CHAPTER V

CONCLUSION

5.1 Summary

In Chapter I, we briefly reviewed the one-dimensional white noise model for which the density of states can be computed exactly. This fact was first pointed out by Frisch and Lloyd[3], and has been subsequently studied in detail by Halperin[2] and Zittartz and Langer[4]. Defining

$$A(E) = \frac{8}{\pi}(-E), \tag{5.1.1}$$

$$B(E) = \frac{8\sqrt{2}}{3} \cdot \frac{\hbar}{\sqrt{m}} \cdot \frac{(-E)^{3/2}}{\xi}, \tag{5.1.2}$$

we can express the exact result for $\xi \to 0$ as

$$\rho_{as}(E) = \frac{A(E)}{2\xi} \exp\{-\frac{B(E)}{2\xi}\}. \tag{5.1.3}$$

The expression (5.1.3) provides us with an exact expression which can be used to check the validity of more general approximation schemes.

In Chapter II, we examine the method of Halperin and Lax[5,9] used to compute the density of states for the random model. Their theory is based on Schrödinger formulation of quantum mechanics. They assumed that all eigenstates in the low-energy tail of a given energy have the same shape. Using this assumption, they first approximate the density of states[5], and show that, for their first order approximation,

$$\rho_1(E) = \frac{1}{\sqrt{5}} \cdot \frac{A(E)}{2\xi} \cdot \exp\{-\frac{B(E)}{2\xi}\}. \qquad 5.1.4$$

Since their assumption is not exact, the density of states $\rho_1(E)$ turns out to be too small by a factor of $\sqrt{5} = 2.236$. However, in their second order approximation, they calculate the correction $C(E)$, and show that the corrected density of states is given by[9]

$$\rho_2(E) = \exp\{\mu C(E)\}\rho_1(E), \qquad 5.1.5$$

where

$$\mu C(E) = \frac{13}{18}. \qquad 5.1.6$$

It follows that

$$\rho_2(E) = \frac{e^{13/18}}{\sqrt{5}} \cdot \frac{A(E)}{2\xi} \cdot \exp\{-\frac{B(E)}{2\xi}\}, \qquad 5.1.7$$

where the unexact factor $e^{13/18}/\sqrt{5} = 0.921$.

In Chapter III, we review the Sa-yakanit theory[10,7] and his calculation of the density of states for the random model. His theory is based on Feynman formulation of quantum mechanics. He introduce the non-local harmonic oscillator trial action to model the potential of the random model. He show that for the leading term of the first cumulant, the approximate density of states[7] is given by

$$\rho_\ell(E) = \frac{\sqrt{2\pi}}{6} \cdot \frac{A(E)}{2\xi} \cdot \exp\{-(\frac{\pi}{3})^{1/2} \cdot \frac{(B(E)}{2\xi}\}, \qquad 5.1.8$$

where the unexact factors are $\frac{\sqrt{2\pi}}{6} = 0.418$ and $(\frac{\pi}{3})^{1/2} = 1.0233$.

In Chapter IV, we extend Sa-yakanit's theory[7,10] to include the leading term in the second cumulant by using the method of **steepest** descent, and show that the corrected density of states corresponding to the correction $R(\xi t_o)$ can be put into the form

$$\rho_c(E) = \exp\{R(\xi t_o)\}\rho_\ell(E). \qquad 5.1.9$$

For the complete first cumulant, the corrected density of states $\rho_c(E)$ is $\rho_1(E)$ and the correction $R(\xi t_o)$ is $R_1(\xi t_o)$, where

$$R_1(\xi t_o) = -\frac{1}{2} + \ell n\, 4; \qquad 5.1.10$$

then
$$\rho_1(E) = e^{-1/2}\cdot\frac{4\sqrt{2\pi}}{6}\cdot\frac{A(E)}{2\xi}\cdot\exp\{-(\frac{\pi}{3})^{1/2}\cdot\frac{B(E)}{2\xi}\}. \qquad 5.1.11$$

For the second cumulant approximation, the corrected density of states $\rho_c(E)$ is $\rho_2(E)$, and the correction $R(\xi t_o)$ is $R_1(\xi t_o) + R_2(\xi t_o)$, where

$$R_2(\xi t_o) = +\frac{1}{4}\left(\frac{3}{64} + \frac{5}{768}\right)\left(\frac{\pi}{3}\right)^{1/2}\cdot\frac{B(E)}{2\xi}. \qquad 5.1.12$$

$$\rho_2(E) = e^{-1/2}\cdot\frac{4\sqrt{2\pi}}{6}\cdot\frac{A(E)}{2\xi}\cdot\exp\{-\left(\frac{3031}{3072}\right)\left(\frac{\pi}{3}\right)^{1/2}\cdot\frac{B(E)}{2\xi}\}, \qquad 5.1.13$$

and the unexact factors are $e^{-1/2}\cdot\frac{4\sqrt{2\pi}}{6} = 1.014$ and $\left(\frac{3031}{3072}\right)\left(\frac{\pi}{3}\right)^{1/2} = 1.0097$.

5.2 Discussion

As seen in the preceding section, all of the approximate density[5,9,7] of states do not have the exact numerical factors in front of the exponential term and in the exponent. We have computed the percentage errors of them. Denoting these errors as Δ_1 and Δ_2 respectively,

Table 5.1 The percentage errors of the numerical factors in front of the exponential and in the exponent for the correspond density of states : The simbols Δ_1 and Δ_2 here denote the percentage errors respectively. For convenience in comparison we write superscript HL to specify the Halperin and Lax results.

