

Solutions to Pathria's Statistical Mechanics

Chapter 2

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Problem 2.1

The key of the problem is to prove the Jacobian of the transformation equals 1, i.e.

$$D = \frac{\partial(Q_1, \dots, Q_s, P_1, \dots, P_s)}{\partial(q_1, \dots, q_s, p_1, \dots, p_s)} = 1$$

As indicated by $|AB| = |A||B^{-1}|$ (A and B are matrices), we can decompose our transformation into two steps and write

$$D = \frac{\partial(Q_1, \dots, Q_s, P_1, \dots, P_s)}{\partial(q_1, \dots, q_s, P_1, \dots, P_s)} \bigg/ \frac{\partial(q_1, \dots, q_s, p_1, \dots, p_s)}{\partial(q_1, \dots, q_s, P_1, \dots, P_s)}$$

If we write $\frac{\partial(Q_1, \dots, Q_s, P_1, \dots, P_s)}{\partial(q_1, \dots, q_s, P_1, \dots, P_s)}$ explicitly, i.e.

$$\begin{vmatrix} \frac{\partial Q_i}{\partial q_j} & \frac{\partial Q_i}{\partial P_j} \\ 0 & \delta_j^i \end{vmatrix}$$

So, we have

$$\begin{aligned} \frac{\partial(Q_1, \dots, Q_s, P_1, \dots, P_s)}{\partial(q_1, \dots, q_s, P_1, \dots, P_s)} &= \left\{ \frac{\partial(Q_1, \dots, Q_s)}{\partial(q_1, \dots, q_s)} \right\}_{P=\text{constants}} \\ D &= \left\{ \frac{\partial(Q_1, \dots, Q_s)}{\partial(q_1, \dots, q_s)} \right\}_{P=\text{constants}} \bigg/ \left\{ \frac{\partial(p_1, \dots, p_s)}{\partial(P_1, \dots, P_s)} \right\}_{q=\text{constants}} \end{aligned}$$

We suppose that the generating function of canonical transformation are $\Phi(q, P, t)$, then we have

$$p_i = \frac{\partial \Phi}{\partial q_i}$$

$$Q_i = \frac{\partial \Phi}{\partial P_i}$$

So,

$$\begin{aligned} \left\{ \frac{\partial(Q_1, \dots, Q_s)}{\partial(q_1, \dots, q_s)} \right\}_{P=\text{constants}} &= \left| \frac{\partial^2 \Phi}{\partial P_i \partial q_j} \right| \\ \left\{ \frac{\partial(p_1, \dots, p_s)}{\partial(P_1, \dots, P_s)} \right\}_{q=\text{constants}} &= \left| \frac{\partial^2 \Phi}{\partial q_i \partial P_j} \right| \end{aligned}$$

$$D = \left| \frac{\partial^2 \Phi}{\partial P_i \partial q_j} \right| \bigg/ \left| \frac{\partial^2 \Phi}{\partial q_i \partial P_j} \right| = 1$$

Problem 2.2

(a)

$$x = r \sin \theta \cos \phi, \quad y = r \sin \theta \sin \phi, \quad z = r \cos \theta$$

$$\frac{\partial(x, y, z)}{\partial(r, \theta, \phi)} = r^2 \sin \theta$$

$$\frac{\partial(x, y, z)}{\partial(p_r, p_\theta, p_\phi)} = 0$$

$$p_x = p_r \sin \theta \cos \phi + p_\theta \frac{\cos \theta \cos \phi}{r} - p_\phi \frac{\sin \phi}{r \sin \theta}$$

$$p_y = p_r \sin \theta \sin \phi + p_\theta \frac{\cos \theta \sin \phi}{r} + p_\phi \frac{\cos \phi}{r \sin \theta}$$

$$p_z = p_r \cos \theta - p_\theta \frac{\sin \theta}{r}$$

$$\frac{\partial(p_x, p_y, p_z)}{\partial(p_r, p_\theta, p_\phi)} = \frac{1}{r^2 \sin \theta}$$

$$D = \frac{\partial(x, y, z, p_x, p_y, p_z)}{\partial(r, \theta, \phi, p_r, p_\theta, p_\phi)} = 1$$

