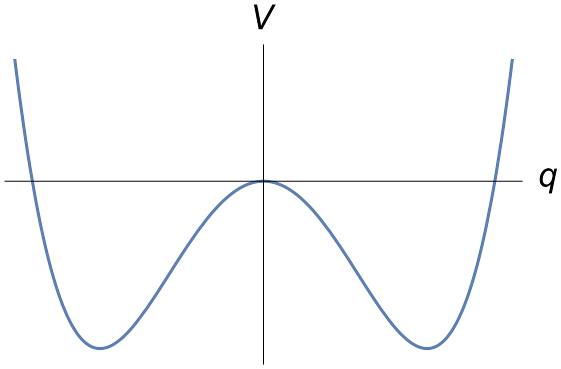
4.5. Spontaneous Broken Symmetry

Consider the 1-D potential

$$V(q) = -\frac{1}{2}\alpha q^2 + \frac{1}{4}\gamma q^4 \qquad \alpha,\ q > 0 \tag{4.99}$$



The Helmholtz free energy is [see eq(4.14)]

$$F_\beta = -\frac{1}{\beta}\ln \int dx \int_x^x \overline{\mathcal{D}}\, q \exp\left\{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau \left(\frac{1}{2} m \dot{q}^2 + V\right)\right\} \tag{4.100}$$

which can't be evaluated in closed form.

Writing eq(4.100) as

$$F_\beta = -\frac{1}{\beta}\ln \int dx\, P_\beta(x) \tag{4.101}$$

where

$$\begin{aligned} P_\beta(x) &= \int_x^x \overline{\mathcal{D}}\, q \exp\left\{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau \left(\frac{1}{2} m \dot{q}^2 + V\right)\right\} \\ &= \left\langle x \,\middle|\, e^{-\beta H} \,\middle|\, x \right\rangle \end{aligned} \tag{4.102}$$

is the partition function density expressed as a Euclidean path integral.

From eq(4.101), we see that F_β is dominated by the region(s) around a maximum of P_β determined by

$$\frac{dP_\beta}{dx} = 0 \qquad \frac{d^2 P_\beta}{dx^2} < 0 \tag{4.103}$$

Introducing the effective potential

$$V_{\text{eff}}(x) = -\frac{1}{\beta}\ln P_\beta(x) \tag{4.104}$$

$$\rightarrow \qquad \frac{dV_{\text{eff}}}{dx} = -\frac{1}{\beta P_\beta}\frac{dP_\beta}{dx}$$

$$\frac{d^2 V_{\text{eff}}}{dx^2} = \frac{1}{\beta P_\beta^2}\left(\frac{dP_\beta}{dx}\right)^2 - \frac{1}{\beta P_\beta}\frac{d^2 P_\beta}{dx^2}$$

From eq(4.102), we see that $P_\beta \geq 0$ if H is hermitian. Thus, if P_β is a maximum, we have

$$\frac{dV_{\text{eff}}}{dx} = 0 \qquad \frac{d^2 V_{\text{eff}}}{dx^2} = -\frac{1}{\beta P_\beta}\frac{d^2 P_\beta}{dx^2} > 0 \tag{4.105}$$

Thus, F_β is dominated by the regions around the minima of V_{eff}. For low enough energies, the system behaves like a harmonic oscillator at these minima.

As in §4.2, F_β is taken as a functional of the expectation value of the position operator, denoted here as $\overline{x} = \langle x \rangle$. We'll assume $\overline{x}$ to be time-independent, which is true at least for $J(t) = 0$. By eq(4.101), we have

$$F_\beta(\overline{x}) \approx -\frac{1}{\beta} \ln\left[P_\beta(\overline{x}) \int dx \right]$$

$$= V_{\text{eff}}(\overline{x}) - \frac{1}{\beta} \ln \int dx \qquad \text{[Eq(4.104) used.]} \qquad (4.106)$$

As in eq(4.29), we define the effective action by the Legendre transform

$$\Gamma_\beta(\overline{x}) = V_{\text{eff}}(\overline{x}) + \frac{1}{\beta \hbar} \int_0^{\beta\hbar} d\tau \, J(\tau) \, \overline{x} \qquad (4.107)$$

where the term $-\frac{1}{\beta} \ln \int dx$ was dropped since it's independent of $\overline{x}$ & J and hence is just a constant with respect to the functional derivatives of interest.

