Chapter 1

LINEAR POLARON MODEL

Let us consider the hamiltonian of the linear polaron system consisting of the energy of one oscillator H_S, oscillator vibration of lattice H_Σ and a linear electron-lattice interaction $H_{S\Sigma}$.

$$
\begin{aligned}
&H = H_{S+\Sigma} = H_S + H_\Sigma + H_{S\Sigma} \\
&H = \frac{\mathbf{p}^2}{2m} + \frac{K^2\mathbf{r}^2}{2} + \frac{1}{2}\sum_f (p_f p_f^* + \nu^2(f) q_f q_f^*) + \frac{i}{\sqrt{V}}\sum_f S(f)(\mathbf{f}\cdot\mathbf{r})q_f \\
&q_{-f} = q_f^* \;, \qquad p_{-f} = p_f^*
\end{aligned}
\tag{1.1}
$$

where $S(f) = S(|\mathbf{f}|)$ is real, $\nu(\mathbf{f}) = \nu(|\mathbf{f}|) > 0$ and is a radially symmetric function. $\mathbf{f} = \left(\frac{2\pi n_1}{L}, \frac{2\pi n_2}{L}, \frac{2\pi n_3}{L}\right)$, n_α are integers and $L^3 = V$ is the volume of the system. The total number N of oscillators is supposed to be finite for finite V. $N \to \infty$ when $V \to \infty$ and is such that $\frac{N}{V}$ = constant.

Note the identity

$$
\begin{aligned}
&\frac{1}{2}\sum_f \nu^2(f)\left(q_f - i\frac{(\mathbf{f}\cdot\mathbf{r})}{\nu^2(f)}\frac{S(f)}{\sqrt{V}}\right)\left(q_f^* + i\frac{(\mathbf{f}\cdot\mathbf{r})}{\nu^2(f)}\frac{S(f)}{\sqrt{V}}\right) \\
&\quad = \frac{1}{2}\sum_f \nu^2(f) q_f q_f^* + \frac{1}{2}\sum_f \nu^2(f)\frac{S^2(f)}{V}(\mathbf{f}\cdot\mathbf{r})^2 \\
&\quad + \frac{1}{2}\sum_f \{i(\mathbf{f}\cdot\mathbf{r})q_f - i(\mathbf{f}\cdot\mathbf{r})q_f^*\}\frac{S(f)}{\sqrt{V}}
\end{aligned}
$$

where

$$-\sum_f i(\mathbf{f}\cdot\mathbf{r})q_f^*\frac{S(f)}{\sqrt{V}} = -\frac{1}{\sqrt{V}}\sum_f i(\mathbf{f}\cdot\mathbf{r})q_{-f}S(-f)$$
$$= \frac{1}{\sqrt{V}}\sum_f i(\mathbf{f}\cdot\mathbf{r})q_f S(f)\ .$$

In view of the radial symmetry,

$$\sum_f F(|\mathbf{f}|)f_\alpha f_\beta = \delta_{\alpha\beta}\frac{1}{3}\sum_f F(|\mathbf{f}|)f^2$$
$$\frac{1}{2V}\sum_f \nu^{-2}(f)S^2(f)(\mathbf{f}\cdot\mathbf{r})^2 = \frac{\mathbf{r}^2}{6V}\sum_f \frac{S^2(f)f^2}{\nu^2(f)}\ .$$

From this we can write the potential energy

$$\begin{aligned} U &= \frac{K^2\mathbf{r}^2}{2} + \frac{1}{2}\sum_f \nu^2(f)q_f q_f^* + \frac{i}{\sqrt{V}}\sum_f S(f)(\mathbf{f}\cdot\mathbf{r})q_f \\ &= \frac{(K^2-K_0^2)}{2}\mathbf{r}^2 + \frac{1}{2}\sum_f \nu^2(f)\left(q_f - i\frac{(\mathbf{f}\cdot\mathbf{r})}{\nu^2(f)}\frac{S(f)}{\sqrt{V}}\right)\left(q_f^* + i\frac{(\mathbf{f}\cdot\mathbf{r})}{\nu^2(f)}\frac{S(f)}{\sqrt{V}}\right) \end{aligned} \tag{a}$$

where

$$K_0^2 = \frac{1}{3V}\sum_f \frac{S^2(f)f^2}{\nu^2(f)}\ . \tag{1.2}$$

If $K = K_0$, $U \geq 0$. We also see that $U = 0$ when

$$q_f = i\frac{(\mathbf{f}\cdot\mathbf{r})}{\nu^2(f)}\frac{S(f)}{\sqrt{V}}\ . \tag{b}$$

The total kinetic energy $\frac{\mathbf{p}^2}{2m} + \frac{1}{2}\sum_f |p_f|^2$ is evidently positive definite.

Let us introduce normal coordinates Q_λ. Then $\mathbf{r}, q_f$ will be linear combinations of Q_λ and

$$\ddot{Q}_\lambda + \Omega_\lambda^2 Q_\lambda = 0\ .$$

For $K = K_0$, (a) shows that U becomes zero only if q_f belongs to the 3-dimensional manifold (b). In other words, we note that H is an invariant with respect to the 3-dimensional translation group

$$\mathbf{r}\to\mathbf{r}+\mathbf{R}\ ;\qquad q_f \to q_f + i\frac{(\mathbf{f}\cdot\mathbf{R})}{\nu^2(f)}\frac{S(f)}{\sqrt{V}}\ .$$

Therefore exactly three of Ω_λ^2 will be zero, all other Ω_λ^2 being positive. We thus have three modes

$$\ddot{Q}_\alpha = 0$$

corresponding to the inertial motion. Thus $\mathbf{r}(t)$ contains uniform inertial movement on which harmonic vibrations will be superimposed. Also note that when $K < K_0$, the form U is not positive so that some Ω_λ^2 must be negative and the movements will be of unstable type characterized by exponentially increasing function of t.

Here we shall be interested in the case $K = K_0$. But from technical consideration it will be more convenient to take

$$K = K_0 + \eta^2 \tag{1.3}$$

and then perform the limiting process ($\eta \to 0$) (before the usual limiting process $V \to \infty$). Note that as $\eta^2 > 0$ the form U is positive definite and hence all Ω_λ^2 will be positive. Thus in this situation all $\mathbf{r}, \mathbf{p}, q_f, p_f$ will be represented as sums of harmonic vibrations.

We now introduce the Bose amplitudes

$$q_f = \left(\frac{\hbar}{2\nu(f)}\right)^{\frac{1}{2}} (b_f + b^\dagger_{-f}); \quad p_f = i\left(\frac{\hbar\nu(f)}{2}\right)^{\frac{1}{2}} (b_f^\dagger - b_f) .$$

It is easy to see that

$$q_{-f} = q_f^* ; \quad p_{-f} = p_f^*$$

and

$$[q_f, p_f] = \frac{q_f p_f - p_f q_f}{i\hbar} = 1 .$$

The hamiltonian (1.1) can be transformed into

$$H = \frac{\mathbf{p}^2}{2m} + \frac{1}{2}(K_0^2 + \eta^2)\mathbf{r}^2 + i\sum_f \frac{1}{\sqrt{V}} S(f)\left(\frac{h}{2\nu(f)}\right)^{\frac{1}{2}} (\mathbf{f}\cdot\mathbf{r})(b_f + b^\dagger_{-f})$$
$$+ \sum_f h\nu(f) b_f^\dagger b_f + \frac{1}{2}\sum_f h\nu(f) . \tag{1.4}$$

The Hamilton equations of motion from Eq. (1.4) are

$$m\frac{d\mathbf{r}}{dt} = \mathbf{p}$$
$$\frac{d\mathbf{p}}{dt} = -(K_0^2 + \eta^2)\mathbf{r} - \frac{i}{\sqrt{V}}\sum_f S(f)\left(\frac{h}{2\nu(f)}\right)^{\frac{1}{2}} \mathbf{f}(b_f + b_f^\dagger) . \tag{1.5}$$

The Heisenberg equation for operators $b_f, b^\dagger_{-f}$ will be:

$$i\hbar\frac{db_f}{dt} = h\nu(f)b_f - \frac{i}{\sqrt{V}}\left(\frac{\hbar}{2\nu(f)}\right)^{\frac{1}{2}} S(f)(\mathbf{f}\cdot\mathbf{r})\,;$$

$$i\hbar\frac{db^\dagger_{-f}}{dt} = -h\nu(f)b^\dagger_{-f} + \frac{i}{\sqrt{V}}\left(\frac{\hbar}{2\nu(f)}\right)^{\frac{1}{2}} S(f)(\mathbf{f}\cdot\mathbf{r})$$

and on changing $f \rightarrow -f$

$$-i\hbar\frac{db^\dagger_f}{dt} = h\nu(f)b^\dagger_f + \frac{i}{\sqrt{V}}\left(\frac{\hbar}{2\nu(f)}\right)^{\frac{1}{2}} S(f)(\mathbf{f}\cdot\mathbf{r})\,.$$

Here we shall draw attention to the study of the equilibrium correlation and two-time Green functions constructed with the help of Eq. (1.4). We introduce correlation and Green functions defined by the relations

$$\begin{aligned}
\langle A(t)B(\tau)\rangle_{\mathrm{eq}} &= \int_{-\infty}^{\infty} I_{A,B}(\omega)e^{-i\omega(t-\tau)}d\omega \\
\langle B(\tau)A(t)\rangle_{\mathrm{eq}} &= \int_{-\infty}^{\infty} I_{A,B}(\omega)e^{-\beta\omega\hbar}e^{-i\omega(t-T)}d\omega\,,\ \ \beta = \frac{1}{k_B T} \qquad (1.6)\\
\langle\langle A(t), B(\tau)\rangle\rangle_{\mathrm{ret}} &= \theta(t-\tau)\langle[A(t), B(\tau)]\rangle_{\mathrm{eq}} \\
&= \theta(t-\tau)\frac{\langle A(t)B(\tau) - B(\tau)A(t)\rangle}{i\hbar} \\
\langle\langle A(t), B(\tau)\rangle\rangle_{\mathrm{adv}} &= -\theta(\tau - t)\langle[A(t), B(\tau)]\rangle_{\mathrm{eq}}\,.
\end{aligned}$$

Introduce a function of a complex variable $\Omega(\mathrm{Im}\,\Omega \not\equiv 0)$,

$$\langle\langle A, B\rangle\rangle_{\Omega} = \frac{1}{\hbar}\int_{-\infty}^{\infty} I_{A,B}(\omega)\frac{1 - e^{-\beta\omega\hbar}}{\Omega - \omega}d\omega \qquad (1.7)$$

which is regular in the complex Ω plane except the real axis. The function (1.7) defines the frequency representation of the retarded and advanced Green function by means of the relations

$$\langle\langle A(t), B(\tau)\rangle\rangle_{\mathrm{ret}} = \frac{1}{2\pi}\int_{-\infty}^{\infty} \langle\langle A, B\rangle\rangle_{\omega+i0}e^{-i\omega(t-\tau)}d\omega \qquad (1.8)$$

$$\langle\langle A(t), B(\tau)\rangle\rangle_{\mathrm{adv}} = \frac{1}{2\pi}\int_{-\infty}^{\infty} \langle\langle A, B\rangle\rangle_{\omega-i0}e^{-i\omega(t-\tau)}d\omega \qquad (1.9)$$

which yield

$$\langle\langle A, B\rangle\rangle_{\omega+i0} - \langle\langle A, B\rangle\rangle_{\omega-i0} = -2\pi i\frac{1 - e^{-\beta\hbar\omega}}{\hbar}I_{A,B}(\omega)\,. \qquad (1.10)$$

