi-classical approximation.

(c) Calculate $Z(\beta)$ and show that it can be written as a product of "kinetic" term and "spin" term.

The solution:

(a) The trajectories of a particle in a confining potential are those of constant energy

$$E = \frac{p^2}{2m} + V(x) \qquad \rightarrow \qquad p(x) = \pm\sqrt{2m\,(E - V(x))}. \tag{1}$$

Therefore for $|E| \leq \frac{\epsilon}{2}$ we have

$$0 < x < \frac{L}{2} \qquad p(x) = \pm\sqrt{2m\left(E + \frac{\epsilon}{2}\right)}, \tag{2}$$

while for $E > \frac{\epsilon}{2}$ we have

$$0 < x < L \qquad p(x) = \begin{cases} \pm\sqrt{2m\left(E + \frac{\epsilon}{2}\right)} & 0 < x \leq \frac{L}{2} \\ \pm\sqrt{2m\left(E - \frac{\epsilon}{2}\right)} & \frac{L}{2} < x < L \end{cases}$$

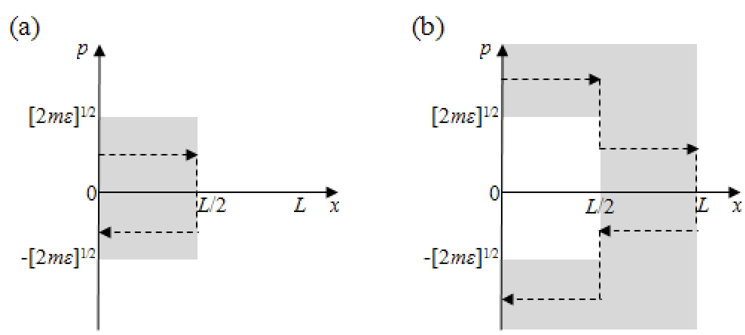

Figure 1: The possible trajectories in the phase space for a particle in the given well for (a) $|E| \leq \frac{\epsilon}{2}$ and (b) $E > \frac{\epsilon}{2}$.

(b) In the semi-classical approximation x and p are taken to be independent variables, and a "state" in phase space is of volume $(2\pi\hbar)^d$.
$N(E)$ are the number of states with energy smaller than E,

$$N(E) = \int \frac{d^dx d^dp}{(2\pi\hbar)^d}\Theta(E - H(x,p)), \tag{3}$$

where $\Theta(x)$ is the step function. Thus according to the above,

$$N\left(|E| < \frac{\epsilon}{2}\right) = \frac{L/2}{2\pi\hbar} 2\sqrt{2m\left(E + \frac{\epsilon}{2}\right)} = \frac{L}{2\pi\hbar}\sqrt{2m\left(E + \frac{\epsilon}{2}\right)} \tag{4}$$

$$N\left(E > \frac{\epsilon}{2}\right) = \frac{L}{2\pi\hbar}\left[\sqrt{2m\left(E + \frac{\epsilon}{2}\right)} + \sqrt{2m\left(E - \frac{\epsilon}{2}\right)}\right]. \tag{5}$$

(c) The partition function $Z(\beta)$ is given by

$$Z(\beta) = \int_{-\infty}^{\infty} \frac{dxdp}{2\pi\hbar} e^{-\beta(p^2/2m + V(x))} = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dpe^{-\beta p^2/2m} \times \int_{-\infty}^{\infty} dxe^{-\beta V(x)}$$

$$= \frac{1}{2\pi\hbar}\sqrt{\frac{2m\pi}{\beta}}\frac{L}{2}\left(e^{\beta\frac{\epsilon}{2}} + e^{-\beta\frac{\epsilon}{2}}\right) = \frac{1}{\hbar}\sqrt{\frac{m}{2\pi\beta}} L\cosh\left(\beta\frac{\epsilon}{2}\right). \tag{6}$$

We can see that Z can be expressed as (kinetic term)$\times$(spin term).