For $J \neq 0$, eq(4.102) becomes

$$P_\beta(x) = \int_x^x \overline{\mathcal{D}} q \exp\left\{ -\frac{1}{\hbar} \int_0^{\beta\hbar} d\tau \left(\frac{1}{2} m \dot{q}^2 + V + J q \right) \right\} \qquad (4.108)$$

Writing

$$q = x + y \qquad \text{with} \qquad y(0) = y(\beta\hbar) = 0$$

we have

$$\int_x^x \overline{\mathcal{D}} q = \int_0^0 \overline{\mathcal{D}} y$$

$$\frac{1}{2} m \dot{q}^2 + V + J q = \frac{1}{2} m \dot{x}^2 + \frac{1}{2} m \dot{y}^2 + m \dot{x} \dot{y} + J x$$

$$+ V(x) + \left[\frac{d V(x)}{d x} + J \right] y + \frac{1}{2} \frac{d^2 V(x)}{d x^2} y^2 + \ldots$$

Using

$$\dot{\overline{x}} = 0$$

we have

$$P_\beta(\overline{x}) = \exp\left[-\beta V(\overline{x}) - \overline{x} \frac{1}{\hbar} \int_0^{\beta\hbar} d\tau \, J(\tau) \right] \qquad (4.109)$$

$$\times \int_0^0 \overline{\mathcal{D}} y \exp\left\{ -\frac{1}{\hbar} \int_0^{\beta\hbar} d\tau \right.$$

$$\left. \times \left[\frac{1}{2} m \dot{y}^2 + \left(\frac{d V(\overline{x})}{d x} + J \right) y + \frac{1}{2} \frac{d^2 V(\overline{x})}{d x^2} y^2 + \ldots \right] \right\}$$

If the $O(y^3)$ terms are negligible, the integrals in eq(4.109) are all Gaussians & hence be readily evaluated.

Unfortunately, this approximation fails if $\frac{d^2 V(\overline{x})}{d x^2} < 0$ so that the Gaussian integrals diverge. In which case higher order terms are needed to keep P_β finite. Even so, special care is required to get meaningful results. For example, evaluation for the potential eq(4.99) by means of Taylor expansion involves integration of the type

$$\int_{-\infty}^{\infty} dx \exp\left(\frac{1}{2} \alpha x^2 - \frac{1}{4} \gamma x^4 \right) = \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} dx \frac{1}{n!} \left(-\frac{1}{4} \gamma x^4 \right)^n e^{\alpha x^2/2} \qquad (4.110)$$

For $\alpha > 0$, every term in the series is singular.

An often used approximation is the method of steepest descent in which the path integral is approximated by

$$Z_{a\,b} \approx Z_2\, e^{-S_c/\hbar}$$

where Z_2 is the path integral for the quadratic part of the hamiltonian & S_c is the action evaluated on its classical path for which $\delta S = 0$.

If we drop the linear term to avoid un-illuminating mathematical complexities, the steepest descent method gives

$$P_\beta(\overline{x}) \approx \sqrt{\frac{m\,\omega}{2\,\pi\,\hbar\,\sinh\beta\hbar\omega}}\;\exp\left[-\beta\,V(\overline{x}) - \overline{x}\,\frac{1}{\hbar}\int_0^{\beta\,\hbar} d\,\tau\,J(\tau)\right] \quad (4.111)$$

where

$$m\,\omega^2 = \frac{d^2\,V(\overline{x})}{d\,x^2} \quad (4.112)$$

Using eq(4.111) on eq(4.104) gives

$$V_{\text{eff}}(\overline{x}) = -\frac{1}{2\,\beta}\ln\left(\frac{m\,\omega}{2\,\pi\,\hbar\,\sinh\beta\hbar\omega}\right) + V(\overline{x}) + \overline{x}\,\frac{1}{\beta\,\hbar}\int_0^{\beta\,\hbar} d\,\tau\,J(\tau) \quad (4.114)$$