The equation of motion for Green functions are

$$\begin{aligned} i\frac{d}{dt}\langle\langle A(t),B(\tau)\rangle\rangle_{\substack{\text{ret}\\ \text{adv}}} &= \delta(t-\tau)\frac{1}{\hbar}\langle AB-BA\rangle+\langle\langle i\frac{dA(t)}{dt},B(\tau)\rangle\rangle_{\substack{\text{ret}\\ \text{adv}}}\\ \Omega\langle\langle A,B\rangle\rangle_\Omega &= \frac{1}{\hbar}\langle AB-BA\rangle+\langle\langle i\frac{dA}{dt},B\rangle\rangle_\Omega \\ -i\Omega\langle\langle A,B\rangle\rangle_\Omega &= \frac{1}{i\hbar}\langle AB-BA\rangle+\langle\langle\frac{dA}{dt},B\rangle\rangle_\Omega \ . \end{aligned} \tag{1.11}$$

From Eq. (1.6) we get one useful identity

$$\langle B(\tau)A(t)\rangle_{\text{eq}}=\int_{-\infty}^{\infty}I_{B,A}(\omega)e^{-i\omega(t-\tau)}d\omega=\int_{-\infty}^{\infty}I_{B,A}(-\omega)e^{-i\omega(t-\tau)}d\omega$$

and $I_{B,A}(-\omega)=I_{A,B}(\omega)e^{-\beta\omega\hbar}$.

From Eq. (1.7) it is easy to see that

$$\begin{aligned} \langle\langle B,A\rangle\rangle_\Omega &= \frac{1}{\hbar}\int_{-\infty}^{\infty}I_{B,A}(\omega)\frac{1-e^{-\beta\omega\hbar}}{\Omega-\omega}d\omega=\frac{1}{\hbar}\int_{-\infty}^{\infty}I_{B,A}(-\omega)\frac{1-e^{\beta\omega\hbar}}{\Omega+\omega}d\omega\\ &= \frac{1}{\hbar}\int_{-\infty}^{\infty}I_{A,B}(\omega)e^{-\beta\omega\hbar}\frac{1-e^{\beta\omega\hbar}}{\Omega+\omega}d\omega\\ &= \frac{1}{\hbar}\int_{-\infty}^{\infty}I_{A,B}(\omega)\frac{1-e^{-\beta\omega\hbar}}{-\Omega-\omega}d\omega \ . \end{aligned}$$

Therefore

$$\langle\langle B,A\rangle\rangle_\Omega=\langle\langle A,B\rangle\rangle_{-\Omega}\,;\qquad \text{Im}\,\Omega\neq 0\ . \tag{1.12}$$

Starting from Eqs. (1.5) and (1.11) we get

$$\begin{aligned} &im\Omega\langle\langle r_\alpha,r_\beta\rangle\rangle_\Omega=\langle\langle p_\alpha,r_\beta\rangle\rangle_\Omega\\ &(\mathbf{r}=(r_1,r_2,r_3),\mathbf{p}=(p_1,p_2,p_3)\,,p_\alpha r_\beta-r_\beta p_\alpha=-i\hbar\delta_{\alpha,\beta})\ ; \end{aligned} \tag{1.13}$$

$$\begin{aligned} -i\Omega\langle\langle p_\alpha,r_\beta\rangle\rangle_\Omega = &-\delta_{\alpha,\beta}-(K_0^2+\eta^2)\langle\langle r_\alpha,r_\beta\rangle\rangle_\Omega\\ &-\frac{i}{\sqrt{V}}\sum_f S(f)\left(\frac{\hbar}{2\nu(f)}\right)^{\frac{1}{2}}f_\alpha\langle\langle b_f+b_{-f}^\dagger,r_\beta\rangle\rangle_\Omega\ ; \end{aligned} \tag{1.14}$$

$$\begin{aligned} \hbar\Omega\langle\langle b_f,r_\beta\rangle\rangle_\Omega &= h\nu(f)\langle\langle b_f,r_\beta\rangle\rangle_\Omega-\frac{i}{\sqrt{V}}\left(\frac{\hbar}{2\nu(f)}\right)^{\frac{1}{2}}S(f)\langle\langle\mathbf{f}\cdot\mathbf{r},r_\beta\rangle\rangle_\Omega\ ;\\ \hbar\Omega\langle\langle b_{-f}^\dagger,r_\beta\rangle\rangle_\Omega &= -h\nu(f)\langle\langle b_{-f}^\dagger,r_\beta\rangle\rangle_\Omega+\frac{i}{\sqrt{V}}\left(\frac{\hbar}{2\nu(f)}\right)^{\frac{1}{2}}S(f)\langle\langle\mathbf{f}\cdot\mathbf{r},r_\beta\rangle\rangle_\Omega\ . \end{aligned} \tag{1.15}$$

From Eq. (1.15) it follows that

$$\langle\langle b_f, r_\beta\rangle\rangle_\Omega = -\frac{i}{\sqrt{V}}\frac{1}{(\Omega-\nu(f))}\left(\frac{1}{2\nu(f)\hbar}\right)^{\frac{1}{2}} S(f)\langle\langle \mathbf{f}\cdot\mathbf{r}, r_\beta\rangle\rangle_\Omega$$

$$\langle\langle b^\dagger_{-f}, r_\beta\rangle\rangle_\Omega = \frac{i}{\sqrt{V}}\frac{1}{\Omega+\nu(f)}\left(\frac{1}{2\nu(f)\hbar}\right)^{\frac{1}{2}} S(f)\langle\langle \mathbf{f}\cdot\mathbf{r}, r_\beta\rangle\rangle_\Omega\ .$$

Thus

$$\langle\langle b_f + b^\dagger_{-f}, r_\beta\rangle\rangle = \frac{i}{\sqrt{V}}\left\{\frac{1}{\Omega+\nu(f)} - \frac{1}{\Omega-\nu(f)}\right\}\left(\frac{1}{2\nu(f)\hbar}\right)^{\frac{1}{2}} S(f)\langle\langle \mathbf{f}\cdot\mathbf{r}, r_\beta\rangle\rangle\ .$$

By substituting this formula into Eqs. (1.13) and (1.14) we get

$$\begin{aligned}-m\Omega^2\langle\langle r_\alpha, r_\beta\rangle\rangle_\Omega = &-(K_0^2+\eta^2)\langle\langle r_\alpha, r_\beta\rangle\rangle_\Omega - \delta_{\alpha,\beta}\\ &+\frac{1}{V}\sum_f \frac{S^2(f)}{2\nu(f)} f_\alpha\left\{\frac{1}{\Omega+\nu(f)}+\frac{1}{\nu(f)-\Omega}\right\}\\ &\times\langle\langle \mathbf{f}\cdot\mathbf{r}, r_\beta\rangle\rangle_\Omega\ .\end{aligned}$$

Since

$$\sum_f F(|\mathbf{f}|) f_\alpha f_\beta = \delta_{\alpha,\beta}\frac{1}{3}\sum_f F(|\mathbf{f}|) f^2 \tag{1.16}$$

it follows that

$$\begin{aligned}-m\Omega^2\langle\langle r_\alpha, r_\beta\rangle\rangle_\Omega &= -\eta^2\langle\langle r_\alpha, r_\beta\rangle\rangle_\Omega\\ &-\frac{1}{3V}\sum_f \frac{S^2(f)f^2}{\nu^2(f)}\langle\langle r_\alpha, r_\beta\rangle\rangle_\Omega\\ &+\frac{1}{V}\sum_f \frac{S^2(f)}{6\nu(f)} f^2\left\{\frac{1}{\Omega+\nu(f)}+\frac{1}{\nu(f)-\Omega}\right\}\\ &\times\langle\langle r_\alpha, r_\beta\rangle\rangle_\Omega - \delta_{\alpha,\beta}\ .\end{aligned}$$

But

$$\begin{aligned}&\frac{1}{\Omega+\nu(f)} - \frac{1}{\nu(f)} + \frac{1}{\nu(f)-\Omega} - \frac{1}{\nu(f)}\\ &= \frac{-\Omega}{\nu(f)(\Omega+\nu(f))} + \frac{\Omega}{(\nu(f)-\Omega(\nu)f)}\\ &= -\Omega\left\{\frac{1}{\nu(f)(\nu(f)+\Omega)} + \frac{1}{(\Omega-\nu(f))\nu(f)}\right\}\ ,\end{aligned}$$

therefore Eq. (1.16) gives

$$\left[m\Omega^2 - \eta^2 - \Omega\frac{1}{V}\sum_f \frac{S^2(f)}{6\nu^2(f)}f^2\left\{\frac{1}{\nu(f)+\Omega}+\frac{1}{\Omega-\nu(f)}\right\}\right] \times \langle\langle r_\alpha, r_\beta\rangle\rangle_\Omega = \delta_{\alpha,\beta}\ . \tag{1.17}$$

Denote

$$\Delta(\Omega) = \frac{-1}{V}\sum_f \frac{S^2(f)}{6\nu^2(f)}f^2\left\{\frac{1}{\nu(f)+\Omega}+\frac{1}{\Omega-\nu(f)}\right\} \tag{1.18}$$

and note that

$$\Delta(-\Omega) = -\Delta(\Omega)\ . \tag{1.19}$$

Equation (1.17) yields

$$\langle\langle r_\alpha, r_\beta\rangle\rangle_\Omega = \frac{\delta_{\alpha,\beta}}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)}\ . \tag{1.20}$$

From Eqs. (1.5) and (1.11) we have

$$\langle\langle p_\alpha, r_\beta\rangle\rangle_\Omega = \frac{-im\Omega\delta_{\alpha,\beta}}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)} \tag{1.21}$$

and Eqs. (1.12) and (1.19) yield

$$\langle\langle r_\beta, p_\alpha\rangle\rangle_\Omega = \frac{im\Omega\delta_{\alpha,\beta}}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)}\ . \tag{1.22}$$

By using Eqs. (1.5) and (1.11) we further have

$$-i\Omega m\langle\langle r_\beta, p_\alpha\rangle\rangle_\Omega = \frac{m}{i\hbar}\langle r_\beta p_\alpha - p_\alpha r_\beta\rangle + \langle\langle p_\beta, p_\alpha\rangle\rangle_\Omega$$

and

$$\begin{aligned}\langle\langle p_\beta, p_\alpha\rangle\rangle_\Omega &= -m\delta_{\alpha,\beta} + \frac{(m\Omega)^2\delta_{\alpha,\beta}}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)}\\ &= -\delta_{\alpha,\beta}m\frac{\Omega\Delta(\Omega) - \eta^2}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)}\ .\end{aligned} \tag{1.23}$$