ρ \ Δ %	Δ_1	Δ_2
ρ_{as}	0	0
ρ_1^{HL}	-55	0
ρ_2^{HL}	-7.9	0
ρ_ℓ	-58	2.3
ρ_1	1.4	2.3
ρ_2	1.4	0.97

the errors are listed in Table 5.1

We first consider the Halperin and Lax results : Both ρ_1^{HL} and ρ_2^{HL} have the same zero-values of Δ_2's, but have non-zero values for Δ_1's. The effect of the second order correction changes ρ_1^{HL} to ρ_2^{HL}, and changes the values of Δ_1's from -55 to -7.9 %. Next we consider the results of Sa-yakanit's theory : All of the approximate density of states have non-zero values for both Δ_1's and Δ_2's. Both ρ_ℓ and ρ_1 have the same values of 2.3 % for Δ_2's, but have different values for Δ_1's. The effect of the complete first cumulant changes ρ_ℓ to ρ_1, and changes the values of Δ_1's from -58 to + 1.4 %. For ρ_2 the value of Δ_1 is still 1.4 %, but the value of Δ_2 is changed from 2.3 to 0.97 % according to the effect of the second cumulant correction. Finally we consider the results from the theories of both Halperin and Lax and Sa-yakanit : We see that our Δ_2's are not as good as of Halperin and Lax. In principle it is certainly possible to further correct our results until they agree exactly with the exact expression. However, the leading terms in the higher cumulants affect the value of Δ_2 to a much lesser extent than the leading term in the second cumulant. The values of both Δ_1 and Δ_2 of ρ_2 are very close to the exact values. Our result therefore appears to be satisfactory and so we have chosen to stop our calculation at this step. However, if one neglects few percents of Δ_2's of both ρ_ℓ and ρ_1 , one finds that ρ_ℓ and ρ_1^{HL} as well as ρ_1 and ρ_2^{HL} have nearly the same values of Δ_1's. We see that ρ_ℓ and ρ_1 are nearly equal to ρ_1^{HL} and ρ_2^{HL} respectively. Our method[10,7] has, however, several advantages over the method of Halperin and Lax[5,9].

Firstly, the mathematical details of calculating the Halperin and Lax relation (2.6.4)[9] is very complicated. However, our equivalent relation (4.3.9) is easily obtained by the method of steepest descent.

Secondly, the minimization of the exponent of (2.4.3) in the Halperin and Lax method[5] leads to a nonlinear differential equation

$$-\frac{1}{2} f''(x) - \frac{1}{2}\mu f(x)^3 \quad = \quad Ef(x), \qquad 2.5.5$$

whereas in our work, the minimization leads to a simple algebraic equation

$$E_\omega \quad = \quad -\frac{4}{3} E . \qquad 3.5.18$$

We clearly see that (3.5.18) is more simpler than (2.5.5).

Thirdly, the variational equation (3.5.18) which is the minimization of the exponent can be reduced from the maximization of the pressure

$$P(E) \quad = \int_{-\infty}^{E} dE' \int_{-\infty}^{E'} dE'' \rho(E''), \qquad F.1$$

as formulated by Lloyd and Best.[24] This means that we are able to determine the variational parameter ω by the Lloyd-Best variational principle[24]. No such determination appears in the Halperin and Lax theory[5,9]. Mathematically our method is more rigorous than their method

Finally, Halperin and Lax's method[5,9] can not be extended to find the density of states for a free electron model, whereas our method can. In the limit of small time, it is obvious that (3.5.5) of our calculation reduces to

$$\rho_1(E) = \frac{1}{2\pi\hbar}\left(\frac{m}{2\pi\hbar}\right)^{1/2} \cdot \int_{-\infty}^{\infty} dt(it)^{-1/2} \exp\left\{\frac{iEt}{\hbar} - \frac{1}{2\hbar^2}\cdot\frac{\xi}{\sqrt{\pi}L}\cdot t^2\right\}. \qquad 5.2.1$$

By using the formula (3.5.17) and the asymptotic expansion[23] of $D_p(z)$

$$D_p(z)_{z\to-\infty} \approx -\frac{\sqrt{2\pi}}{\Gamma(-p)}\cdot e^{p\pi i}\, e^{z^2/4}\, z^{-p-1}, \qquad 5.2.2$$

where $\Gamma(\nu)$ denotes the complete gamma function, we get

$$\rho_1(E) = \frac{1}{2\pi\hbar}\cdot\sqrt{\frac{2m}{E}} \qquad 5.2.3$$

which is usually the density of states for the free electron model.