Using

$$\begin{aligned}\lim_{\beta\to\infty}\frac{1}{2\,\beta}\ln\sin\beta\hbar\omega &= \lim_{\beta\to\infty}\frac{1}{2\,\beta}\ln\frac{e^{\beta\,\hbar\,\omega} - e^{-\beta\,\hbar\,\omega}}{2} \\ &= \lim_{\beta\to\infty}\frac{1}{2\,\beta}\ln e^{\beta\,\hbar\,\omega} \\ &= \frac{1}{2}\,\hbar\,\omega\end{aligned}$$

we have, for $J = 0$,

$$V_{\text{eff}}^{\infty}(\overline{x}) = \frac{1}{2}\,\hbar\,\omega + V(\overline{x}) \quad (4.115)$$

For the potential in eq(4.99), we have

$$V_{\text{eff}}^{\infty}(\overline{x}) = \frac{1}{2}\,\hbar\,\omega - \frac{1}{2}\,\alpha\,\overline{x}^2 + \frac{1}{4}\,\gamma\,\overline{x}^4 \quad (4.116)$$

where we’ve used

$$\lim_{\beta\to\infty}\frac{1}{2\,\beta}\ln\left(\frac{m\,\omega}{2\,\pi\,\hbar}\right) = 0 \quad (4.116a)$$

Using

$$\frac{d\,V(x)}{d\,x} = -\alpha\,x + \gamma\,x^3$$

$$\frac{d^2\,V(x)}{d\,x^2} = -\alpha + 3\,\gamma\,x^2$$

eq(4.112) becomes

$$m\,\omega^2 = -\alpha + 3\,\gamma\,\overline{x}^2$$

$$\omega = \sqrt{\frac{1}{m}\left(-\alpha + 3\,\gamma\,\overline{x}^2\right)} \quad (4.116b)$$

$$\to \qquad \frac{d\omega}{d\bar{x}} = \frac{3\gamma\bar{x}}{\sqrt{m\left(-\alpha + 3\gamma\bar{x}^2\right)}}$$

The minimum of eq(4.116) is given by

$$\frac{d V_{\text{eff}}^{\infty}(\bar{x})}{d\bar{x}} = 0 = \frac{1}{2}\hbar \frac{3\gamma\bar{x}}{\sqrt{m\left(-\alpha + 3\gamma\bar{x}^2\right)}} - \alpha\bar{x} + \gamma\bar{x}^3 \qquad \text{(a)}$$

For γ small, we have, to the lowest order,

$$-\alpha\bar{x} + \gamma\bar{x}^3 = 0$$

Since $\bar{x}$ is a maximum, we have

$$\bar{x}_{\min} \approx \pm\sqrt{\frac{\alpha}{\gamma}} \qquad \text{(b)}$$

whereupon eq(4.116b) gives

$$\omega \approx \sqrt{\frac{2\alpha}{m}} \qquad (4.118)$$

To improve the accuracy, we put eq(b) back into eq(a) to get

$$\frac{1}{2}\hbar\frac{3\gamma}{\sqrt{2\alpha m}} - \alpha + \gamma\bar{x}^2 = 0$$

$$\to \qquad \bar{x}_{\min} \approx \pm\frac{1}{\sqrt{\gamma}}\sqrt{\alpha - \frac{1}{2}\hbar\frac{3\gamma}{\sqrt{2\alpha m}}}$$

$$\approx \pm\sqrt{\frac{\alpha}{\gamma}}\left(1 - \frac{1}{4\alpha}\hbar\frac{3\gamma}{\sqrt{2\alpha m}}\right)$$

$$= \pm\left(\sqrt{\frac{\alpha}{\gamma}} - \frac{3\hbar}{4\alpha}\sqrt{\frac{\gamma}{2m}}\right) \qquad (4.117)$$

Eq(4.117) is a non-perturbative result owing to the $\gamma^{-1/2}$ dependence on the coupling strength that becomes singular as $\gamma \to 0$. By definition, perturbative result is a power series in γ so that it must be finite as $\gamma \to 0$.