For $|\mathrm{Im}\ \Omega| > 0$, we may perform in Eqs. (1.20–1.23) the limiting procedure $\eta \to 0$, thus obtaining

$$\begin{aligned}\langle\langle r_\alpha, r_\beta\rangle\rangle &= \frac{\delta_{\alpha,\beta}}{M\Omega^2 + \Omega\Delta(\Omega)}\\ \langle\langle p_\alpha, r_\beta\rangle\rangle_\Omega &= -\langle\langle r_\beta, p_\alpha\rangle\rangle_\Omega = \frac{-im\Omega\delta_{\alpha,\beta}}{M\Omega^2 + \Omega\Delta(\Omega)} = \frac{-im\delta_{\alpha,\beta}}{m\Omega + \Delta(\Omega)}\\ \langle\langle p_\alpha, p_\beta\rangle\rangle_\Omega &= -m\delta_{\alpha,\beta} + \frac{(m\Omega)^2\delta_{\alpha,\beta}}{m\Omega^2 + \Omega\Delta(\Omega)} = -\delta_{\alpha,\beta}\frac{\Delta(\Omega)}{M\Omega + \Delta(\Omega)}\ .\end{aligned} \tag{1.24}$$

It should be stressed that in calculating the spectral intensity $I_{A,B}(\omega)$ for example, $I_{p_\alpha,p_\beta}(\omega)$, we must use the form (1.23) before letting $\eta \to 0$. In view of Eq. (1.10)

$$I_{p_\alpha,p_\beta}(\omega) = \delta_{\alpha,\beta}\frac{i\hbar}{2\pi}(1 - e^{-\beta\hbar\omega})^{-1}\frac{m\Omega^2}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)}\Bigg|_{\omega-i0}^{\omega+i0}$$

$$= -\delta_{\alpha,\beta}m\frac{i\hbar}{(1 - e^{-\beta\omega\hbar})2\pi}\left\{\frac{\Omega\Delta(\Omega) - \eta^2}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)}\right\}\Bigg|_{\omega-i0}^{\omega+i0} \quad (1.25)$$

Here we shall begin to use the short-hand notation

$$F(\Omega)\Big|_a^b = F(b) - F(a)\ ,$$

keeping in mind that the division by $1 - e^{-\beta\hbar\omega}$ in Eq.(1.25) may introduce a delta function $K\delta(\omega)$ with some unknown coefficient K.

When $\eta^2 > 0$, the expressions

$$\ldots\Big|_{\omega-i0}^{\omega+i0}$$

in Eq. (1.25) are zero in a neighbourhood of the point $\omega = 0$. On the other hand we know that in this case $\eta^2 > 0$, $p_\alpha(t)$ is a sum of harmonic oscillations with frequencies not equal to zero, therefore the corresponding spectral intensity

$$I_{p_\alpha,p_\beta}(\omega) = 0$$

in the neighbourhood of the point $\omega = 0$ (which does not contain the frequencies of the mentioned harmonic oscillator). So we must first compute (1.25) for $\eta^2 > 0$ and only after this may we go to the limit $\eta \to 0$. Let us consider in some detail the simplest example when

$$\nu(f) = \nu = \text{const} > 0\ . \quad (1.26)$$

In this case, Eqs. (1.1), (1.2) and (1.18) yield

$$\Delta(\Omega) = \frac{-K_0^2}{2}\left\{\frac{1}{\Omega+\nu} + \frac{1}{\Omega-\nu}\right\} = \frac{-K_0^2\Omega}{\Omega^2 - \nu^2}\ . \quad (1.27)$$

From Eq.(1.25) it follows that

$$I_{p_\alpha,p_\beta}(\omega) = \delta_{\alpha,\beta}\frac{i\hbar}{2\pi}(1 - e^{-\beta\hbar\omega})^{-1}\frac{m^2\Omega^2}{m\Omega^2 - \eta^2 - \frac{K_0^2\Omega^2}{\Omega^2-\nu^2}}\Bigg|_{\omega-i0}^{\omega+i0}$$

$$= \delta_{\alpha,\beta}\frac{i\hbar}{2\pi}(1 - e^{-\beta\hbar\omega})^{-1}\frac{m^2\Omega^2(\Omega^2 - \nu^2)}{m\Omega^4 - \Omega^2(K_0^2 + \eta^2 + m\nu^2) + \eta^2\nu^2}\Bigg|_{\omega-i0}^{\omega+i0}. \quad (1.28)$$

Here the denominator has two roots in Ω^2, namely

$$\begin{aligned} \omega_1^2 &= \frac{\nu^2\eta^2}{K_0^2+\nu^2 m} + O(\eta^4) \\ \omega_2^2 &= \frac{K_0^2+\nu^2 m}{m} + O(\eta^2) \end{aligned} \tag{1.29}$$

so that

$$m\Omega^4 - \Omega^2(K_0^2+\eta^2+\nu^2 m) + \nu^2\eta^2 = m(\Omega^2-\omega_1^2)(\Omega^2-\omega_2^2)\ .$$

Therefore

$$\begin{aligned} &\frac{m^2\Omega^2(\Omega^2-\nu^2)}{m\Omega^4-\Omega^2(K_0^2+\nu^2 m+\eta^2)+\nu^2\eta^2} \\ &= \frac{m\omega_1^2(\omega_1^2-\nu^2)}{\omega_1^2-\omega_2^2}\frac{1}{\Omega^2-\omega_1^2} + \frac{m\omega_2^2(\omega_2^2-\nu^2)}{\omega_2^2-\omega_1^2}\frac{1}{\Omega^2-\omega_2^2} + \varepsilon \end{aligned}$$

where ε is regular and does not have any singularity on the real axis. On the other hand

$$\frac{1}{\Omega^2-\omega_j^2} = \frac{1}{2\omega_j}\cdot\left\{\frac{1}{\Omega-\omega_j}-\frac{1}{\Omega+\omega_j}\right\}\ ; \qquad j=1,2$$

and

$$\frac{1}{\Omega^2-\omega_j^2} = -\frac{2\hbar i}{2\omega_j}\{\delta(\omega-\omega_j)-\delta(\omega+\omega_j)\}\ .$$

We thus get from Eq. (1.28)

$$\begin{aligned} I_{p_\alpha,p_\beta} &= \frac{1}{2}\delta_{\alpha,\beta}\left\{\frac{\hbar\omega_1}{1-e^{-\beta\hbar\omega_1}}\delta(\omega-\omega_1)+\frac{\hbar\omega_1}{e^{\beta\hbar\omega_1}-1}\delta(\omega+\omega_1)\right\}\frac{m(\nu^2-\omega_1^2)}{\omega_2^2-\omega_1^2} \\ &+ \frac{1}{2}\delta_{\alpha,\beta}\left\{\frac{\hbar}{1-e^{-\beta\hbar\omega_2}}\delta(\omega-\omega_2)+\frac{\hbar}{e^{\hbar\omega_2}-1}\delta(\omega+\omega_2)\right\}\frac{m\omega_2(\omega_2^2-\nu^2)}{\omega_2^2-\omega_1^2}\ . \end{aligned}$$

In view of Eq. (1.29), in the limit $\omega_1 \to 0$ when $\eta \to 0$,

$$\frac{\hbar\omega_1}{1-e^{-\beta\hbar\omega_1}} \longrightarrow \frac{1}{\beta} = \theta\ , \qquad \frac{\hbar\omega_1}{e^{\beta\hbar\omega_1}-1} \longrightarrow \frac{1}{\beta} = \theta\ ,$$

$$\omega_2 \longrightarrow \mu = \sqrt{\frac{K_0^2}{m}+\nu^2}\ .$$

Thus, by performing in Eq. (1.30) the limiting process $\eta \to 0$ we finally get

$$\begin{aligned} I_{p_\alpha,p_\beta}(\omega) &= \delta_{\alpha,\beta}\frac{m^2\theta}{\left(\frac{K_\Omega}{\nu}\right)^2 + m}\delta(\omega) \\ &\quad + \frac{K_0^2\delta_{\alpha,\beta}}{2\mu}\left\{\frac{\hbar}{1-e^{-\beta\hbar\mu}}\delta(\omega-\mu) + \frac{\hbar}{e^{\beta\hbar\mu}-1}\delta(\omega+\mu)\right\}, \end{aligned} \tag{1.30}$$

which yields

$$\begin{aligned} \langle p_\alpha(t)p_\beta(\tau)\rangle_{\text{eq}} &= 0, \quad \alpha \neq \beta \\ \langle p_\alpha(t)p_\alpha(\tau)\rangle_{\text{eq}} &= \frac{m^2\theta}{m + \left(\frac{K_\Omega}{\nu}\right)^2} \\ &\quad + \frac{K_0^2}{2\mu}\left\{\frac{\hbar}{1-e^{-\beta\hbar\mu}}e^{-i\mu(t-\tau)} + \frac{\hbar}{e^{\beta\hbar\mu}-1}e^{i\mu(t-\tau)}\right\}. \end{aligned} \tag{1.31}$$

Consider now the more general case when $\nu(f)$ becomes a continuous spectrum in the limit $V \to \infty$.

Let us return to Eq. (1.25). We have

$$I_{p_\alpha,p_\beta}(\omega) = \delta_{\alpha,\beta}m\frac{i\hbar\omega}{2\pi(1-e^{-\beta\hbar\omega})}\frac{1}{\omega}f_\eta(\Omega)\Big|_{\omega-i0}^{\omega+i0} \tag{1.32}$$

where

$$-f_\eta(\Omega) = \frac{\Omega\Delta(\Omega)-\eta^2}{m\Omega^2-\eta^2+\Omega\Delta(\Omega)}.$$

We see that

$$f_\eta(0) = -1; \qquad f_\eta(\Omega)\Big|_{\omega-i0}^{\omega+i0} = 0, \quad \text{for sufficiently small } \omega.$$

Therefore for sufficiently small ω:

$$\begin{aligned} \frac{1}{\Omega}f_\eta(\Omega)\Big|_{\omega-i0}^{\omega+i0} &= f_\eta(\omega)\left(\frac{1}{\omega+i\varepsilon} - \frac{1}{\omega-i\varepsilon}\right) = -2\pi i f_\eta(\omega)\delta(\omega) \\ &= 2\pi i\delta(\omega). \end{aligned}$$

Note that $\frac{1}{\Omega}$ has only one singular point $\Omega = 0$. For this reason, for arbitrary real ω:

$$\frac{1}{\Omega}f_\eta(\Omega)\Big|_{\omega-i0}^{\omega+i0} = +2\pi i\delta(\omega) + \frac{1}{\Omega}f_\eta(\Omega)\Big|_{\omega-i0}^{\omega+i0}$$

or

$$\frac{1}{\omega}f_\eta(\Omega)\Big|_{\omega-i0}^{\omega+i0} = -2\pi i\delta(\omega) + \frac{1}{\Omega}f_\eta(\Omega)\Big|_{\omega-i0}^{\omega+i0}.$$

Thus Eq. (1.32) yields:

$$\mathcal{I}_{p_\alpha,p_\beta}(\omega) = \delta_{\alpha,\beta}\frac{i\hbar\omega m}{2\pi(1-e^{-\beta\hbar\omega})}\left\{ -2\pi i\delta(\omega) + \frac{1}{\Omega}f_\eta(\Omega)\Big|_{\omega-i0}^{\omega+i0}\right\}.$$