5.3 Conclusion

As discussed in the preceding section, we see that our method has several advantages over Halperin and Lax's method. However, both of these theories were formulated from the same idea by assuming that the random potential of the system is the same shape. The results of these two different approaches should not be different. To summerize our results, the curves of Equations (5.1.4),(5.1.7), (5.1.8), (5.1.11), (5.1.13), and (5.1.3) are plotted together in Figure 5.1. For clarity of the curves, Table 5.2 is presented. From this figure and table, we can make the following conclusions:

Firstly, we see that ρ_ℓ is not as good as ρ_1^{HL} in comparison with ρ_{as}. This can be seen easily by considering the percentage errors of ρ_ℓ and ρ_1^{HL}. For example at E = -2, the percentage error of ρ_ℓ is -67.5 %, while that of ρ_1^{HL} is-55.4 %. The reason may be thought of as follows: In our method the shape of potential wells is always fixed in the form of harmonic well, while in Halperin and Lax's method the wave function f is allowed to vary in shape in order to fit the random potential. Fortunately, in one dimension the function f can be solved exactly for the nonlinear differential equation (2.5.5). This fact enable the first order approximation of Halperin and Lax's method to get better results than the leading term of the first cumulant. However, in the complete first cumulant the values of ρ_1 is much better than ρ_1^{HL} as compared to ρ_{as}. For example at E = -2, the percentage error of ρ_1 equals -21.2 %, while that of ρ_1^{HL} equals -67.5 %. This implies that the complete first cumulant give better results than the first order approximation of Halperin and Lax's method. Furthermore, our method can be performed beyond the first cumulant to obtain the leading term of the second cumulant(ρ_2). By comparing ρ_2 and ρ_2^{HL} with ρ_{as}, we find that the results of both ρ_2 and ρ_2^{HL} are closed to ρ_{as}. At high energies, for example at E = -0.5, the percentage error of ρ_2 is extremely small, while that of ρ_2^{HL} is equal to -8.04 %. At low energies, for example at E = -2, the percentage error of ρ_2^{HL} is -8.40 %. From this example, we see that our result ρ_2 is better than ρ_2^{HL} at high energies, and is nearly the same as ρ_2^{HL} at low energies. This indicates that our ρ_2 is approximately equal to ρ_2^{HL}, and that the second cumulant approximation in our method is approximately equal to the second order approximation of Halperin and Lax's method.

Secondly, as discussed in the preceding section, our method has several advantages over Halperin and Lax's method. Firstly, the cumulant correction to the density of states can be calculated directly in our method, but Halperin and Lax must solve the modified Green's function $\hat{G}$. Secondly, our method give the variational equation which is easier to solve than that of Halperin and Lax's method. Thirdly, we derive the variational equation from the Lloyd-Best variational principle. Finally, we point out that our method can be extended to high energies to obtain the free-electron density of states. This extension does not appear in Halperin and Lax's method. From all of the above discussion, we conclude that our method is more practical than Halperin and Lax's method. We believe that the idea developed in this thesis based on Sa-yakanit's theory should be applicable to the other problems in three dimensions.