For $\bar{x} \approx 0$, eq(4.116b) gives

$$\omega = \sqrt{-\frac{\alpha}{m}\left(1 - \frac{3\gamma}{\alpha}\bar{x}^2\right)} \approx i\sqrt{\frac{\alpha}{m}}\left(1 - \frac{3\gamma}{2\alpha}\bar{x}^2\right)$$

Hence

$$\ln\omega = \ln\left(i\sqrt{\frac{\alpha}{m}}\right) - \frac{3\gamma}{2\alpha}\bar{x}^2 + \ldots$$

$$\sinh\beta\hbar\omega \approx i\sin\beta\hbar\sqrt{\frac{\alpha}{m}}\left(1 - \frac{3\gamma}{2\alpha}\bar{x}^2\right)$$

$$= i \sin\left(\beta \hbar \sqrt{\frac{\alpha}{m}}\right)\left[1 - \cot\left(\beta \hbar \sqrt{\frac{\alpha}{m}}\right)\left(\frac{3 \beta \hbar \gamma}{2 \sqrt{m \alpha}} \bar{x}^2\right)\right]$$

$$\rightarrow \qquad -\frac{1}{2\beta} \ln\left(\frac{m \omega}{2 \pi \hbar \sinh \beta\hbar\omega}\right) \approx C + \frac{3 \gamma}{4 \beta \alpha} (1 + A) \bar{x}^2 + \ldots \qquad (4.118a)$$

where

$$A = \beta \hbar \sqrt{\frac{\alpha}{m}} \cot\left(\beta \hbar \sqrt{\frac{\alpha}{m}}\right)$$

$$C = -\frac{1}{2\beta} \ln\left(\frac{\sqrt{m \alpha}}{2 \pi \hbar \sin\left(\beta \hbar \sqrt{\frac{\alpha}{m}}\right)}\right)$$

Putting eq(4.118a) into eq(4.114), eq(4.116) is modified to read

$$V_{\text{eff}}(\bar{x}) \approx \left(\frac{3 \gamma}{4 \beta \alpha} - \frac{1}{2} \alpha\right) \bar{x}^2 + \frac{1}{4} \gamma \bar{x}^4 \qquad (4.119)$$

where we've dropped the constant term C & assumed $A << 1$ or

$$\beta \hbar \sqrt{\frac{\alpha}{m}} << \tan\left(\beta \hbar \sqrt{\frac{\alpha}{m}}\right) \qquad (4.119a)$$

Since $\tan(4.5\,\pi) = 10$, eq(4.119) holds for

$$0.45\,\pi < \beta \hbar \sqrt{\frac{\alpha}{m}} < \frac{\pi}{2}$$

The extrema of V_{eff} in eq(4.119) are given by

$$\frac{d\,V_{\text{eff}}(\bar{x})}{d\,x} \approx \left(\frac{3 \gamma}{2 \beta \alpha} - \alpha\right) \bar{x} + \gamma \bar{x}^3 = 0$$

$$\rightarrow \qquad \bar{x} = 0 \qquad \text{or} \qquad \bar{x}^2 = -\frac{3}{2 \beta \alpha} + \frac{\alpha}{\gamma}$$

$$\frac{d^2\,V_{\text{eff}}(\bar{x})}{d\,x^2} \approx \frac{3 \gamma}{2 \beta \alpha} - \alpha + 3 \gamma \bar{x}^2$$

$$\rightarrow \qquad \left.\frac{d^2\,V_{\text{eff}}(\bar{x})}{d\,x^2}\right|_{\bar{x}=0} \approx \frac{3 \gamma}{2 \beta \alpha} - \alpha$$

Setting the critical temperature by

$$\frac{3 \gamma}{2 \beta_c \alpha} = \alpha \qquad \rightarrow \qquad k_B T_c = \frac{2 \alpha^2}{3 \gamma}$$

we see that

1. For $T > T_c$,
   there is only one minimum at $\bar{x} = 0$ as the other two roots are imaginary.
2. For $T < T_c$,

there're two minima at $\overline{x} = \pm\sqrt{-\frac{3}{2\beta\alpha} + \frac{\alpha}{\gamma}}$ & one maximum at $\overline{x} = 0$.