But the function

$$\frac{h\Omega}{1-e^{-\beta h\Omega}}$$

is regular in the neighbourhood of the real axis and because of this

$$\frac{h\omega}{1-e^{-\omega\beta h}}\frac{1}{\Omega}f_\eta(\Omega)\Big|_{\omega-i0}^{\omega+i0} = \frac{\hbar}{1-e^{-\beta\Omega\hbar}}f_\eta(\Omega)\Big|_{\omega-i0}^{\omega+i0}.$$

Therefore

$$\mathcal{I}_{p_\alpha,p'_\alpha}(\omega) = 0\,, \qquad \alpha \neq \alpha'\,;$$
$$\mathcal{I}_{p_\alpha,p_\alpha}(\omega) = m\theta\delta(\omega) - m\frac{i\hbar}{2\pi(1-e^{-\hbar\beta\Omega})}\frac{\Omega\Delta(\Omega)-\eta^2}{m\Omega-\eta^2+\Omega\Delta(\Omega)}\Big|_{\omega-i0}^{\omega+i0}.$$

We thus have

$$\langle p_\alpha(t)p_{\alpha'}(\tau)\rangle_{\mathrm{eq}} = 0\,, \quad \alpha \neq \alpha'\,;$$
$$\langle p_\alpha(t)p_\alpha(\tau)\rangle_{\mathrm{eq}} = m\theta - \int_{-\infty}^{\infty}\frac{i\hbar m e^{-i\Omega(t-\tau)}}{2\pi(1-e^{-\hbar\beta\Omega})}\frac{\Omega\Delta(\Omega)-\eta^2}{m\Omega^2-\eta^2+\Omega\Delta(\Omega)}\Big|_{\omega-i0}^{\omega+i0}d\omega\,. \tag{1.33}$$

Consider the function

$$\begin{aligned} f_\eta(\Omega) &= -\frac{\Omega\Delta(\Omega)-\eta^2}{m\Omega^2-\eta^2+\Omega\Delta(\Omega)} \\ &= -1+\frac{m\Omega^2}{m\Omega^2-\eta^2+\Omega\Delta(\Omega)} \\ &= -1+\frac{m\Omega}{m\Omega+\Delta(\Omega)-\frac{\eta^2}{\Omega}} \end{aligned}$$

for $\Omega = \varepsilon + i\omega$ and $\Omega = -\varepsilon + i\omega$; $\varepsilon > 0$.
In virtue of Eq. (1.18),

$$\begin{aligned} &-\operatorname{Im}\Delta(\omega+i\varepsilon) \\ &= \frac{\pi\varepsilon}{V}\sum_f \frac{S^2(f)}{6\nu^2(f)}f^2\left\{\frac{1}{(\nu(f)+\omega)^2+\varepsilon^2}+\frac{1}{(\nu(f)-\omega)^2+\varepsilon^2}\right\} > 0\,. \end{aligned}$$

Furthermore

$$\mathrm{Im}\ -\frac{\eta^2}{\Omega} = \pi\frac{\eta^2\varepsilon}{\omega^2+\varepsilon^2} > 0 \ .$$

Therefore

$$\mathrm{Im}\ \left(m\Omega + \Delta(\Omega) - \frac{\eta^2}{\Omega}\right) > \varepsilon\ , \quad \Omega = \omega + i\varepsilon$$

and

$$\left|m\Omega + \Delta(\Omega) - \frac{\eta^2}{\Omega}\right| > \varepsilon\ . \tag{1.34}$$

In the same manner, we have

$$\left|\mathrm{Im}\ \Omega + \Delta(\Omega) - \frac{\eta^2}{\Omega}\right| > \varepsilon\ , \qquad \text{where } \varepsilon = -\mathrm{Im}\ \Omega > 0\ .$$

We thus see that the function $f_\eta(\Omega)$ of the complex variable Ω is regular in the two half-planes

$$\begin{aligned} &\mathrm{Im}\ \Omega > 0\ , \\ &\mathrm{Im}\ \Omega < 0\ . \end{aligned} \tag{1.35}$$

Further let us note that the poles of the function

$$\frac{1}{1-e^{-\beta\hbar\Omega}}$$

in the region (1.35) nearest to the real axis are respectively

$$\Omega = \frac{2\pi i}{\hbar\beta}\ ; \qquad \Omega = -\frac{2\pi i}{\hbar\beta}\ .$$

Hence if we have a normal closed contour C in the region

$$0 < \mathrm{Im}\ \Omega < \frac{2\pi}{\hbar\beta}$$

or in the region

$$0 > \mathrm{Im}\ \Omega > \frac{2\pi}{\hbar\beta}\ ,$$

then

$$\int_C \frac{e^{-i\Omega(t-\tau)}}{1-e^{-\hbar\beta\Omega}} f_\eta(\Omega) d\Omega = 0\ .$$

Writing down Eq. (1.18),

$$\Delta(\Omega) = \frac{-1}{V}\sum_f \frac{S^2(f)}{6\nu^2(f)} f^2 \left\{ \frac{1}{\nu(f)+\Omega} + \frac{1}{\Omega-\nu(f)} \right\}, \tag{1.36}$$

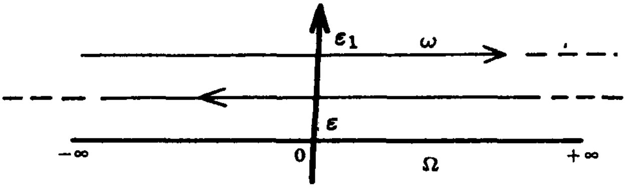
we see that it is an expression which contains only a finite number of terms (f) when V is held fixed. Therefore for sufficiently large $|\Omega|$

$$|\Omega \cdot \Delta(\Omega)| \leq \text{const} \qquad |\text{Im } \Omega| \geq \varepsilon > 0 \tag{1.37}$$

and

$$|\Delta(\Omega)| \leq \text{const.}$$

$$0 < \varepsilon < \varepsilon_1 < \frac{2\pi}{\hbar\beta} .$$



We thus take for C an infinite contour

$$i\varepsilon_1 - \infty < \vec{\omega} < i\varepsilon_1 + \infty$$
$$i\varepsilon - \infty < \overleftarrow{\omega} < i\varepsilon + \infty$$

and obtain

$$-\frac{mi\hbar}{2\pi}\int_{i\varepsilon_1-\infty}^{i\varepsilon_1+\infty} \frac{e^{-i\Omega(t-\tau)}}{1-e^{-\hbar\beta\Omega}} \frac{\Omega\Delta(\Omega)-\eta^2}{M\Omega^2-\eta^2+\Omega\Delta(\Omega)} d\Omega$$
$$+\frac{mi\hbar}{2\pi}\int_{i\varepsilon-\infty}^{i\varepsilon+\infty} \frac{e^{-i\Omega(t-\tau)}}{1-e^{-\hbar\beta\Omega}} \frac{\Omega\Delta(\Omega)-\eta^2}{M\Omega^2-\eta^2+\Omega\Delta(\Omega)} d\Omega$$

from which it follows that the integral

$$-\frac{mi\hbar}{2\pi}\int_{i\varepsilon-\infty}^{i\varepsilon+\infty} \frac{e^{-i\Omega(t-\tau)}}{1-e^{-\hbar\beta\Omega}} \frac{\Omega\Delta(\Omega)-\eta^2}{M\Omega^2-\eta^2+\Omega\Delta(\Omega)} d\Omega$$

does not depend upon ε when

$$0 < \varepsilon < \frac{2\pi}{\hbar\beta} \, . \tag{1.38}$$

In the same way, we see that the integral taken over the interval $(-i\varepsilon - \infty, -i\varepsilon + \infty)$ does not depend upon ε when ε is in the region (1.38). We can write Eq. (1.33) in the form

$$\begin{aligned} \langle p_\alpha(t)p_\alpha(\tau)\rangle_{\mathrm{eq}} = m\theta &- \frac{i\hbar m}{2\pi}\int_{i\varepsilon-\infty}^{i\varepsilon+\infty} \frac{e^{-i\Omega(t-\tau)}}{1-e^{-\hbar\beta\Omega}} \frac{\Omega\Delta(\Omega)-\eta^2}{m\Omega-\eta^2+\Omega\Delta(\Omega)}d\Omega \\ &+ \frac{i\hbar m}{2\pi}\int_{-i\varepsilon-\infty}^{-i\varepsilon+\infty} \frac{e^{-i\Omega(t-\tau)}}{1-e^{-\hbar\beta\Omega}} \frac{\Omega\Delta(\Omega)-\eta^2}{m\Omega^2-\eta^2+\Omega\Delta(\Omega)}d\Omega \, . \end{aligned}$$

In view of Eqs. (1.34) and (1.37) we may go to the limit $\eta \to 0$ and write

$$\begin{aligned} \langle p_\alpha(t)p_\alpha(\tau)\rangle_{\mathrm{eq}} = m\theta &- \frac{i\hbar m}{2\pi}\int_{i\varepsilon-\infty}^{i\varepsilon+\infty} \frac{e^{-i\Omega(t-\tau)}}{1-e^{-\hbar\beta\Omega}} \frac{\Omega\Delta(\Omega)}{m\Omega+\Delta(\Omega)}d\Omega \\ &+ \frac{i\hbar m}{2\pi}\int_{-i\varepsilon-\infty}^{i\varepsilon+\infty} \frac{e^{-i\Omega(t-\tau)}}{1-e^{-\hbar\beta\Omega}} \frac{\Delta(\Omega)}{m\Omega+\Delta(\Omega)}d\Omega \, . \end{aligned} \tag{1.39}$$

Consider now the standard limiting process $V \to \infty$. From Eq. (1.18) we have

$$\Delta(\Omega) = -\int_{-\infty}^{\infty} E_V(\nu)\frac{d\nu}{\Omega-\nu}$$

where

$$\begin{aligned} &E_V(\omega) = \frac{1}{V}\sum \frac{S^2(f)}{6\nu^2(f)} f^2\{\delta(\nu(f)+\omega)+\delta(\nu(f)-\omega)\} \, , \\ &E_V(\omega) \geq 0 \, ; \qquad E_V(-\omega) = E_V(\omega) \, . \end{aligned}$$

Suppose that this generalised function $E_V(\omega)$ tends to

$$\underset{V \longrightarrow \infty}{E_V(\omega) \longrightarrow} E(\omega) = \frac{1}{(2\pi)^3}\int \frac{S^2(f)}{6\nu^2(f)} f^2\{\delta(\nu(f)+\omega)+\delta(\nu(f)-\omega)\}d\mathbf{f}$$

in such a way that

(i) the limit is taken uniformly in any finite interval of the region

$$i\varepsilon - \infty < \omega < i\varepsilon + \infty \, , \qquad \varepsilon > 0 \tag{1.40}$$

and

$$-i\varepsilon - \infty < \omega < -i\varepsilon + \infty \ , \qquad \varepsilon > 0$$

so that

$$\int_{-\infty}^{\infty} E_V(\nu)\frac{d\nu}{\Omega - \nu} \longrightarrow -\Delta_\infty(\Omega) = \int_{-\infty}^{\infty} \frac{E(\nu)d\nu}{\Omega - \nu} \ ; \tag{1.41}$$