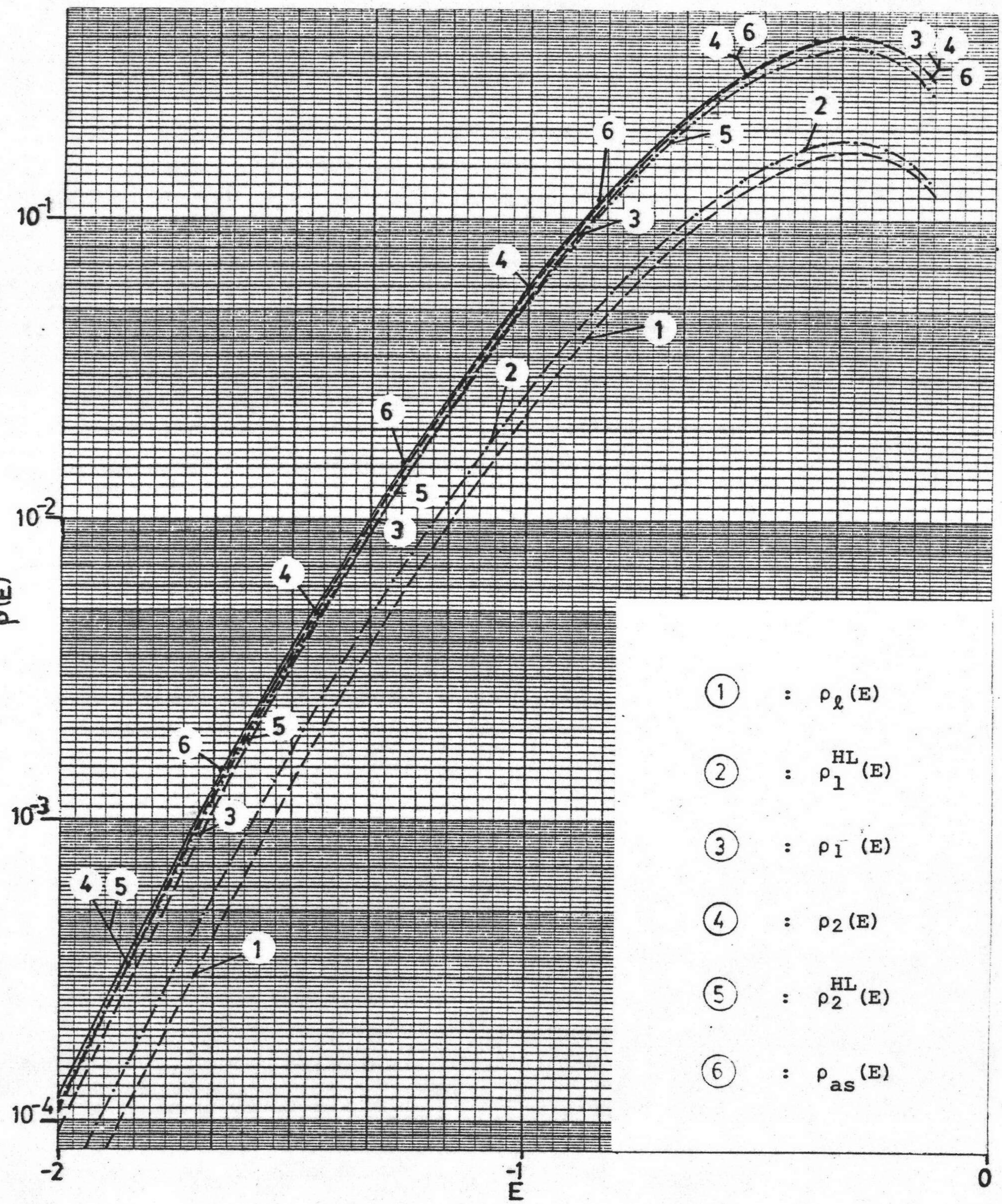


Figure 5.1 Density of states $\rho(E)$ for the one-dimensional white noise model, compared with its asymptotic form for low energies, $\rho_{as}(E)$.

All of the curves are plotted in units of $\hbar = 1$, $m = 1$, and $2\xi = 1$. The numbers from one to six indicate the following density of states :

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

$$\rho_1^{HL}(E) = \frac{1}{\sqrt{5}} \cdot \frac{A(E)}{2\xi} \exp\{-\frac{B(E)}{2\xi}\},$$

$$\rho_1(E) = e^{-1/2} \cdot \frac{4\sqrt{2\pi}}{6} \cdot \frac{A(E)}{2\xi} \cdot \exp\{-(\tfrac{\pi}{3})^{1/2} \cdot \frac{B(E)}{2\xi}\} ,$$

$$\rho_2(E) = e^{-1/2} \cdot \frac{4\sqrt{2\pi}}{6} \cdot \frac{A(E)}{2\xi} \exp\{-(\tfrac{3031}{3072})(\tfrac{\pi}{3})^{1/2} \cdot \frac{B(E)}{2\xi}\},$$

$$\rho_2^{HL}(E) = \frac{e^{13/18}}{\sqrt{5}} \cdot \frac{A(E)}{2\xi} \cdot \exp\{-\frac{B(E)}{2\xi}\} ,$$

and

$$\rho_{as}(E) = \frac{A(E)}{2\xi} \cdot \exp\{-\frac{B(E)}{2\xi}\} ,$$

where the functions $A(E)$ and $B(E)$ are defined by

$$A(E) = \frac{8}{\pi} (-E) ,$$

$$B(E) = \frac{8\sqrt{2}}{3} (-E)^{3/2} .$$

$-E$ \ ρ	$\rho_{\ell}(E)$	$\rho_1^{HL}(E)$	$\rho_1(E)$	$\rho_2(E)$	$\rho_2^{HL}(E)$	$\rho_{as}(E)$
2.0	3.87-05	5.31-05	9.38-05	1.09-04	1.09-04	1.19-04
1.5	1.33-03	1.67-03	3.23-03	3.55-03	3.45-03	3.74-03
1.0	2.24-02	2.62-02	5.44-02	5.73-02	5.40-02	5.86-02
0.5	1.36-01	1.50-01	3.30-01	3.36-01	3.09-01	3.36-01
1/3	1.69-01	1.84-01	4.09-01	4.13-01	3.78-01	4.11-01
1/6	1.36-01	1.47-01	3.31-01	3.32-01	3.02-01	3.28-01

Table 5.2 Numerical results of the corresponding density of states which we use to plot Figure 5.1. The forms of all are shown in the page 56. All of the results is written in the computational notation, for example, 3.87-05 = 3.87×10^{-5}.

APPENDIX A

EVALUATION OF $G_o(\vec{X}_2,\vec{X}_1;t)$

To evaluate the non-local harmonic oscillator propagator[20] G_o, we rewrite the trial action S_o in the form

$$S_o(\omega) = S_{HO} + \frac{m\omega^2}{2t}\left(\int_o^t d\tau\, \vec{X}(\tau)\right)^2, \qquad \text{A.1}$$

where S_{HO} is familiarly the simple harmonic oscillator action[12],

$$S_{HO} = \int_o^t d\tau \frac{m}{2}\{\dot{\vec{X}}^2(\tau) - \omega^2\vec{X}(\tau)\}. \qquad \text{A.2}$$

The second term on the right-hand side of (A.1) can be converted to an integral form by an identity[23],

$$\exp\{\frac{i}{\hbar} \cdot \frac{m\omega^2}{2t}\left(\int_o^t d\tau\vec{X}(\tau)\right)^2\}$$

$$= \left(\frac{it}{2\pi\hbar m\omega^2}\right)^{d/2} \cdot \int_{-\infty}^{\infty} d\vec{f}\, \exp\left\{-\frac{i}{\hbar}\left(\frac{t}{2m\omega^2}\vec{f}^2 - \int_o^t d\tau\vec{X}(\tau)\cdot\vec{f}\right)\right\}. \qquad \text{A.3}$$