3. At $T = T_c$, all three extrema coalesce into one minimum at $\overline{x} = 0$.

Quoting eq(4.98) of §4.4, we have, for a harmonic oscillator,

$$Z_{ab} = \exp\left[\frac{i}{2\hbar}(q_a p_a - q_b p_b)\right]\int_{q_a,p_a}^{q_b,p_b} \mathcal{D}p\,\mathcal{D}q\,\exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b} dt\,\mathcal{L}\right] \qquad (4.120)$$

where

$$\mathcal{L} = p\dot{q} - H \qquad (4.120a)$$

$$= p\dot{q} - \frac{1}{2}m\omega^2 q^2 - \frac{p^2}{2m} \qquad (4.120b)$$

& the measure is [see eq(4.97)]

$$\mathcal{D}p\,\mathcal{D}q = \prod_{j=1}^{N-1}\frac{dp_j\,dq_j}{2\pi\hbar} \qquad (4.121)$$

The p integrals are of the type

$$\int_{-\infty}^{\infty}\frac{dp_j}{2\pi\hbar}\exp\frac{i}{\hbar}\left(p_j\dot{q}_j - \frac{p_j^2}{2m}\right) = \sqrt{\frac{m}{2\pi\hbar i}}\,\exp\left(\frac{i}{\hbar}\frac{m\dot{q}_j^2}{2}\right)$$

so that eq(4.120) becomes

$$Z_{ab} = \exp\left[\frac{i}{2\hbar}(q_a p_a - q_b p_b)\right]\int_{q_a}^{q_b}\overline{\mathcal{D}}q\,\exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b} dt\,\mathcal{L}\right]$$

where

$$\mathcal{L} = \frac{1}{2}m\dot{q}^2 - \frac{1}{2}m\omega^2 q^2$$

$$= \frac{1}{2}m\dot{q}^2 - V \qquad (4.121a)$$

$$\overline{\mathcal{D}}q = \left(\frac{m}{2\pi\hbar i}\right)^{N-1}\prod_{j=1}^{N-1}dq_j \qquad (4.121b)$$

Assuming eq(4.121a) to hold for all V, we have, for the potential of eq(4.99)

$$Z_{00} = \int_{q_0}^{q_0}\overline{\mathcal{D}}q\,\exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b}dt\left(\frac{1}{2}m\dot{q}^2 + \frac{1}{2}\alpha q^2 - \frac{1}{4}\gamma q^4\right)\right\} \qquad (4.122)$$

where we've set

$$q_a = q_b = q_0 \qquad \& \qquad p_a = p_b = 0$$

Setting

$$q \to q - q_0$$

we have

$$Z_{00} = \int_0^0\overline{\mathcal{D}}q\,\exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b}dt\left(\frac{1}{2}m\dot{q}^2 + \frac{1}{2}\alpha(q+q_0)^2 - \frac{1}{4}\gamma(q+q_0)^4\right)\right\}$$

$$= \int_0^0\overline{\mathcal{D}}q\,\exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b}dt\left(\frac{1}{2}m\dot{q}^2 + \frac{1}{2}\alpha q_0^2 - \frac{1}{4}\gamma q_0^4\right.\right. \qquad (4.123)$$

$$\left.\left. -(\gamma q_0^3 - \alpha q_0)q - \frac{1}{2}(3\gamma q_0^2 - \alpha)q^2 - \gamma q_0 q^3 - \frac{1}{4}\gamma q^4\right)\right\}$$

The assumption $p_a = p_b = 0$ implies the center of mass of the system is stationary, which means the linear term in V must vanish, i.e.,

$$\gamma q_0^3 - \alpha q_0 = 0 \quad \rightarrow \qquad q_0 = 0 \qquad \text{or} \qquad q_0 = \pm\sqrt{\frac{\alpha}{\gamma}}$$

For $T < T_c$, $q_0 = 0$ is a maximum of V so that a stable oscillation is possible only for $q_0 = \pm\sqrt{\frac{\alpha}{\gamma}}$, which is the dominant part of eq(4.117).

Furthermore, the action in eq(4.123) no longer possesses the reflection symmetry $q \to -q$ owing to the presence of the q^3 term. In other words, the system has undergone a spontaneous symmetry breaking when the temperature drops below T_c.

What happened is this: for $T < T_c$, the system develops 2 equivalent ground states. If the energy barrier between these states are high enough to prevent significant tunneling, the system can be in only one of them. Symmetry of the system is then broken.

See Swanson’s text for further discussions.