CHAPTER IV

SECOND CUMULANT CORRECTION



4.1 Introduction

A few years after Sa-yakanit¹⁰ established his theory, Gross⁸ worked out the effect of the second cumulant on the density of states calculated with respect to the first cumulant. He used the path integral representation of a single-particle partition function to evaluate the density of states. His work was not systematically presented, and is not the same as Sa-yakanit's work¹⁰. We will now present our calculation of the density of states which includes the effect of the correction up to the second cumulant along the lines of Sa-yakanit's idea.^{10,7}

4.2 Leading Term Approximation in First Cumulant

We begin by considering the density of states for the onedimensional white noise potential

$$\rho_{g}(E) = \frac{i^{1/2}}{2\pi h} (\frac{m\omega^{2}}{2\pi h})^{1/2} \int_{-\infty}^{\infty} dt \ t^{1/2} \cdot \exp\left\{-\frac{i}{h}(\frac{E}{4}\omega - E)t\right\}$$

$$-\frac{1}{2h^{2}} \cdot \frac{\xi}{2\pi h} (\frac{m\omega}{2\pi h})^{1/2} t^{2}.$$
3.5.11

The integral in (3.5.11) can not be easily integrated by the usual methods of elementary calculus. To carry out the integration in (3.5.11), we consider an integral of the following form

$$I(s) = \int_{-\infty}^{\infty} dsg(s) \exp\{\alpha_{o}F(s)\}, \qquad 4.2.1$$

where α is a large parameter, and the functions F(s) and g(s) are analytic functions. We are especially interested in function F(s) of the form

$$F(s) = \alpha s + \beta s^2, \qquad 4.2.2$$

where the functions α and β will be defined in the next step. By means of the method of steepest descent 25,26, the integral (4.2.1) can be worked out asymptotically as

I(s) =
$$i \sqrt{\frac{2\pi}{\alpha_0}} \cdot \frac{g(s_0)}{[F''(s_0)]^{1/2}} \cdot \exp \{\alpha_0 F(s_0)\}, 4.2.3$$

where so is formally determined by

$$\frac{d}{ds} F(s)|_{s=s_0} = 0$$
, 4.2.4

$$F''(s_0) = \frac{d^2}{ds^2} F(s)|_{s=s_0}$$
 4.2.5

For its application to (3.5.11), we take

$$g(s) = s^{1/2},$$
 4.2.6

and F(s) to be the exponent of the exponential in (3.5.11). If one sets

$$\alpha_{\circ} = \frac{1}{\xi}, \qquad 4.2.7$$

$$\alpha = -\frac{i}{\hbar} \left(\frac{E}{\mu} - E \right), \qquad 4.2.8$$

and
$$\beta = -\frac{1}{2h^2} \cdot (\frac{m\omega}{2\pi h})^{1/2}$$
, 4.2.9

then one obtains the following minimum value to

$$\xi t_0 = s_0 = -\frac{\alpha}{2\beta}$$
 4.2.10

The asymptotic integration of (3.5.11) is thus given by

$$\rho_{\ell}(E) = \frac{i^{1/2}}{2\pi\hbar} \left(\frac{m\omega^{2}}{2\pi\hbar}\right)^{1/2} \cdot \frac{\sqrt{2\pi}}{\xi} \cdot \frac{i s_{o}^{1/2}}{[F''(s_{o})]^{1/2}} \exp\left\{\frac{1}{\xi}F(s_{o})\right\},$$

4.2.11

where
$$F(s_0) = -\frac{\alpha^2}{4\beta}$$
, 4.2.12

and
$$F''(s_0) = 2\beta$$
. 4.2.13

We now determine the variational parameter w using the Lloyd - Best variational principle (see Appendix F). The complete variational equation is

$$0 = \frac{9}{4} z^{1/2} \{ \Gamma(\frac{5}{4}, z) - z^{1/2} \Gamma(\frac{3}{4}, z) \} - \omega \Gamma(\frac{3}{4}, z) \cdot \frac{dz}{d\omega}, F.15$$

where $\Gamma(\alpha,y)$ denotes the incomplete gamma function, and z is the exponent of the exponential in (4.2.11), or refer to (F.18). As shown in Appendix F, the two terms in the parenthesis $\{\}$ cancel each other. Hence (F.15) reduces to the familiar condition

$$\frac{\mathrm{d}z}{\mathrm{d}\omega} = \frac{\mathrm{d}}{\mathrm{d}\omega} \left(\frac{\alpha^2}{4\beta\xi}\right) = 0 . \qquad F.19$$