Inserting (A.1) and (A.3) into (3.4.3), we then find that the propagator G_o can be expressed as

$$G_o(\vec{X}_2,\vec{X}_1;t) = \left(\frac{it}{2\pi\hbar m\omega^2}\right)^{d/2} \cdot \int\mathcal{D}[\vec{X}(\tau)] \int_{-\infty}^{\infty} d\vec{f}\,.$$

$$\cdot\exp\{\frac{i}{\hbar}\left(S_{HO} - \frac{t}{2m\omega^2}\vec{f}^2 + \int_o^t d\tau\vec{X}(\tau)\cdot\vec{f}\right)\}. \qquad \text{A.4}$$

Changing the order of integration, (A.4) becomes

$$G_o(\vec{X}_2,\vec{X}_1;t) = \left(\frac{it}{2\pi\hbar m\omega^2}\right)^{d/2} \cdot \int_{-\infty}^{\infty} d\vec{f}\, \exp\left\{-\frac{i}{\hbar}\left(\frac{t}{2m\omega^2}\right)\vec{f}^2\right\} \cdot$$

$$\cdot G_f(\vec{X}_2,\vec{X}_1;t,\vec{f}), \qquad \text{A.5}$$

where

$$G_f(\vec{X}_2,\vec{X}_1;t,\vec{f}) = \int \mathcal{D}[\vec{X}(\tau)]\exp\{\frac{i}{\hbar}(S_{HO} + \int_0^t d\tau\vec{X}(\tau).\vec{f})\}. \qquad \text{A.6}$$

The propagator (A.6) is the forced harmonic oscillator propagator which is evaluated in the literature[12]. With a constant external force $\vec{f}$ we have

$$G_f(\vec{X}_2,\vec{X}_1;t,\vec{f}) = \left(\frac{m\omega}{2\pi i\hbar\sin\omega t}\right)^{d/2} \cdot \exp\{\frac{i}{\hbar}(\frac{m\omega}{4}[\cot\frac{\omega t}{2}(\vec{X}_2-\vec{X}_1)^2$$

$$-\tan\frac{\omega t}{2}(\vec{X}_2+\vec{X}_1)^2] + \frac{1}{\omega}\cdot\tan\frac{\omega t}{2}(\vec{X}_2+\vec{X}_1)\cdot\vec{f}$$

$$-[\frac{1}{m\omega^3}\cdot\tan\frac{\omega t}{2} - \frac{t}{2m\omega^2}\cdot\vec{f}^2])\} . \qquad \text{A.7}$$

Substituting (A.7) into (A.5), and performing the $\vec{f}$ - integration. We get

$$G_o(\vec{X}_2,\vec{X}_1;t) = \left(\frac{m}{2\pi i\hbar t}\right)^{d/2} \cdot \left(\frac{\omega t}{2\sin\frac{\omega t}{2}}\right)^{d} \cdot$$

$$\cdot\exp[\frac{i}{\hbar}\cdot\frac{m\omega}{4}\cot\frac{\omega t}{2}(\vec{X}_2-\vec{X}_1)^2] . \qquad \text{A.8}$$

APPENDIX B

EVALUATION OF $S_{o,c\ell}$

The classical action $S_{o,c\ell}$ is the extremum of the action S_o, and the action S_o can be written as

$$S_o'(\vec{X}_2,\vec{X}_1;\omega) = S_o(\vec{X}_2,\vec{X}_1;\omega) + \int_o^t d\tau \vec{f}(\tau)\cdot\vec{X}(\tau), \qquad \text{B.1}$$

where the action S_o corresponds to the classical action $S_{o,c\ell}$, and is the action $S_o(\omega)$ of (3.4.1), and where the external force $\vec{f}(\tau)$ is an arbitrary function of time.

To calculate the action $S'_{o,c\ell}$, we substitute (3.4.1) into (B.1), and get

$$S_o'(\vec{X}_2,\vec{X}_1;\omega) = \int_o^t d\tau\frac{m}{2}\{\dot{X}^2(\tau) - \frac{\omega^2}{2t}\cdot\int_o^t d\sigma[\vec{X}_c(\tau) - \vec{X}_c(\sigma)]^2\}$$

$$+ \int_o^t d\tau\, \vec{f}(\tau)\cdot\vec{X}_c(\tau). \qquad \text{B.2}$$

If $\vec{X}_c(\tau)$ denotes the classical path, then $S'_{o,c\ell}$ is given by

$$S'_{o,c\ell}(\vec{X}_2,\vec{X}_1;\omega) = \int_o^t d\tau\frac{m}{2}\{\dot{X}_c^2(\tau) - \frac{\omega^2}{2t}\cdot\int_o^t d\sigma[\vec{X}_c(\tau) - \vec{X}_c(\sigma)]^2\}$$

$$+ \int_o^t d\tau\vec{f}(\tau)\cdot\vec{X}_c(\tau). \qquad \text{B.3}$$

Taking variational on S_o', we obtain the classical equation

$$\ddot{\vec{X}}_c(\tau) + \omega^2\vec{X}_c(\tau) = \frac{\omega^2}{t}\cdot\int_0^t d\sigma\vec{X}_c(\sigma) + \frac{\vec{f}}{m}(\tau). \qquad \text{B.4}$$

If we integrate by parts the first term on the right hand side of (B.3), and use (B.4), we obtain

$$S'_{o,c\ell}(\vec{X}_2,\vec{X}_1;\omega) = \frac{m}{2}\left[\dot{\vec{X}}_c(\tau)\cdot\vec{X}_c(\omega)\right]\Big|_{\tau=o}^{\tau=t} + \frac{1}{2}\int_0^t d\tau\vec{f}(\tau)\cdot\vec{X}_c(\tau). \qquad \text{B.5}$$