(ii) for $|\mathrm{Im}\ \Omega| \geq \varepsilon$, $|\Omega\Delta(\Omega)| \leq K_\varepsilon$ where K_ε is a constant independent of V. In this situation we may go to the limit $V \to \infty$ in Eq. (1.39) and write

$$\begin{aligned}\langle p_\alpha(t)p_\alpha(\tau)\rangle &= m\theta - \frac{i\hbar m}{2\pi}\int_{i\varepsilon-\infty}^{i\varepsilon+\infty} \frac{e^{-i\Omega(t-\tau)}}{1-e^{-\beta\hbar\Omega}}\frac{\Delta_\infty(\Omega)}{m\Omega + \Delta_\infty(\Omega)}d\Omega \\ &\quad + \frac{i\hbar m}{2\pi}\int_{-i\varepsilon-\infty}^{-i\varepsilon+\infty} \frac{e^{-i\Omega(t-\tau)}}{1-e^{-\beta\hbar\Omega}}\frac{\Delta_\infty(\Omega)}{m\Omega + \Delta_\infty(\Omega)}d\Omega \\ &= m\theta - \frac{i\hbar m}{2\pi}\int_{-\infty}^{\infty} \frac{e^{-i\Omega(t-\tau)}}{1-e^{-\beta\hbar\Omega}}\frac{\Delta_\infty(\Omega)}{m\Omega + \Delta_\infty(\Omega)}\Bigg|_{\omega-i\varepsilon}^{\omega+i\varepsilon} d\omega \ .\end{aligned} \tag{1.42}$$

Here

$$\begin{aligned}\Delta_\infty(\Omega) &= -\int_{-\infty}^{\infty} \frac{E(\nu)}{\Omega - \nu}d\nu \\ E(\nu) &= E(-\nu) \geq 0\end{aligned} \tag{1.43}$$

and by virtue of (ii),

$$|\Omega\Delta_\infty(\Omega)| \leq K_\varepsilon \ , \qquad \text{for } |\mathrm{Im}\ \Omega| \geq \varepsilon \ . \tag{1.44}$$

The right hand side of Eq. (1.42) does not depend upon ε if ε is positive and sufficiently small. We thus may perform in Eq. (1.42) the limiting process $\varepsilon > 0$, $\varepsilon \to 0$ and obtain

$$\langle p_\alpha(t)p_\alpha(\tau)\rangle_{\mathrm{eq}} = m\theta - \frac{i\hbar m}{2\pi}\int_{-\infty}^{\infty} \frac{\omega}{1-e^{-\beta\hbar\omega}}e^{-i\omega t}\frac{1}{\Omega}\frac{\Delta_\infty(\Omega)}{m\Omega + \Delta_\infty(\Omega)}\Bigg|_{\omega-i0}^{\omega+i0} d\omega \ .$$

We assume that the discontinuity

$$\frac{1}{\Omega}\frac{\Delta_\infty(\Omega)}{m\Omega + \Delta_\infty(\Omega)}\Bigg|_{\omega-i0}^{\omega+i0}$$

is of the first order, so that if $F(\Omega)$ is an analytic function in the neighbourhood of the real axis (for example $F(\Omega) = \frac{\Omega}{1-e^{-\beta\hbar\Omega}}$), then

$$\left(F(\Omega) - F(\omega)\right)\frac{1}{\Omega}\frac{\Delta_\infty(\Omega)}{m\Omega + \Delta_\infty(\Omega)}\Bigg|_{\omega-i0}^{\omega+i0} = 0 \, .$$

As

$$-\frac{\Delta_\infty(\Omega)}{m\Omega + \Delta_\infty(\Omega)} = -1 + \frac{m\Omega}{m\Omega + \Delta_\infty(\Omega)}$$

and

$$-\frac{i\hbar m}{2\pi}\frac{\omega}{1 - e^{-\beta\omega\hbar}}\frac{1}{\Omega}\Bigg|_{\omega-i\epsilon}^{\omega+i\epsilon} = -\frac{m}{\beta}\delta(\omega) = -m\theta\delta(\omega)$$

we finally get

$$\langle p_\alpha(t)p_\alpha(\tau)\rangle_{\mathrm{eq}} = \int_{-\infty}^{\infty} \mathcal{I}(\omega)e^{-i\omega t}d\omega \, ,$$
$$\mathcal{I}(\omega) = \frac{i\hbar m^2}{2\pi}\frac{\omega}{1 - e^{-\beta\hbar\omega}}\frac{1}{m\Omega + \Delta_\infty(\Omega)}\Bigg|_{\omega-i0}^{\omega+i0} \tag{1.45}$$

From Eq. (1.43)

$$\Delta_\infty(\omega \pm i0) = -\int E(\nu)\mathcal{P}\left(\frac{1}{\omega - \nu}\right)d\nu \pm i\pi E(\omega)$$

it follows that

$$i\frac{1}{m\Omega + \Delta_\infty(\Omega)}\Bigg|_{\omega-i0}^{\omega+i0} \geq 0 \, .$$

Since

$$\frac{\omega}{1 - e^{-\beta\omega\hbar}} \geq 0 \, ,$$

we easily see that

$$\mathcal{I}(\omega) \geq 0 \, . \tag{1.46}$$

It is to be noted that if we take

$$E(\omega) = \frac{K_0^2}{2}\{\delta(\omega - \nu_0) + \delta(\omega - \nu_0)\} \, ,$$

we shall obtain from Eq. (1.45) our previous formula (1.31).

Let us now turn to the calculation of the free energy of the dynamical system under consideration,

$$F' = -\theta \ln \mathrm{Sp}\, e^{-\beta H}$$

The free energy of one particle of mass m not interacting with the phonons is

$$F_S = -\theta \ln \mathrm{Sp}\, e^{-\mathbf{p}^2\beta/2m} = -\theta \lim_{\eta \to 0} \ln \mathrm{Sp} \exp -\left(\frac{\mathbf{p}^2}{2m} + \frac{\eta^2}{2}\mathbf{r}^2\right)\beta$$

The free energy of Σ is given by

$$F_\Sigma = -\theta \ln \mathrm{Sp}\, e^{-H_\Sigma \beta} \,,$$

$$H_\Sigma = \frac{1}{2}\sum (p_f p_f^* + \nu^2(f) q_f q_f^*)$$

As these energies are well-known we need only to calculate that part of the total free energy which corresponds to the interaction of our particle with the phonon field

$$F_{\mathrm{int}} = F - F_S - F_\Sigma$$

In order to perform such a calculation let us introduce a parameter λ (between 0 and 1) in the total hamiltonian H

$$H(\lambda) = \frac{\mathbf{p}^2}{2m} + \frac{\eta^2\mathbf{r}^2}{2} + \frac{1}{6}\frac{1}{V}\sum_f \frac{\lambda^2 S_f^2 f^2}{\nu^2(f)}\mathbf{r}^2 + i\frac{1}{\sqrt{V}}\sum_f \lambda S_f q_f(\mathbf{f}\ \mathbf{r}) + H_\Sigma$$

We see that

$$H(0) = H_S + H_\Sigma \,,$$

$$H(1) = H \,,$$

and thus

$$\begin{aligned} F_{\mathrm{int}} &= \int_0^1 \frac{\partial F(\lambda)}{\partial \lambda} d\lambda = -\theta \int_0^1 \frac{\partial}{\partial \lambda} \ln \mathrm{Sp}\, e^{-\beta H(\lambda)} d\lambda \\ &= \int_0^1 \frac{\mathrm{Sp}\, \frac{\partial H}{\partial \lambda} e^{-\beta H(\lambda)}}{\mathrm{Sp}\, e^{-\beta H(\lambda)}} = \int_0^1 \langle \frac{\partial H}{\partial \lambda} \rangle_{\lambda,\mathrm{eq}} d\lambda \end{aligned} \tag{1.47}$$

Here the index λ in

$$\langle \cdot \quad \rangle_{\lambda,\mathrm{eq}}$$

indicates that averaging is performed with the Gibbs statistical operator, corresponding to $H(\lambda)$. On one hand, we have

$$\frac{\partial H(\lambda)}{\partial\lambda}=\frac{1}{3}\frac{1}{V}\sum_f\frac{\lambda S_f^2 f^2}{\nu^2(f)}\mathbf{r}^2+i\frac{1}{\sqrt{V}}\sum_f S_f q_f(\mathbf{f}\cdot\mathbf{r})\ ,$$

and on the other hand we may write the equation of motion (1.5) for the hamiltonian $H(\lambda)$ as

$$-m\frac{d^2\mathbf{r}}{dt^2}-\eta^2\mathbf{r}=\frac{1}{3}\frac{1}{V}\sum_f\frac{\lambda^2 S_f^2 f^2}{\nu^2(f)}\mathbf{r}+i\frac{1}{\sqrt{V}}\sum_f\lambda S_f q_f(\mathbf{f})\ .$$

Therefore

$$\lambda\Big\langle\frac{\partial H(\lambda)}{\partial\lambda}\Big\rangle_{\lambda,\mathrm{eq}}=-\Big\langle\Big(m\frac{d^2\mathbf{r}}{dt^2}+\eta^2\mathbf{r}\Big)\cdot\mathbf{r}\Big\rangle_{\lambda,\mathrm{eq}}\ . \tag{1.48}$$

In view of Eqs. (1.6), (1.10) and (1.24)

$$\begin{aligned}&\langle r_\alpha(t)r_{\alpha'}(\tau)\rangle_{\lambda,\mathrm{eq}}=0\ ,\qquad \alpha\neq\alpha'\ ;\\&\langle r_\alpha(t)r_\alpha(\tau)\rangle_{\lambda,\mathrm{eq}}=\frac{\hbar i}{2\pi}\int_{-\infty}^{\infty}\frac{e^{-i\omega(t-\tau)}}{1-e^{-\beta\omega\hbar}}\frac{1}{m\Omega^2-\eta^2+\Omega\lambda^2\Delta(\Omega)}\Bigg|_{\omega-i0}^{\omega+i0}d\omega\ ,\end{aligned} \tag{1.49}$$

because by changing H to $H(\lambda)$ we introduce a factor λ into S_f and thus $\Delta(\Omega)$ is to be replaced by $\lambda^2\Delta(\Omega)$.
Therefore

$$\begin{aligned}&\Big\langle\Big(-m\frac{d^2r_\alpha(t)}{dt^2}-\eta^2r_\alpha(t)\Big)r_\alpha(\tau)\Big\rangle\\&=\frac{i\hbar}{2\pi}\int_{-\infty}^{\infty}\frac{m\omega^2-\eta^2}{1-e^{-\beta\omega\hbar}}e^{-i\omega(t-\tau)}\frac{1}{m\Omega^2-\eta^2+\Omega\lambda^2\Delta(\Omega)}\Bigg|_{\omega-i0}^{\omega+i0}d\omega\\&=\frac{i\hbar}{2\pi}\int_{-\infty}^{\infty}\frac{e^{-i\omega(t-\tau)}}{1-e^{-\beta\omega\hbar}}\frac{m\Omega^2-\eta^2}{m\Omega^2-\eta^2+\Omega\lambda^2\Delta(\Omega)}\Bigg|_{\omega-i0}^{\omega+i0}d\omega\ ,\end{aligned}$$

and because of Eq. (1.48)

$$\lambda\Big\langle\frac{\partial H(\lambda)}{\partial\lambda}\Big\rangle_{\lambda,\mathrm{eq}}=3\frac{i\hbar}{2\pi}\int_{-\infty}^{\infty}\frac{1}{1-e^{-\beta\omega\hbar}}\frac{m\Omega^2-\eta^2}{m\Omega^2-\eta^2+\Omega\lambda^2\Delta(\Omega)}\Bigg|_{\omega-i0}^{\omega+i0}d\omega\ .$$