It follows then

$$E_{\omega} = -\frac{4}{3} E . \qquad F.20$$

As we see, the variational equation (F.20) is identical to the variational equation (3.5.18)

Since the approximate density of states (4.2.11) depends explicitly on α and β , and both of them are dependent on the energy E through (F.20); the approximate density of states must also depend explicitly on the energy E. Thus (F.20) leads us to

$$\rho_{\ell}(E) = (\frac{\sqrt{2\pi}}{6}) \cdot \frac{1}{\pi} \cdot \frac{(-E)}{\xi} \cdot \exp\{-(\frac{\pi}{3})^{1/2} \cdot \frac{1}{3} \cdot \frac{1}{\sqrt{m}} \cdot (\frac{-E)^{3/2}}{\xi}\},$$

$$4.2.14$$

which is exactly equal to (3.5.19)

Before ending this section, we should note that throughout our work, the limit $\xi \to 0$ is used and the minimum value t_0 is unique, even if more terms in the cumulant expansion are kept. This means that the minimum value t_0 come only from the following equations: (4.2.10), (4.2.8), (4.2.9), and (F.20). Thus we have

$$t_o = 2\sqrt{2} \left(\frac{\pi}{3}\right)^{1/2} \cdot \frac{E^{1/2}}{\xi} \cdot \frac{h^2}{\sqrt{m}}$$
 4.2.15

4.3 Correction to the Density of States

Now we consider an integral of the following form

$$J(s) = \int_{-\infty}^{\infty} dsG(s) \exp{\{\alpha_{O}F(s) + R(s)\}}, \qquad 4.3.1$$

where a is a large parameter, and the function G(s) is given by

$$G(s) = s^{1/2}$$
. 4.3.2

The function F(s) is taken to be the function F(s) in the preceding section, while R(s) is taken to be the rest of the terms in the cumulant expansion. This integral is easily carried out by the method of steepest descent 25,26 since

$$\alpha_{o}^{F(s)} >> R(s).$$
 4.3.3

Condition (4.3.3) implies that the function R(s) is the correction to the function α_0 F(s). Also, the condition (4.3.3) implies that (4.3.1) can be rewritten as

$$J(s) = \int_{-\infty}^{\infty} dsg(s)exp\{\alpha_{o}F(s)\}, \qquad 4.3.4$$

where
$$g(s) = G(s) \exp \{R(s)\}.$$
 4.3.5

We see that F(s) in (4.3.4) is the same as F(s) in the preceding section. It means that we will find the minimum value t_0 in the form (4.2.10) with (4.2.8) and (4.2.9) still valid. Since we find that (4.3.4) is the same as (4.2.1), Eq. (4.2.3) can be applied. We thus have

$$J(s) = i \sqrt{\frac{2\pi}{\alpha_0}} \cdot \frac{g(s_0)}{[F''(s_0)]^{1/2}} \exp \{\alpha_0 F(s_0)\}, 4.3.6$$

where s_0 and $F''(s_0)$ are determined by (4.2.4) and (4.2.5) respectively, and the function $g(s_0)$ is

$$g(s_0) = G(s_0) \exp{R(s_0)}$$
 4.3.7

Comparing (4.3.6) with (4.2.3), the quantities s_0 , $F(s_0)$, and $F''(s_0)$ in (4.3.6) are the same as the quantities s_0 , $F(s_0)$, and $F''(s_0)$ in (4.2.3) respectively. Moreover, the function g(s) in (4.2.6) is the function G(s) in (4.3.2). This means that if we redefine g(s) in (4.2.6) by G(s), we can replace $g(s_0)$ in the integral (4.2.3) by $G(s_0)$. Dividing (4.3.6) by (4.2.3), one finds the relation between I(s) and J(s), i.e.,