(b)

$$T = \frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2} + \frac{p_\phi^2}{2mr^2 \sin^2 \theta}$$

$$\begin{aligned} & \int_{-\infty}^{\infty} dp_\theta \int_{-\infty}^{\infty} dp_\phi f(r, \theta, \phi, T) \\ = & 2 \int_{-\infty}^{\infty} dp_\theta \int_{\frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2}}^{\infty} \frac{mr^2 \sin^2 \theta dT}{p_\phi} f(r, \theta, \phi, T) \\ = & 2mr \sin \theta \int_{-\infty}^{\infty} dp_\theta \int_{\frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2}}^{\infty} \frac{dT}{\sqrt{2mT - p_r^2 - \frac{p_\theta^2}{r^2}}} f(r, \theta, \phi, T) \end{aligned}$$

Problem 2.3

The Hamiltonian of the rotator is a function of the angular momentum L .

$$H = f(L)$$

Now we divide the phase space into cells with volume h by lines with constant energies:

Since the angle φ varies between 0 and 2π , angular momentum should be quantized as shown:

$$h = 2\pi \Delta L \quad \Rightarrow \quad \Delta L = \hbar$$

Since we starting from the zero line, the eigenvalues of energy should be

$$E_m = f(m\hbar) \tag{1}$$

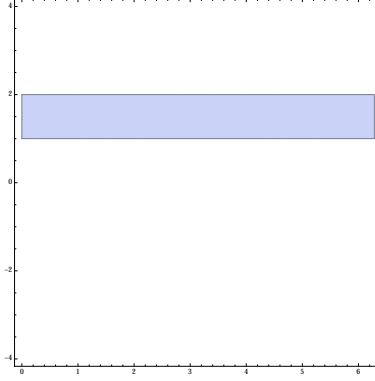


Figure 1: A quantum state in phase space

Notice that we get this result by cutting the phase space into slices without solving the Schrödinger Equation. Because the Hamiltonian commutes with the angular momentum, the eigenenergy is given by eigenvalues of the angular momentum:

$$-i\hbar \frac{\partial \psi}{\partial \varphi} = L\psi \quad \psi(\varphi) = \psi(\varphi + 2\pi)$$

solve the differential equation and the result is:

$$L = m\hbar \quad m \in \mathbb{Z}.$$

Now we find that the result we get from the eigenfunction of angular momentum operator is the same as we get from cutting the phase space into cells.

Problem 2.4

If we just consider about the orbital angular momentum, it can be written as a function of p_θ and p_φ which are the canonical momentum conjugate to the spherical coordinate variables θ and φ :

$$L^2 = p_\theta^2 + \frac{p_\varphi^2}{\sin^2 \theta} \quad (2)$$

thus the phase volume of the region which satisfies $L^2 \leq M^2$ is

$$\begin{aligned} \Omega &= \int_0^\pi d\theta \int_0^{2\pi} d\varphi \int_{L^2 \leq M^2} dp_\theta dp_\varphi \\ &= \int_0^\pi d\theta \int_0^{2\pi} d\varphi \pi M^2 \sin \theta \\ &= 4\pi^2 M^2 \end{aligned} \quad (3)$$

Thus the number of microstates is $\Omega = \Omega/\hbar^2 = M^2/\hbar^2$. Then let us calculate the number by quantized angular momentum. By summing up all the eigenstates of the angular momentum, we get:

$$\Omega = \sum_{j=0}^{j_{\max}} (2j+1) = (j_{\max} + 1)^2 \quad (4)$$

Now we have to determine the number j_{\max} . Since we want the absolute value of the angular momentum $\sqrt{j_{\max}(j_{\max} + 1)}\hbar < M$, we can find that j_{\max} is determined by the following equation:

$$j_{\max} = \left\lfloor \frac{\sqrt{1 + \frac{4M^2}{\hbar^2}} - 1}{2} \right\rfloor \quad (5)$$

It is obvious that $j_{\max} = \lfloor M/\hbar \rfloor - 1$ or $j_{\max} = \lfloor M/\hbar \rfloor$. So the total number of microstates will be:

$$\Omega = \left\lfloor \frac{M}{\hbar} \right\rfloor^2 \text{ or } \left(\left\lfloor \frac{M}{\hbar} \right\rfloor + 1 \right)^2 \quad (6)$$