Note that

$$\frac{m\Omega^2-\eta^2}{m\Omega^2-\eta^2+\Omega\lambda^2\Delta(\Omega)}=1-\frac{\Omega\lambda^2\Delta(\Omega)}{m\Omega^2-\eta^2+\Omega\lambda^2\Delta(\Omega)}\,,$$

$$\left.\frac{m\Omega^2-\eta^2}{m\Omega^2-\eta^2+\Omega\lambda^2\Delta(\Omega)}\right|_{\omega-i0}^{\omega+i0}=-\left.\frac{\Omega\lambda^2\Delta(\Omega)}{m\Omega^2-\eta^2+\Omega\lambda^2\Delta(\Omega)}\right|_{\omega-i0}^{\omega+i0}.$$

Therefore Eq. (1.48) yields

$$\left\langle\frac{\partial H(\lambda)}{\partial\lambda}\right\rangle_{\lambda,\mathrm{eq}}=-3\frac{i\hbar}{2\pi}\int_{-\infty}^{\infty}\frac{1}{1-e^{-\beta\omega\hbar}}\left.\frac{\Omega\lambda\Delta(\Omega)}{m\Omega^2-\eta^2+\lambda^2\Omega\Delta(\Omega)}\right|_{\omega-i0}^{\omega+i0}d\omega$$

By applying literally the reasoning used for the calculation of $\langle p_\alpha(t)p_\alpha(\tau)\rangle_{\mathrm{eq}}$, we get in the limit $\eta\to 0$, $V\to\infty$

$$\left\langle\frac{\partial H(\lambda)}{\partial\lambda}\right\rangle_{\lambda,\mathrm{eq}}=-\frac{3i\hbar}{2\pi}\int_{-\infty}^{\infty}\frac{\Omega}{1-e^{-\beta\hbar\Omega}}\frac{1}{\Omega}\left.\frac{\lambda\Delta_\infty(\Omega)}{m\Omega+\lambda^2\Delta_\infty(\Omega)}\right|_{\omega-i\varepsilon}^{\omega+i\varepsilon}d\omega\,. \qquad (1.50)$$

The right hand side does not depend on ε when $0<\varepsilon<\frac{2\pi}{\hbar\beta}$. So, putting $\varepsilon>0$, $\varepsilon\to 0$ from Eq. (1.47) we obtain

$$F_{\mathrm{int}}=-\frac{3i\hbar}{2\pi}\int_0^1 d\lambda\int_{-\infty}^{\infty}\frac{\Omega}{1-e^{-\beta\hbar\Omega}}\frac{1}{\Omega}\left.\frac{\lambda\Delta_\infty(\Omega)}{m\Omega+\lambda^2\Delta_\infty(\Omega)}\right|_{\omega-i0}^{\omega+i0}d\omega\,. \qquad (1.51)$$

Consider a special example

$$E(\omega)=\frac{K_0^2}{2}\{\delta(\omega-\nu_0)+\delta(\omega+\nu_0)\}\,, \qquad (1.52)$$

then

$$\Delta_\infty(\Omega)=-\frac{K_0^2\Omega}{\Omega^2-\nu^2}$$

and

$$-\frac{1}{\Omega}\frac{\lambda\Delta_\infty(\Omega)}{m\Omega+\lambda^2\Delta_\infty(\Omega)}=\frac{1}{\Omega}\frac{\lambda K_0^2}{m\Omega^2-(m\nu^2+\lambda^2K_0^2)}\,.$$

This expression has three poles

$$\Omega=0\,,\quad \Omega=\mu(\lambda)\,,\quad \Omega=-\mu(\lambda)\,;\quad \mu(\lambda)=\sqrt{\nu_0^2+\lambda^2\frac{K_0^2}{m}}\,.$$

Note that

$$\frac{1}{\Omega^2-\mu^2(\lambda)}=\frac{1}{2\mu(\lambda)}\left\{\frac{1}{\Omega-\mu(\lambda)}-\frac{1}{\Omega+\mu(\lambda)}\right\}.$$

We then see that

$$\begin{aligned}&-\frac{1}{\Omega}\frac{\lambda\Delta_\infty(\Omega)}{m\Omega+\lambda^2\Delta_\infty(\Omega)}\Bigg|_{\omega-i0}^{\omega+i0}\,.\\ &=\frac{2\pi i\delta(\omega)\lambda K_0^2}{m\nu_0^2+\lambda^2K_0^2}-\frac{2\pi\lambda K_0^2 i}{2\mu^2(\lambda)m}\{\delta(\omega-\mu(\lambda))+\delta(\omega+\mu(\lambda))\}\end{aligned}$$

and.

$$\begin{aligned}&-\frac{3i\hbar}{2\pi}\int_{-\infty}^{\infty}\frac{\Omega}{1-e^{-\beta\hbar\Omega}}\frac{1}{\Omega}\frac{\lambda\Delta_\infty(\Omega)}{m\Omega+\lambda^2\Delta_\infty(\Omega)}\Bigg|_{\omega-i0}^{\omega+i0}d\omega\\ &=-3\theta\frac{\lambda K_0^2}{m\nu_0^2+\lambda^2K_0^2}+\frac{3\lambda K_0^2\hbar}{2m\mu(\lambda)}\left\{\frac{1}{1-e^{-\beta\hbar\mu(\lambda)}}+\frac{e^{-\beta\hbar\mu(\lambda)}}{1-e^{-\beta\hbar\mu(\lambda)}}\right\}\\ &=-3\theta\frac{\lambda K_0^2}{m\nu_0^2+\lambda^2K_0^2}+\frac{3\lambda K_0^2\hbar}{2m\mu(\lambda)}+\frac{3\lambda K_0^2\hbar}{m\mu(\lambda)}\frac{e^{-\beta\hbar\mu(\lambda)}}{1-e^{-\beta\hbar\mu(\lambda)}}\\ &=\frac{d}{d\lambda}\left\{-\frac{3\theta}{2}\ln(m\nu_0^2+\lambda^2K_0^2)+\frac{3\hbar}{2}\frac{\partial\mu(\lambda)}{\partial\lambda}+3\theta\ln(1-e^{-\beta\hbar\mu(\lambda)})\right\}\,.\end{aligned}$$

Therefore

$$\begin{aligned}F_{\text{int}}&=-3\theta\ln\sqrt{\frac{m+\frac{K_0^2}{\nu_0^2}}{m}}+\frac{3\hbar}{2}(\mu-\nu)-3\theta\ln\frac{1-e^{-\beta\hbar\nu_0}}{1-e^{-\beta\hbar\mu}}\,,\\ \mu&=\sqrt{\nu_0^2+\frac{K_0^2}{m}}\qquad\qquad(\lambda=1)\,.\end{aligned}\tag{1.53}$$

As we have seen, all the Green's functions and correlation functions corresponding to the particle S as well as F_{int} are defined by $E(\nu)$ and the influence of the photon field on these quantities is also specified only by the spectral intensity $E(\nu)$. Therefore, if we have two different systems of oscillators interacting with our particle (in the way considered) for which $E(\nu)$ will be the same, all mentioned quantities will remain unchanged.

Consider for example the two-body problem

$$\begin{aligned}\mathcal{H}&=\frac{\mathbf{p}^2}{2m}+\frac{K_0^2}{2}(\mathbf{r}-\mathbf{R})^2+\frac{\mathbf{P}^2}{2M}=\sum_{\alpha=1}^{3}\mathcal{H}_\alpha\,,\\ \mathcal{H}_\alpha&=\frac{p_\alpha^2}{2m}+\frac{K_0^2}{2}(r_\alpha-R_\alpha)^2+\frac{P_\alpha^2}{2M}\,,\end{aligned}$$

and the corresponding one-body hamiltonian

$$H_S = \frac{\mathbf{p}^2}{2m} = \frac{1}{2m}\sum_{\alpha=1}^{3} p_\alpha^2 ,$$
$$H_\Sigma = \frac{\mathbf{P}^2}{2M} + \frac{K_0^2}{2}\mathbf{R}^2 = \sum_{\alpha=1}^{3}\left(\frac{P_\alpha^2}{2M} + \frac{K_0^2}{2}R_2^2\right) .$$

Let us compute

$$F_{\text{int}} = -\theta \ln \frac{\operatorname{Sp} e^{-H\beta}}{\operatorname{Sp} e^{-H_S\beta}\operatorname{Sp} e^{-H_\Sigma\beta}} ,$$

where the one-dimensional hamiltonians $\mathcal{H}, \mathcal{H}_S, \mathcal{H}_\Sigma$ are

$$\mathcal{H} = \frac{1}{2m}p^2 + \frac{K_0^2}{2}(x-X)^2 + \frac{1}{2M}P^2 ,$$
$$\mathcal{H}_S = \frac{1}{2m}p^2 ; \qquad \mathcal{H}_\Sigma = \frac{1}{2M}P^2 + \frac{1}{2}K_0^2 X^2 .$$

To diagonalize the one-dimensional hamiltonian $\mathcal{H}$, we introduce normal coordinates q, Q and corresponding momenta y, Y:

$$\frac{mx + MX}{m+M} = q , \qquad x - X = Q . \tag{1.54}$$

Noticing that

$$\frac{\partial}{\partial x} = \frac{m}{m+M}\frac{\partial}{\partial q} + \frac{\partial}{\partial Q} ,$$
$$\frac{\partial}{\partial X} = \frac{M}{m+M}\frac{\partial}{\partial q} - \frac{\partial}{\partial Q} ,$$

we put

$$\begin{aligned} p &= \frac{m}{m+M}y + Y , \\ P &= \frac{M}{m+M}y - Y . \end{aligned} \tag{1.55}$$

We have

$$\mathcal{H} = \frac{1}{2(m+M)}y^2 + \frac{1}{2}\frac{M+m}{Mm}Y^2 + \frac{K_0^2}{2}Q^2 = \mathcal{H}_{\text{in}} + \mathcal{H}_{\text{osc}} ,$$
$$\mathcal{H}_{\text{in}} = \frac{y^2}{2(m+M)} ; \qquad \mathcal{H}_{\text{osc}} = \frac{1}{2}\frac{M+m}{Mm}Y^2 + \frac{K_0^2}{2}Q^2 .$$

Therefore

$$F_{\text{int}} = -3\theta \ln \frac{\mathrm{Sp}\, e^{-\mathcal{H}_{\text{in}}\beta}}{\mathrm{Sp}\, e^{-\mathcal{H}_S\beta}} - 3\theta \frac{\ln \mathrm{Sp}\, e^{-\mathcal{H}_{\text{osc}}\beta}}{\ln \mathrm{Sp}\, e^{-\mathcal{H}_\Sigma\beta}} \; .$$