The integro-differential equation (B.4) is solvable and so the complete solution of $\vec{X}_c(\tau)$ with the boundary conditions $\vec{X}(o) = \vec{X}_1$ and $\vec{X}(t) = \vec{X}_2$ can be obtained. Inserting $\vec{X}_c(\tau)$ into (B.5), we get

$$\begin{aligned} S'_{o,c\ell}(\vec{X}_2,\vec{X}_1;\omega) &= \frac{m\omega}{4}\cot\frac{\omega t}{2}\,|\vec{X}_2-\vec{X}_1|^2 \\ &+ \frac{m\omega}{2\sin\omega t}\left[\frac{2\vec{X}_2}{m\omega}\cdot\int_0^t d\tau\vec{f}(\tau)\left(\sin\omega\tau - 2\sin\frac{\omega t}{2}\cdot\sin\frac{\omega}{2}(t-\tau)\sin\frac{\omega\tau}{2}\right)\right. \\ &+ \frac{2\vec{X}_1}{m\omega}\cdot\int_0^t d\tau\vec{f}(\tau)\left(\sin\omega(t-\tau) - 2\sin\frac{\omega t}{2}\cdot\sin\frac{\omega}{2}(t-\tau)\sin\frac{\omega\tau}{2}\right) \\ &- \frac{2}{m^2\omega^2}\cdot\int_0^t\int_0^\tau d\tau d\sigma\vec{f}(\tau)\cdot\vec{f}(\sigma)\Big(\sin\omega(t-\tau)\sin\omega\sigma \\ &\left.- 4\sin\frac{\omega}{2}(t-\tau)\sin\frac{\omega\tau}{2}\cdot\sin\frac{\omega}{2}(t-\sigma)\cdot\sin\frac{\omega\sigma}{2}\Big)\right]. \end{aligned} \qquad \text{B.6}$$

By means of (B.1), the action S'_o becomes the action S_o when $\vec{f}$ equals zero. This means that the classical action $S'_{o,c\ell}$ becomes the classical action $S_{o,c\ell}$ when $\vec{f}$'s equal zero. Hence, we find

$$S_{o,c\ell}(\vec{X}_2,\vec{X}_1;\omega) = \frac{m\omega}{4}\cot\frac{\omega t}{2}|\vec{X}_2-\vec{X}_1|^2 . \qquad \text{B.7}$$

APPENDIX C

INTEGRAL FORM OF $<S^n>$

To find the integral form of $<S^n>$, we insert (3.3.19) into (3.4.7), and write the average of S^n, for an integer n, in the form

$$<S^n> = \left(\frac{i}{2h}\right)^n \frac{\xi^n}{(2\pi)^{dn}} \cdot \int_0^t\int_0^t \cdots \int_0^t\int_0^t d\tau_1 d\sigma_1 \ldots d\tau_n d\sigma_n \int_{-\infty}^{\infty} d\vec{k}_1 \ldots \int_{-\infty}^{\infty} d\vec{k}_n e^{-\frac{L^2}{4}\cdot\sum_{m=1}^{n}\vec{k}_m^2}$$

$$\cdot <\exp\{\frac{i}{\hbar}\int_0^t du\, \vec{f}(u)\cdot\vec{X}(u)\}> , \qquad \text{C.1}$$

where the quantity ξ denotes the fluctuation which is defined by (2.5.3), and where the force $\vec{f}$ is given by

$$\vec{f}(u) \equiv \hbar \sum_{m=1}^{n} \vec{k}_m \{\delta(u-\tau_m) - \delta(u-\sigma_m)\}. \qquad \text{C.2}$$

According to Feynman and Hibbs[12], the averaging in (C.1) is called the characteristic functional, and can be done exactly as follows

$$<\exp\{\frac{i}{\hbar}\int_0^t du\vec{f}(u).\vec{X}(u)\}> = \exp\{\frac{i}{\hbar}(S'_{o,c\ell}(\vec{X}_2,\vec{X}_1;\omega) - S_{o,c\ell}(\vec{X}_2,\vec{X}_1;\omega))\}, \qquad \text{C.3}$$

where the actions $S_{o,c\ell}$ and $S'_{o,c\ell}$ are the extremum of the actions S_o and S'_o respectively, and where the function $\vec{f}$ depends explicitly on time, and satisfies (B.1).

To compute $<S>$, we let n = 1 in (C.1), thus, we have

$$\frac{i}{\hbar}\langle S\rangle = -\frac{1}{2\hbar^2}\cdot\frac{\xi}{(2\pi)^d}\cdot\int_o^t\int_o^t d\tau_1 d\sigma_1 \int_{-\infty}^{\infty} d\vec{k}_1 e^{-L^2\vec{k}^2/4}$$

$$\cdot\langle\exp\{\frac{i}{\hbar}\int_o^t du\vec{f}(u)\cdot\vec{X}(u)\}\rangle \quad , \qquad \text{C.4}$$

where $\vec{f}(u) = \hbar\vec{k}_1\{\delta(u-\tau_1) - \delta(u-\sigma_1)\}$. C.5