If we take the classical limit that $M \gg \hbar$, the result will be:

$$\Omega \simeq \frac{M^2}{\hbar^2} \quad (7)$$

Problem 2.5

In this problem we need to use the WKB approximation in Quantum Mechanics. In D. Griffiths' book we find that the

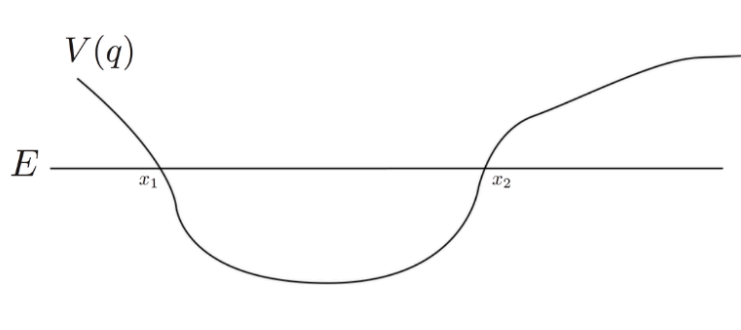


Figure 2: WKB Approximation

WKB wave function between two classical turning point x_1 and x_2 is:

$$\psi(x) = \frac{2D}{\sqrt{p(x)}} \sin \left[\frac{1}{\hbar} \int_x^{x_2} p(x') dx' + \frac{\pi}{4} \right] \quad x < x_2$$

or

$$\psi(x) = -\frac{2D'}{\sqrt{p(x)}} \sin \left[-\frac{1}{\hbar} \int_{x_1}^x p(x') dx' - \frac{\pi}{4} \right] \quad x > x_1$$

in which $p(x) = \sqrt{2m[E - V(x)]}$. We can define:

$$\begin{aligned} \theta_1(x) &= \frac{1}{\hbar} \int_{x_1}^x p(x') dx' + \frac{\pi}{4} \\ \theta_2(x) &= \frac{1}{\hbar} \int_x^{x_2} p(x') dx' + \frac{\pi}{4} \end{aligned}$$

Since the two solutions should be the same, the difference between the two θ functions should be $n\pi, n \in \mathbb{Z}$:

$$n\pi - \frac{\pi}{2} = \frac{1}{\hbar} \int_{x_1}^{x_2} p(x') dx' \quad (8)$$

The integral in classical phase space is

$$\oint p dq = 2 \int_{x_1}^{x_2} p(x') dx'$$

so finally we can find that

$$\oint p dq = h \left(n - \frac{1}{2} \right) \quad n \in \mathbb{Z}. \quad (9)$$

Problem 2.6

The equation of phase space orbit is:

$$\frac{1}{2} m l^2 \dot{\theta}^2 + \frac{1}{2} m g l \theta^2 = E$$

This is a ellipse whose area is:

$$S = \pi \sqrt{2 E m l^2} \sqrt{\frac{2 E}{m g l}} = 2 \pi E \sqrt{\frac{l}{g}} = E \tau$$

Problem 2.7

- (i) Assume that these N SHOs are distinguishable. To distribute total energy E into such N SHOs, there are

$$C_{E/\hbar\omega + N/2 - 1}^{N-1}$$

ways. Let $E/\hbar\omega \gg N$, we get the approximate result:

$$\frac{1}{(N-1)!} \left(\frac{E}{\hbar\omega} \right)^{N-1}$$

- (ii) The total energy of N classical SHOs is:

$$\sum_{i=1}^N \left(\frac{p_i^2}{2m} + \frac{k x_i^2}{2} \right) = E$$

The phase space volume is:

$$\left(\frac{2}{\omega} \right)^N E^{N-1} \pi^N \frac{1}{(N-1)!} dE$$

while $dE = \hbar\omega$, we get $\omega_0 = h^N$

Problem 2.8

Assume that

$$V_{3N} = \int \cdots \int \prod_{i=1}^N (4\pi r_i^2 dr_i) = C_N R^{3N} \quad (10)$$