The free energy of the one-dimensional oscillator H_Σ with frequency $\nu = \sqrt{K_0/M}$ is known to be

$$F_\Sigma = \frac{\hbar\nu}{2} - \theta \ln \frac{1}{1 - e^{-\beta\hbar\nu}} \; ,$$

and as the oscillator H has the frequency

$$\mu = \sqrt{\frac{K_0^2(M+m)}{Mm}} = \nu\sqrt{1 + \frac{M}{m}} \; ,$$

F_{osc} will be

$$F_{\text{osc}} = \frac{\hbar\mu}{2} - \theta \ln \frac{1}{1 - e^{-\beta\hbar\mu}} \; ; \quad \text{one-dimensional} \; .$$

So

$$F_{\text{int}} = -3\theta \ln \frac{\mathrm{Sp}\, e^{-\mathcal{H}_{\text{in}}\beta}}{\mathrm{Sp}\, e^{-\mathcal{H}_S\beta}} - 3\theta \ln \frac{1 - e^{-\beta\hbar\nu}}{1 - e^{-\beta\hbar\mu}} + \frac{3}{2}\hbar(\mu - \nu) \; .$$

As x is the coordinate in the interval $-\frac{L}{2} < x < \frac{L}{2}$, the proper value of the corresponding momentum will be $\frac{2\pi}{L}n\hbar$ and

$$\begin{aligned} \frac{\mathrm{Sp}\, e^{-\mathcal{H}_{\text{in}}\beta}}{\mathrm{Sp}\, e^{-\mathcal{H}_S\beta}} &= \frac{\sum\limits_n \exp\left\{ -\left(\frac{2\pi}{L}n\hbar\right)^2 \frac{\beta}{2(m+M)} \right\}}{\sum\limits_n \exp\left\{ -\left(\frac{2\pi}{L}n\hbar\right)^2 \frac{\beta}{2m} \right\}} \\ &\xrightarrow[L\to\infty]{} \frac{\left(\frac{1}{2\pi\hbar}\right)^3 \int_{-\infty}^{\infty} \exp\left\{ -\frac{\beta p^2}{2(m+M)} \right\} dp}{\left(\frac{1}{2\pi\hbar}\right)^3 \int_{-\infty}^{\infty} \exp\left\{ -\frac{\beta p^2}{2m} \right\} dp} \\ &= \sqrt{\frac{m+M}{m}} \; . \end{aligned}$$

So

$$F_{\text{int}} = -3\theta \ln \sqrt{\frac{m+M}{m}} + \frac{3}{2}\hbar(\mu - \nu) - 3\theta \ln \frac{1 - e^{-\beta\hbar\nu}}{1 - e^{-\beta\hbar\mu}} \; ,$$

which coincides with Eq. (1.53) if we take

$$\frac{K_0^2}{\nu^2} = M \; .$$

It is also easy to obtain formula (1.31) starting from the two-body problem by putting

$$y = i(a^\dagger - a)\left(\frac{\hbar \mathcal{M}\mu}{2}\right)^{\frac{1}{2}} ,$$
$$Q = (a^\dagger + a)\left(\frac{\hbar}{2\mathcal{M}\mu}\right)^{\frac{1}{2}} , \tag{1.56}$$

where $a, a^\dagger$ are Bose amplitudes, $\mathcal{M} = \frac{Mm}{M+m}$, and so μ is given by

$$\mu^2 = \frac{K_0^2}{\mathcal{M}} .$$

We further have

$$\mathcal{H}_{\rm osc} = \frac{\hbar\mu}{2} + \hbar\mu a^\dagger a$$

and

$$i\hbar\frac{da}{dt} = \hbar\mu a \; ; \qquad a(t) = e^{-i\mu t} ,$$
$$a^\dagger(t) = e^{-i\mu t}a^\dagger ,$$

as

$$\frac{dy}{dt} = 0 , \qquad y = \text{const} .$$

From Eq. (1.56),

$$p_\alpha(t) = \frac{m}{m+M}y + i(a^\dagger e^{i\mu t} - ae^{-i\mu t})\left(\frac{\hbar\mathcal{M}\mu}{2}\right)^{\frac{1}{2}} . \tag{1.57}$$

Hence

$$\langle p_\alpha(t)p_\alpha(\tau)\rangle_{\rm eq} = \left(\frac{m}{m+M}\right)^2\langle y^2\rangle_{\rm eq} + \frac{\hbar\mathcal{M}\mu}{2}\left(\langle aa^\dagger\rangle e^{-i\mu(t-\tau)} + \langle a^\dagger a\rangle e^{i\mu(t-\tau)}\right) .$$

Since

$$\langle y^2\rangle_{\rm eq} = (m+M)\theta ,$$
$$\langle aa^\dagger\rangle = \frac{1}{1-e^{-\hbar\beta\mu}} , \qquad \langle a^\dagger a\rangle = \frac{1}{e^{\hbar\beta\mu}-1} ,$$
$$\mathcal{M}_\mu = \frac{\mathcal{M}\mu^2}{\mu} = \frac{K_0^2}{\mu} ,$$

we see that Eq. (1.31) results. Thus the correlation equilibrium (two-time) averages corresponding to S-particle for the hamiltonian Eq. (1.1) are the same as for two-body problem Eqs. (1.54–1.57) in the "one frequency" case, that is, when $\nu(f) = \nu$ or $E(\omega) = \frac{K^2}{2}[\delta(\omega - \nu_0) + \delta(\omega + \nu_0)]$.

Let us return now to the expression of the F_{int} in this case and consider it in the limit of classical mechanics. By putting in Eq. (1.53) $\hbar \to 0$ we get the classical value $F_{\text{int}} = 0$. It is easy to see that zero value of F_{int} occurs always in classical mechanics for dynamical systems characterized by the hamiltonian 1 with value of K^2. This fact may be established directly, starting from Eq. (1.50) which we rewrite in the form

$$\left\langle \frac{\partial H(\lambda)}{\partial \lambda} \right\rangle_{\lambda,\text{eq}} = -\frac{3i\hbar}{2\pi} \int_{-\infty}^{\infty} \frac{\Omega}{1 - e^{-\hbar\beta\Omega}} \frac{\lambda\Delta(\Omega)}{m\Omega^2 - \eta^2 + \lambda^2\Omega\Delta(\Omega)} \Bigg|_{\omega - i\varepsilon}^{\omega + i\varepsilon} d\omega\,, \tag{1.58}$$

where $0 < \varepsilon < \frac{2\pi}{\hbar\beta}$. In the classical limit,

$$\lim_{\hbar \to 0} \frac{\hbar\Omega}{1 - e^{-\hbar\beta\Omega}} = \frac{1}{\beta} = \theta\,.$$

So for classical mechanics we can write

$$\left\langle \frac{\partial H(\lambda)}{\partial \lambda} \right\rangle_{\lambda,\text{eq}} = -\frac{3i\theta}{2\pi} \left\{ \int_{i\varepsilon - \infty}^{i\varepsilon + \infty} F(\Omega)d\Omega - \int_{-i\varepsilon - \infty}^{-i\varepsilon + \infty} F(\Omega)d\Omega \right\}\,, \tag{1.59}$$

where

$$F(\Omega) = \frac{\lambda\Delta(\Omega)}{m\Omega^2 - \eta^2 + \lambda^2\Omega\Delta(\Omega)}\,. \tag{1.60}$$

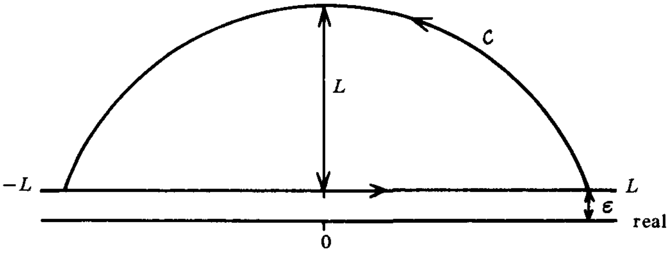
We see that $F(\Omega)$ is a regular analytic function in the half-plane

$$\text{Im}\,\Omega \geq \varepsilon > 0\,.$$

Therefore

$$\int_C F(\Omega)d\Omega = 0 \tag{1.61}$$

for any closed contour lying in this half-plane. Take for C the contour of the type



consisting of the interval $(i\varepsilon - R, i\varepsilon + R)$ and the semi-circle C with the centre at $i\varepsilon$ and radius R. As at C

$$F(\Omega) = \mathrm{O}\left(\frac{1}{L^2}\right) ,$$

we see that

$$\int_C F(\Omega)d\Omega = \mathrm{O}\left(\frac{1}{L}\right) \longrightarrow 0 .$$

Therefore

$$\int_{i\varepsilon-\infty}^{i\varepsilon+\infty} F(\Omega)d\Omega = 0 .$$

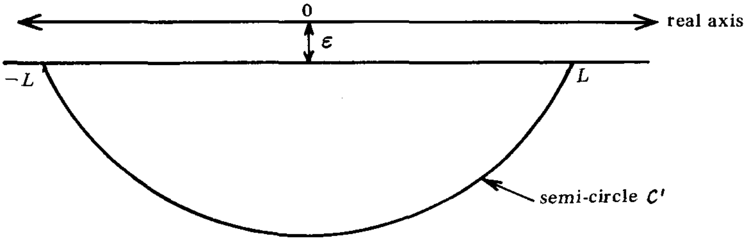
Similar reasoning may be applied to

$$\int_{-i\varepsilon-\infty}^{-i\varepsilon+\infty} F(\Omega)d\Omega = 0 .$$

In fact, $F(\Omega)$ is a regular analytic function in the half-plane

$$\mathrm{IM}\, \Omega \leq -\varepsilon < 0 .$$

We take the closed contour as follows:



and repeat the reasoning, then we will obtain

$$\int_{-i\varepsilon-\infty}^{-i\varepsilon+\infty} F(\Omega)d\Omega \; .$$

Using Eqs. (1.47) and (1.59), we get

$$F_{\text{int}} = 0 \; .$$

We wish to point out that this result is due entirely to classical mechanics. In quantum mechanics, Eq. (1.58) shows that the corresponding

$$F(\Omega) = \frac{\hbar\Omega}{1 - e^{-\beta\hbar\Omega}} \frac{\lambda\Delta(\Omega)}{m\Omega^2 - \eta^2 + \lambda^2\Delta(\Omega)}$$

has poles on the imaginary axis

$$\Omega = \frac{2\pi i n}{\beta\hbar} \; ; \qquad n\text{: integer} \; , \tag{1.62}$$

and for this reason the integrals of the type (1.61) will not be equal to zero (they will be equal to sum of residues of the corresponding poles in Eq. (1.62)).