Refering to (B.7) and (B.6), when $\vec{X}_2 = \vec{X}_1 = 0$, we can easily show that, for dummy variables τ and σ,

$$S_{o,c\ell}(o,o;\omega) = 0, \qquad \text{C.6}$$

$$S'_{o,c\ell}(o,o;\omega) = -\frac{1}{m\omega\sin\frac{\omega t}{2}}\int_o^t\int_o^\tau d\tau d\sigma\vec{f}(\tau)\cdot\vec{f}(\sigma)\{\sin\omega(t-\tau)\sin\omega\sigma$$

$$-4\sin\frac{\omega}{2}(t-\tau)\sin\frac{\omega\tau}{2}\sin\frac{\omega}{2}(t-\sigma)\sin\frac{\omega\sigma}{2}\} \ . \qquad \text{C.7}$$

By performing the integration and grouping the trigonometric function, (C.7) becomes

$$\frac{i}{\hbar}S'_{o,c\ell}(o,o;\omega) = -\frac{i\hbar}{m\omega}\cdot\vec{k}_1^2\cdot\frac{\sin\frac{\omega t}{2}(|\tau-\sigma|)\sin\frac{\omega}{2}(t-|\tau-\sigma|)}{\sin\frac{\omega t}{2}} \ , \qquad \text{C.8}$$

or $$\frac{i}{\hbar}S'_{o,c\ell}(o,o;\omega) = \frac{i\hbar}{2m\omega}\cdot\cot\frac{\omega t}{2}\ \vec{k}_1^2\{1-\Delta(|\tau-\sigma|)\}, \qquad \text{C.9}$$

where $$\Delta(x) = \tan\frac{\omega t}{2}\sin\omega x + \cos\omega x \ . \qquad \text{C.10}$$

Substituting (C.8) and (C.6) into (C.3); and substituting (C.3) into (C.4), we find after performing the $\vec{k}$ - integration

$$\frac{i}{\hbar}\langle S\rangle = -\frac{1}{2\hbar^2}\cdot\frac{\xi}{(4\pi)^{d/2}}\cdot\int_0^t\int_0^t d\tau_1 d\sigma_1\left\{\frac{L^2}{4}+\frac{i\hbar}{m\omega}\cdot\frac{\sin\frac{\omega x}{2}\sin\frac{\omega}{2}(t-x)}{\sin\frac{\omega t}{2}}\right\}^{-d/2}, \qquad \text{C.11}$$

where $x = |\tau - \sigma|$. C.12

Letting $\tau > \sigma$, and setting

$$x = \tau - \sigma , \qquad \text{C.13}$$

and

$$y = \tau + \sigma , \qquad \text{C.14}$$

the integral in (C.11) can be reduced to

$$\int_0^t\int_0^t d\tau d\sigma j(x,\omega;t)^{-d/2} = t\int_0^t dx j(x,\omega;t)^{-d/2} , \qquad \text{C.15}$$

where $$j(x,\omega;t) = \frac{L^2}{4}+\frac{i\hbar}{m\omega}\cdot\frac{\sin\frac{\omega x}{2}\cdot\sin\frac{\omega}{2}(t-x)}{\sin\frac{\omega t}{2}} . \qquad \text{C.16}$$

Finally we have

$$\frac{i}{\hbar}\langle S\rangle = -\frac{1}{2\hbar^2}\cdot\frac{\xi}{(4\pi)^{d/2}}\cdot t\int_0^t dx j(x,\omega;t)^{-d/2} . \qquad \text{C.17}$$

One, can show that, for $n = 2$, (C.1) becomes

$$\langle S^2\rangle = -\frac{1}{4\hbar^2}\cdot\frac{\xi^2}{(4\pi)^d}\cdot\int_0^t\int_0^t\int_0^t\int_0^t d\tau_1 d\sigma_1 d\tau_2 d\sigma_2\{\text{Det } B\}^{-d/2} , \qquad \text{C.18}$$

where $$\text{Det } B = \left[\left\{\frac{L^2}{4}-\frac{i\hbar}{2m\omega}\cdot\cot\frac{\omega t}{2}(1-\Delta_1)\right\}\left\{\frac{L^2}{4}-\frac{i\hbar}{2m\omega}\cdot\cot\frac{\omega t}{2}(1-\Delta_2)\right\} - \left(-\frac{i\hbar}{2m\omega}\cot\frac{\omega t}{2}\right)^2\cdot\frac{\Delta_{12}^2}{4}\right] , \qquad \text{C.19}$$

$$\Delta_i = \Delta(|\tau_i - \sigma_i|), \quad (i = 1,2), \tag{C.20}$$

and

$$\Delta_{12} = \Delta_1 + \Delta_2 - \Delta(|\sigma_1 - \tau_2|) - \Delta(|\tau_1 - \sigma_2|). \tag{C.21}$$

APPENDIX D

EVALUATION OF THE INTEGRAL IN <S>

To evaluate the integral in <S> , we define the integral as

$$I(t) \equiv \int_0^1 d\xi \left\{\sin\frac{\omega t}{2} \, \sin\frac{\omega t}{2}(1-\xi)/\sin\frac{\omega t}{2}\right\}^{-1/2}. \qquad \text{D.1}$$

An equivalent form of (D.1) is given by

$$I(t) = \left(\sin\frac{\omega t}{2}\right)^{1/2} \int_0^1 d\xi \left\{\sin^2\frac{\omega t}{2} - \sin^2\frac{\omega t}{2}(1-2\xi)\right\}^{-1/2}. \qquad \text{D.2}$$