$0 \leq \sum_{i=1}^N r_i \leq R$

we can easily see that C_N is a constant. And we have

$$\prod_{i=1}^N (4\pi r_i^2 dr_i) = 3N C_N R^{3N-1} dR \quad (11)$$

consider the following equation

$$\left(\int_0^\infty e^{-r} r^2 dr\right)^N = \int \cdots \int_{0 \leq \sum_{i=1}^N r_i \leq R} e^{-R} \prod_{i=1}^N r_i^2 dr_i \quad (12)$$

$$= \int_0^\infty e^{-R} \frac{3^N C_N}{(4\pi)^N} R^{3N-1} dR \quad (13)$$

$$= \frac{(3N)! C_N}{(4\pi)^N} \quad (14)$$

We also have

$$\left(\int_0^\infty e^{-r} r^2 dr\right)^N = 2^N \quad (15)$$

Thus

$$C_N = \frac{(8\pi)^N}{(3N)!} \quad (16)$$

and

$$V_{3N} = \int \cdots \int_{0 \leq \sum_{i=1}^N r_i \leq R} \prod_{i=1}^N (4\pi r_i^2 dr_i) = \frac{(8\pi R^3)^N}{(3N)!} \quad (17)$$

The volume of phase space for relativistic gas ($\varepsilon = pc$) can be obtained by replacing the R in V_N by E/c .

$$V = \int \cdots \int_{0 \leq \sum_{i=1}^N r_i \leq E/c} 4\pi p_i^2 dp_i \quad (18)$$

$$= \frac{(8\pi E^3 V)^N}{(3N)! c^{3N}} \quad (19)$$

The entropy of this system is obtained by

$$S = k \ln \Omega = k \ln \frac{V}{h^{3N}} \quad (20)$$

Using the relations we can get that

$$\frac{\partial S}{\partial E} = \frac{1}{T} = \frac{3Nk}{E} \quad (21)$$

$$\frac{\partial S}{\partial V} = \frac{P}{T} = \frac{Nk}{V} \quad (22)$$

$$C_V = \left(\frac{\partial E}{\partial T}\right)_{N,V} = 3Nk \quad (23)$$

$$C_P = \frac{\partial(E + PV)}{\partial T} = 4Nk \quad (24)$$

$$(25)$$

Problem 2.9

Like problem 2.8,

$$\int \cdots \int_{0 \leq \sum_{i=1}^{3N} |x_i| \leq R} (dx_1 \dots dx_{3N}) = C_N R^{3N} \quad (26)$$

Thus

$$\int \cdots \int_{0 \leq \sum_{i=1}^{3N} |x_i| \leq R} (e^{-R} dx_1 \dots dx_{3N}) = \int e^{-R} C_N R^{3N-1} dR = C_N (3N)! \quad (27)$$

On the other hand,

$$\int \cdots \int_{0 \leq \sum_{i=1}^{3N} |x_i| \leq R} (e^{-R} dx_1 \dots dx_{3N}) = \left(\int_{-\infty}^{\infty} dx_1 \dots dx_{3N} \right)^3 N = 2^{3N} \quad (28)$$

We can see that

$$\int \cdots \int_{0 \leq \sum_{i=1}^{3N} |x_i| \leq R} (dx_1 \dots dx_{3N}) = \frac{(2R)^{3N}}{3N!} \quad (29)$$

The phase space for 3N relativistic particles moving in 1 dimension can be obtained using the integral before.

$$V = \frac{(2EL)^{3N}}{(3N)!(c)^{3N}} \quad (30)$$

The entropy of this system is obtained by

$$S = k \ln \Omega = k \ln \frac{V}{h^{3N}} \quad (31)$$

Using the relations we can get that

$$\frac{\partial S}{\partial E} = \frac{1}{T} = \frac{3Nk}{E} \quad (32)$$

$$\frac{\partial S}{\partial L} = \frac{F}{T} = \frac{3Nk}{L} \quad (33)$$

$$C_V = \left(\frac{\partial E}{\partial T} \right)_{N,V} = 3Nk \quad (34)$$

$$C_P = \frac{\partial(E + FL)}{\partial T} = 6Nk \quad (35)$$

$$(36)$$