$$J(s) = I(s) \exp \{R(s_0)\}.$$
 4.3.8

According to the preceding section, the integral I(s) is related to the approximate density of states $\rho_{\ell}(E)$ by a constant If we multiply both side of (4.3.8) by the constant, we obtain

$$\rho_{c}(E) = \exp\{R(s_{o})\} \cdot \rho_{\ell}(E) , \qquad 4.3.9$$

where the function $\rho_c(E)$ is the corrected density of states (corresponding to the correction $R(s_o)$)

However, the corrected density of states (4.3.9) is still incomplete, since the variational parameter ω has not determined. To determine ω , we will use the Lloyd-Best variational principle. To begin this procedure, we expand the correction in power series of to

$$\exp\{R(s_o)\} = \sum_{n=1}^{\infty} A_n B_n(\omega) t_o^n , \qquad 4.3.10$$

where the function $A_n B_n(\omega)$ is the coefficient of the n th power of t_0 . We now insert (4.3.10) into (4.3.9), and use transformations

where the function $\rho_{\rm c}({\bf x},\,\omega)$ is the corrected density of states $\rho_{\rm c}({\bf E})$, the function $\rho_{\rm n}({\bf x},\omega)$ is the n th term of the corrected density of states in series expansion, and the function $C_{\rm n}F_{\rm n}(\omega)$ is the coefficient of the n th power of x. In Appendix F the maximization of the pressure of (4.3.14) is determined, and is seen to yield the same variational equation (F.20) in the limit $\xi \to 0$. It means that the minimum value $t_{\rm o}$ is conditionally unique, and has the useful form as shown by (4.2.15). The relation (4.3.9) is completely proved for the minimum value (4.2.15) and variational equation (F.20).

4.4 Complete First Cumulant

As discussed in the preceding section, it gives us an idea to correct the density of states. Let us consider the effect of the correction when we keep all terms in the first cumulant. It means that we try to evaluate completely the integral in <S>, and keep the constant factor $e^{-1/2}$ in <S>, for d = 1.

For estimating the integral in $\langle S \rangle$, Eq. (3.5.4) must be considered by setting L = 0 and d = 1, and using a transformation

$$x = \xi t . 4.4.1$$

It then can be written as

$$\frac{i}{h} < S > = -\frac{1}{2h^2} \cdot \frac{\xi}{(4\pi)^{1/2}} \cdot t^2 \int_{0}^{1} d\zeta \, j(\zeta, \omega; t)^{-1/2}, \quad 4.4.2$$

where

$$j(\zeta,\omega;t) = \frac{i\hbar}{m\omega} \cdot \frac{\sin\omega t \sin\omega t (1-\zeta)}{2} \cdot \frac{1}{2} \cdot \frac{1}{2}$$

To evaluate the integral in (4.4.2), see Appendix D, we have

$$\frac{i}{h} < S > = -\frac{\xi}{2h^2} \cdot (\frac{m\omega}{2\pi h})^{1/2} t^2 + \frac{i}{h^2} \cdot \frac{\xi}{\omega^{1/2}} (\frac{m}{2\pi h})^{1/2} (2n4)t. \quad 4.4.4$$

For finding the correction $R(s_0)$, we write

$$R_1(s) = \text{the 2nd terms of } \frac{i}{h} < s - 6 > ,$$
 4.4.5

or equivalently, for s = Et,

$$R_1(\xi t)$$
 = the 2nd terms of $\frac{i}{\hbar} < S - S_0 >$. 4.4.6

The second term of $\frac{1}{h}$ <S $_{\circ}$ is + $\frac{1}{2}$ (see (3.5.3)), and the second term of $\frac{1}{h}$ <S> is also found in (4.4.4); thus

$$R_1(\xi t) = -\frac{1}{2} + \frac{i}{\hbar} 2 \cdot \frac{\xi}{\omega^{1/2}} (\frac{m}{2\pi h})^{1/2} (\ln 4)t.$$
 4.4.7

As shown in Section 4.3, Eq. (4.4.7) must be evaluated at $t = t_0$. Using t_0 , given by (4.2.15), and the variational equation (F.20), we easily find

$$R_1(\xi t_0) = -\frac{1}{2} + \ln 4$$
.