Averages from T-Product

Let us now consider equilibrium averages of the form

$$\langle \mathrm{T}\{(r_\alpha(t) - r_\alpha(\tau)(r_{\alpha'}(t) - r_{\alpha'}(\tau))\}\rangle_{\text{eq}} \; ,$$

where T denotes the sign of the time-ordered product. As

$$\begin{aligned}(r_\alpha(t) &- r_\alpha(\tau))(r_{\alpha'}(t) - r_{\alpha'}(\tau)) \\ &= r_\alpha(t)r_{\alpha'}(t) - r_\alpha(\tau)r_{\alpha'}(t) - r_\alpha(t)r_{\alpha'}(\tau) + r_\alpha(\tau)r_{\alpha'}(\tau)\end{aligned}$$

we have

$$\begin{aligned}
&\mathrm{T}\{(r_\alpha(t) - r_\alpha(\tau))(r_{\alpha'}(t) - r_{\alpha'}(\tau))\} \\
&= \begin{cases} r_\alpha(t)r_{\alpha'}(t) - r_{\alpha'}(t)r_\alpha(\tau) - r_\alpha(t)r_{\alpha'}(\tau) + r_\alpha(\tau)r_{\alpha'}(\tau) & \text{if } t > \tau \\ r_\alpha(t)r_{\alpha'}(t) - r_\alpha(\tau)r_{\alpha'}(t) - r_{\alpha'}(\tau)r_\alpha(t) + r_\alpha(\tau)r_{\alpha'}(\tau) & \text{if } t < \tau \end{cases} .
\end{aligned} \tag{1.63}$$

Thus from Eq. (1.49) (putting $\lambda = 1$), we get

$$\langle \mathrm{T}\{(r_\alpha(t) - r_\alpha(\tau))(r_{\alpha'}(t) - r_{\alpha'}(\tau))\}\rangle_{\mathrm{eq}} = 0\,, \qquad \alpha \neq \alpha' \tag{1.64}$$

and

$$\begin{aligned}
&\langle \mathrm{T}\{(r_\alpha(t) - r_\alpha(\tau))^2\}\rangle \\
&= \frac{\hbar i}{2\pi}\int_{-\infty}^{\infty} \frac{2(1 - e^{-i\omega(t-\tau)})}{1 - e^{-\beta\omega\hbar}} \left.\frac{1}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)}\right|_{\omega - i0}^{\omega + i0} d\omega\,, \quad t > \tau\,;
\end{aligned}$$

$$\begin{aligned}
&\langle \mathrm{T}\{(r_\alpha(t) - r_\alpha(\tau))^2\}\rangle \\
&= \frac{\hbar i}{2\pi}\int_{-\infty}^{\infty} \frac{2(1 - e^{-i\omega(\tau-t)})}{1 - e^{-\beta\omega\hbar}} \left.\frac{1}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)}\right|_{\omega - i0}^{\omega + i0} d\omega\,, \quad t < \tau\,.
\end{aligned}$$

Therefore

$$\begin{aligned}
&\langle \mathrm{T}\{(r_\alpha(t) - r_\alpha(\tau))^2\}\rangle \\
&= \frac{\hbar i}{2\pi}\int_{-\infty}^{\infty} \frac{2(1 - e^{-i\omega(t-\tau)})}{1 - e^{-\beta\omega\hbar}} \left.\frac{1}{m\Omega^2 - \eta^2 + \Omega\Delta(\Omega)}\right|_{\omega - i0}^{\omega + i0} d\omega\,.
\end{aligned} \tag{1.65}$$

For some application it is useful to calculate the time-ordered product on "imaginary time". Put $t = -is$ and take real s as the order parameter:

$$\mathrm{T}\{r_\alpha(-is)r_{\alpha'}(-i\sigma)\} = \begin{cases} r_\alpha(-is)r_{\alpha'}(-i\sigma)\,, & s > \sigma \\ r_{\alpha'}(-i\sigma)r_\alpha(-is)\,, & s < \sigma \end{cases} .$$

By using Eq. (1.49) (with $\lambda = 1$) we obtain

$$\langle \mathrm{T}\{(r_\alpha(-is) - r_\alpha(-i\sigma))(r_{\alpha'}(-is) - r_{\alpha'}(-i\sigma))\}\rangle_{\mathrm{eq}} = 0\,, \qquad \alpha \neq \alpha' \tag{1.66}$$

and

$$\begin{aligned}&\langle \mathrm{T}\{(r_\alpha(-is)-r_\alpha(-i\sigma))^2\}\rangle_{\mathrm{eq}}\\&=\frac{\hbar i}{2\pi}\int_{-\infty}^{\infty}\frac{2(1-e^{-\omega|s-\sigma|})}{1-e^{-\hbar\omega\beta}}\,\frac{1}{m\Omega^2-\eta^2+\Omega\Delta(\Omega)}\Bigg|_{\omega-i0}^{\omega+i0}d\omega\ .\end{aligned}\tag{1.67}$$

Consider the "one-frequency" case:

$$E(\omega)=\frac{K_0^2}{2}\{\delta(\omega-\nu_0)+\delta(\omega+\nu_0)\}\ .$$

In this case we may not use directly the formulae (1.65) and (1.67) and remark that the result will be the same as for the two-body model (1.54).

We have

$$\langle r_\alpha(t)r_\alpha(\tau)\rangle_{\mathrm{eq}}=\langle x(t)x(\tau)\rangle_{\mathrm{eq}}$$

and from Eq. (1.46)

$$x=q-\frac{M}{m+M}Q\ .$$

As the evolutions $q(t)$ and $Q(t)$ are described by independent hamiltonians H_{in} and H_{osc} respectively, we have

$$\langle x(t)x(\tau)\rangle_{\mathrm{eq}}=\langle q(t)q(\tau)\rangle_{\mathrm{eq}}+\frac{M^2}{(m+M)^2}\langle Q(t)Q(\tau)\rangle_{\mathrm{eq}}\ .$$

Hence

$$\begin{aligned}&\langle \mathrm{T}\{(r_\alpha(-is)-r_\alpha(-i\sigma))^2\}\rangle_{\mathrm{eq}}\\&=\langle \mathrm{T}\{(q(-is)-q(-i\sigma))^2\}\rangle_{\mathrm{eq}}+\frac{M}{(m+M)^2}\langle \mathrm{T}\{(Q(-is)-Q(-i\sigma))^2\}\rangle_{\mathrm{eq}}\ .\end{aligned}\tag{1.68}$$

Note that because of Eq. (1.67)

$$\begin{aligned}q(t)-q(\tau)&=\frac{(t-\tau)}{(M+m)}y\ ,\qquad y=\text{const.}\\\langle y^2\rangle_{\mathrm{eq}}&=(m+M)\theta\ ,\end{aligned}$$

thus

$$\langle (q(t)-q(\tau))^2\rangle=\frac{(t-\tau)^2\theta}{M+m}\ .\tag{1.69}$$

We also have

$$q(t)q(\tau) - q(\tau)q(t) = \int_\tau^t \{q'(t)q(\tau) - q(\tau)q'(t)\}dt$$
$$= \frac{1}{M+m}\int_\tau^t (yq(\tau) - q(\tau)y)dt$$
$$= \frac{t\cdot\tau}{M+m}(yq - qy) = i\hbar\frac{t-\tau}{M+m} \;. \tag{1.70}$$

So

$$\langle \mathrm{T}\{(q(-is) - q(-i\sigma))^2\}\rangle_{\mathrm{eq}} = \langle q^2(-is) - 2q(-is)q(-i\sigma) + q^2(-i\sigma)\rangle_{\mathrm{eq}}$$
$$= \langle (q(-is) - q(-i\sigma))^2\rangle_{\mathrm{eq}} + \langle -q(-is)q(-i\sigma) + q(-i\sigma)q(-is)\rangle_{\mathrm{eq}} \;, \quad \text{if } s > \sigma \;,$$

and in virtue of Eqs. (1.69) and (1.70)

$$\langle \mathrm{T}\{(q(-is) - q(-i\sigma))^2\}\rangle_{\mathrm{eq}} = -\frac{(s-\sigma)^2\theta}{M+m} + \frac{\hbar}{M+m}(s-\sigma)\,, \quad \text{if } s > \sigma \;.$$

By interchanging s and σ it is easy to see that

$$\langle \mathrm{T}(q(-is) - q(-i\sigma))^2\}\rangle_{\mathrm{eq}} = -\frac{(s-\sigma)^2\theta}{M+m} + \frac{\hbar}{M+m}|s-\sigma| \;. \tag{1.71}$$

Now to calculate the left hand side of Eq. (1.68) one must find the expression for

$$\langle \mathrm{T}\{(Q(-is) - Q(-i\sigma))^2\}\rangle_{\mathrm{eq}} \;.$$

Note that

$$Q(t) = (e^{i\mu t}a^\dagger + e^{-i\mu t}a)\left(\frac{\hbar}{2M\mu}\right)^{\frac{1}{2}} \;.$$

From which it follows that

$$\mathrm{T}\{(Q(-is) - Q(i\sigma))^2\}$$
$$= \frac{\hbar}{2M\mu}\{(e^{\mu s}a^\dagger + e^{-\mu s}a)(e^{\mu s}a^\dagger + e^{-\mu s}a) + (e^{\mu\sigma}a^\dagger + e^{-\mu\sigma}a)(e^{\mu\sigma}a^\dagger + e^{-\mu\sigma}a)$$
$$+ 2\mathrm{T}((e^{\mu s}a^\dagger + e^{-\mu s}a)(e^{\mu\sigma}a^\dagger + e^{-\mu\sigma}a))\} \;.$$

Therefore

$$\langle \mathrm{T}\{(Q(-is) - Q(-i\sigma))^2\}\rangle_{\mathrm{eq}}$$
$$= \frac{\hbar}{2M\mu}\{2\langle a^\dagger a\rangle + 2\langle aa^\dagger\rangle - 2e^{\mu|s-\sigma|}\langle a^\dagger a\rangle - 2e^{-\mu|s-\sigma|}\langle aa^\dagger\rangle\} \;, \tag{1.72}$$

here

$$\langle a^\dagger a\rangle = \frac{1}{e^{\hbar\beta\mu}-1}\,, \qquad \langle a a^\dagger\rangle = 1 + \frac{1}{e^{\hbar\beta\mu}-1}\,.$$

By noting that

$$\frac{1}{m+M} = \frac{1}{mM}\mathcal{M} = \frac{K_0^2}{\mu^2 Mm} = \left(\frac{\nu_0}{\mu}\right)^2 \frac{1}{\mathcal{M}}\left(\text{recall that } \mathcal{M} = \frac{Mm}{M+m}\right)\,,$$

$$\frac{M^2}{(m+M)^2}\frac{1}{\mathcal{M}\mu} = \frac{\mathcal{M}^2}{m^2}\frac{1}{\mathcal{M}\mu} = \frac{\mathcal{M}}{m^2\mu} = \frac{K_0^2}{m^2\mu^2} = \frac{\mu^2-\nu_0^2}{m\mu^3}\,,$$

we get from Eqs. (1.68), (1.71) and (1.72)

$$\begin{aligned}\langle \mathrm{T}\{(r_\alpha(-is) - r_\alpha(-i\sigma))^2\}\rangle_{\mathrm{eq}} &= -\left(\frac{\nu_0}{\mu}\right)^2\theta(s-\sigma)^2 + \frac{\hbar}{m}\left(\frac{\nu_0}{m}\right)^2|s-\sigma| \\ &+ \frac{\mu^2-\nu^2}{m\mu^3}\hbar\left\{\frac{1}{1-e^{-\hbar\beta\mu}}(1-e^{-\mu(s-\tau)}) - \frac{1}{e^{\hbar\beta\mu}-1}(e^{\mu|s-\tau|}-1)\right\}\,.\end{aligned} \tag{1.73}$$

It is interesting to see that

$$\langle \mathrm{T}\{(r_\alpha(-is) - r_\alpha(-i\sigma))^2\}\rangle_{\mathrm{eq}} \geq 0\,, \quad \text{when } |s-\sigma| \leq \beta\hbar = \frac{\hbar}{\theta}\,. \tag{1.74}$$