Moreover, if $\rho_1(E)$ denotes the corrected density of states corresponding to (4.4.8), then (4.3.9) can be applied. We now have

$$\rho_1(E) = \exp\{-\frac{1}{2} + \ln 4\}\rho_1(E),$$
 4.4.9

where $\rho_{\ell}(E)$ is given by (4.2.14). It follows that

$$\rho_{1}(E) = e^{-1/2} \mu(\frac{\sqrt{2\pi}}{6}) \cdot \frac{\mu}{\pi} \cdot \frac{(-E)}{\xi} \cdot \exp\{-(\frac{\pi}{3})^{1/2} \cdot \frac{4\sqrt{2}}{3} \cdot \frac{h}{m} \cdot \frac{(-E)^{3/2}}{\xi}\}. 4.4.10$$

Comparing (4.4.10) with (1.5.1)

$$\rho_{as}(E) = \frac{4}{\pi} \cdot \frac{(-E)}{\xi} \cdot \exp\{-\frac{4\sqrt{2}}{3} \cdot \frac{h}{\sqrt{m}} \cdot \frac{(-E)}{\xi}^{3/2}\}, \qquad 1.5.1$$

we see that the effect of the correction of the second term in the first cumulant changes the numerical factor in front of the exponential from $\frac{\sqrt{2\pi}}{6}$ to $e^{-1/2}$ $\frac{4\sqrt{2\pi}}{6}$. The factor $e^{-1/2}$ $\frac{2\sqrt{2\pi}}{3} = 1.014$ is very close to the required value, but the numerical factor in the exponent is still to be $\left(\frac{\pi}{3}\right)^{1/2} = 1.0233$. However, it can be corrected by adding the correction of the leading term in the second cumulant. We examine this in the next section.

4.5 Second Cumulant Correction

To correct the numerical factor in the exponent, we must consider the second cumulant, and look only at the leading term. According to (3.4.5), the second cumulant of the average part in (3.4.2) is

the 2nd cumulant =
$$\frac{1}{2}(\frac{1}{h})^2 \{ < (s - s_0)^2 > - < s - s_0 >^2 \},$$
 4.5.1

which is very difficult to evaluate directly. However, it can be expanded and rearranged into the form

the 2nd cumulant =
$$\frac{1}{2}(\frac{1}{\hbar})^2\{[\langle s_0^2 \rangle - \langle s_0 \rangle^2] - 2[\langle s_0^2 \rangle - \langle s_0^2 \rangle] + [\langle s_0^2 \rangle - \langle s_0^2 \rangle]\},$$
 4.5.2

which are more easily evaluated than (4.5.1). The three terms on the right - hand side of (4.5.2) can be estimated for the three leading terms of them. The first two terms can be easily calculated using the formula

$$\frac{i}{\hbar}[\langle ZS_{\circ}\rangle - \langle Z\rangle \langle S_{\circ}\rangle] = \left[\frac{\partial}{\partial \lambda} \langle Z(\omega/\lambda)\rangle\right]\Big|_{\lambda=1}, \qquad 4.5.3$$

where Z is a function of ω To obtain the first two terms, we set $Z = S_O$, and Z = S respectively. Hence we get

$$\left(\frac{1}{\hbar}\right)^{2} \left(\left\langle s_{o}^{2}\right\rangle - \left\langle s_{o}^{2}\right\rangle^{2}\right) = \frac{1}{\hbar} \left[\frac{\partial}{\partial \lambda} \left\langle s_{o}(\omega / \lambda)\right\rangle \right]_{\lambda=1}^{2}, \quad 4.5.4$$

and
$$\left(\frac{i}{\hbar}\right)^2 \left[\left\langle SS_0 \right\rangle - \left\langle S \right\rangle \right] = \frac{i}{\hbar} \left[\frac{\partial}{\partial \lambda} \left\langle S(\omega \lambda) \right\rangle \right]_{\lambda=1}$$
. 4.5.5

It should be remembered that we have only kept the leading terms in (4.5.4) and (4.5.5). If we apply (3.5.2) to (4.5.4), and (4.4.4) to (4.5.5), we find

4.5.7

Neglecting the exponential term of $e^{-i\omega t}$ in the limit of large time, the leading terms of (4.5.6) and (4.5.7), for d=1, can be found. We get

$$\left(\frac{1}{h}\right)^{2} \left[\left(\frac{1}{h}\right)^{2} \left(\frac{1}{h}\right)^{2} \left(\frac{1}{h}\right$$

$$\left(\frac{1}{h}\right)^{2} \left[\left(SS_{0} > - \left(S > S_{0} > 1\right)\right)^{2} \approx \frac{5}{8h^{2}} \left(\frac{m}{2\pi h}\right)^{1/2} \cdot t^{2},$$
 4.5.9

where E_{ω} is referred to (3.5.10). The third term in (4.5.2) can be obtained by taking L=0 and d=1 in (C.18) in Appendix C, We have, in the limit of large time,

where Δ_1 and Δ_{12} are defined in (C.20) and (C.21) respectively. To find <S>2, we double (C.11), and let L = 0 and d = 1. In the limit of large time, we have

$$\left(\frac{1}{h}\right)^{2} < S^{2} = \frac{1}{8\pi h^{5}} \cdot \xi^{2} m_{\omega} \int_{0}^{t} \int_{0}^{t} \int_{0}^{t} d\tau_{1} d\sigma_{1} d\tau_{2} d\sigma_{2} \{(1-\Delta_{1})(1-\Delta_{2})\}^{-1/2}.$$
4.5.11

Subtract (4.5.11) from (4.5.10), we get

$$(\frac{1}{h})^2 [\langle S^2 \rangle - \langle S \rangle^2] = \frac{1}{8\pi h^5} \cdot \xi^2 m \omega \int_{0}^{t} \int_{0}^{t} \int_{0}^{t} d\tau_1 d\sigma_1 d\tau_2 d\sigma_2 \{ (1-\Delta_1)(1-\Delta_2) \}^{-1/2}.$$

$$\frac{1}{(1 - \frac{y}{4})^{-1/2}} \cdot \{(1 - \frac{y}{4})^{-1/2} - 1\}, \qquad 4.5.12$$
here
$$y = \frac{\Delta_{12}^2}{(1 - \Delta_1)(1 - \Delta_2)}. \qquad 4.5.13$$

where

For finding the leading term in (4.5.12), we expand the second factor in the integrand by the binomial series, and neglect both of Δ_1 and Δ_2 in all of the divisors. We get

$$\frac{1}{5} \left[\left(\frac{1}{5} \right)^{2} \left[\left(\frac{5}{5} \right)^{2} - \left(\frac{5}{5} \right)^{2} \right] = \frac{1}{8\pi h^{5}} \xi^{2} m \omega \int_{0}^{t} \int_{0}^{t} \int_{0}^{t} d\tau_{1} d\sigma_{1} d\tau_{2} d\sigma_{2} \left\{ \frac{1}{2} \left(\frac{\Delta_{12}^{2}}{\mu} \right) + \frac{3}{8} \left(\frac{\Delta_{12}^{2}}{\mu} \right)^{2} + \frac{5}{16} \left(\frac{\Delta_{12}^{2}}{\mu} \right)^{3} + \cdots \right\} .$$

$$4.5.14$$

Using transforms as below :

$$\tau_{i} = t_{i}t, \qquad 4.5.15$$
and
$$\sigma_{i} = s_{i}t, \qquad 4.5.16$$

the approximation in Appendix E allows us to evaluate the leading term in (4.5.14) as

$$\frac{1}{2} \left(\frac{1}{h}\right)^{2} \left[\left\langle s^{2} \right\rangle - \left\langle s^{2} \right\rangle^{2}\right] = \frac{1}{16\pi h^{5}} \cdot \xi^{2} m \omega t^{4} \int_{0}^{1} \int_{0}^{1} \int_{0}^{1} \int_{0}^{1} dt_{1} ds_{1} dt_{2} ds_{2} \left\{\frac{1}{2} \left(\frac{\Delta_{12}^{2}}{4}\right)^{2} + \frac{3}{8} \left(\frac{\Delta_{12}^{2}}{4}\right)^{2} + \frac{5}{16} \left(\frac{\Delta_{12}^{2}}{4}\right)^{3} + \cdots\right\}, \quad 4.5.17$$

where And is now transformed by (4.5.15) and (4.5.16)

$$\frac{1}{2} (\frac{1}{h})^{2} [\langle s^{2} \rangle - \langle s \rangle^{2}] \simeq \frac{1}{16\pi h^{5}} \cdot \xi^{2} m \omega t^{4} \int_{0}^{1} \int_{0}^{1} \int_{0}^{1} dt_{1} ds_{1} dt_{2} ds_{2} \left\{ \frac{1}{2} \cdot \frac{4}{4} \left(\frac{\Delta_{1}^{2}}{4} \right)^{2} + \frac{3}{8} \cdot \frac{4}{4} \left(\frac{\Delta_{1}^{2}}{4} \right)^{2} + \frac{5}{16} \cdot \frac{4}{4} \left(\frac{\Delta_{1}^{2}}{4} \right)^{3} + \cdots \right\} \qquad 4.5.18$$

$$\simeq -\frac{1}{16\pi h^{5}} \cdot \xi^{2} m t^{3} \left\{ \frac{1}{2} + \frac{3}{64} + \frac{5}{768} + \cdots \right\} \cdot 4.5.19$$

As mentioned in Section 4.3, we now substitute (4.5.8), (4.5.9), and (4.5.19) into (4.5.2), replace t by t_0 , from (4.2.15), and use the variational equation (F.20). Thus we find the second correction $R_2(\xi t_0)$

corresponding to the leading term in the second cumulant to be

$$R_{2}(\xi t_{0}) = \frac{1}{4} \left\{ \frac{3}{64} + \frac{5}{768} + \cdots \right\} \cdot \left(\frac{\pi}{3} \right)^{1/2} \cdot \frac{4\sqrt{2}}{3} \cdot \frac{\hbar}{\sqrt{m}} \cdot \frac{(-E)^{3/2}}{\xi} \cdot 4.5.20$$

The relation (4.3.9) can be applied when $\rho_2(E)$ is the corrected density of states corresponding to (4.5.20). In other words,

$$\rho_2(E) = \exp\{R_2(\xi t_0)\}\rho_1(E),$$
 4.5.21

where $\rho_1(E)$ refer to (4.4.10). The expression (4.5.21), written out explicitly, is

$$\rho_{2}(E) = e^{-1/2} \cdot \frac{4\sqrt{2\pi}}{6} \cdot \frac{4}{\pi} \cdot \frac{(-E)}{\xi} \exp\{-(\frac{3031}{3072})(\frac{\pi}{3})^{\frac{1}{2}} \cdot \frac{1}{\sqrt{2}} \cdot \frac{h}{\xi} \cdot \frac{(-E)^{3/2}}{\xi}\}.$$

We see that the numerical factor in the exponent in (4.5.22) is changed from $(\frac{\pi}{3})^{1/2}$ to $(\frac{3031}{3072})(\frac{\pi}{3})^{1/2}$ by the effect of the leading term in the second cumulant. This factor $(\frac{3031}{3072})(\frac{\pi}{3})^{1/2} = 1.0097$ is near the exact value.