Using the transformation

$$\cos\emptyset = \frac{\sin\frac{\omega t}{4}(1-2\xi)}{\sin\frac{\omega t}{4}}, \qquad \text{D.3}$$

the integral (D.2) becomes

$$I(t) = \frac{4}{\omega t}\left(\sin\frac{\omega t}{2}\right)^{1/2} \cdot \int_0^{\pi/2} d\emptyset \left(1 - \sin^2\frac{\omega t}{4}\cos^2\emptyset\right)^{-1/2}. \qquad \text{D.4}$$

If we use a relationship between hyperbolic and trigonometric function

$$i \sin(ax) = \sinh(iax), \qquad \text{D.5}$$

and replace

$$it = \beta, \qquad \text{D.6}$$

we obtain

$$I(t) = \frac{4}{\omega t\sqrt{i}} \left(\frac{\sinh\frac{\omega\beta}{2}}{1 + \sinh^2\frac{\omega\beta}{4}} \right)^{1/2} K(k), \tag{D.7}$$

where $K(k) = \int_0^{\pi/2} d\phi(1 - k^2\sin^2\phi)^{-1/2}$, D.8

and $k = \tanh\frac{\omega\beta}{4}$. D.9

The complete elliptic integral $K(k)$ in (D.7) can be simplified for computational reason by the Landen's transformation[23]

$$K(k) = \frac{1}{(1 + k)} K(k'), \tag{D.10}$$

where $k' \equiv \frac{2\sqrt{k}}{1 + k} = \left(\frac{2}{1 + \coth\frac{\omega\beta}{2}} \right)^{1/2}$. D.11

In the limit of large time, we have

$$I(t) = \frac{4}{\omega t\sqrt{2i}} \cdot k'K(k'), \tag{D.12}$$

where the limiting value of the elliptic integral $K(k')$ is given by[27]

$$\lim_{k'\to 1} K(k') = \frac{1}{2} \ln\left(\frac{16}{k^2}\right), \tag{D.13}$$

and here $(k')^2 \equiv 1 - k^2 = 1 - e^{-\omega\beta}$ D.14

Finally we find

$$I(t) = \left(\frac{2}{\omega t}\right)\left(\frac{2}{i}\right)^{1/2} \cdot \left(\frac{i\omega t}{2} + \ln 4\right) \tag{D.15}$$

APPENDIX E

EVALUATION OF THE Δ-INTEGRAL

The Δ-integral occurs when we consider the leading terms in (4.5.17), and is conveniently defined for an integer n by

$$I_n \equiv \int_0^1\int_0^1 dt_1 ds_1 \Delta^n(|t_1 - s_1|), \qquad \text{E.1}$$

where Δ is related to (C.10) by the relation: x = yt. The integral (E.1) can be simplified by an elementary conformal mapping, which is similar to (C.13) and (C.14), into the form

$$I_n = \int_0^1 d\xi\, \Delta^n(\xi) \quad , \qquad \text{E.2}$$

where $\Delta(\xi) = (e^{-i\omega t\xi} + e^{-i\omega t(1-\xi)})/(1 + e^{-i\omega t})$. E.3

In the limit of large time, we can neglect[12] the exponential $e^{-i\omega t}$ and the integral (E.2), for n = 1, is

$$I_1 = \int_0^1 d\xi\, \Delta(\xi) = \frac{2}{i\omega t}\,. \qquad \text{E.4}$$

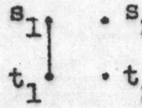
Similarly It can be proved in general that

$$I_n = \left(\frac{2}{i\omega t}\right)\left(\frac{1}{n}\right). \qquad \text{E.5}$$

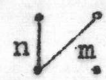
Next we shall show that the leading terms in (4.5.17) are just the I_{2n}'s. To show this, we first consider an integral

$$J_{2n} \equiv \int_0^1\int_0^1\int_0^1\int_0^1 \Delta_{12}^{2n}\, dt_1 ds_1 dt_2 ds_2, \qquad \text{E.6}$$

where Δ_{12} is the same as Δ_{12} in (4.5.17). If one symbolizes the Δ by a line between its points[8], for example,

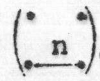
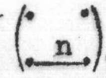
$\Delta(|t_1-s_1|) =$  , E.7

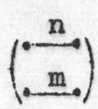
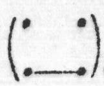
while a product of them can be expressed, e.g.,

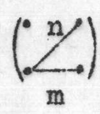
$\Delta^n(|t_1-s_1|)\Delta^m(|t_1-s_2|) =$  , E.8

where each of n and m is an integer.

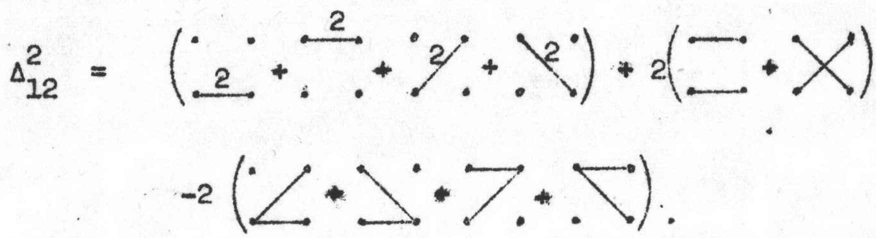
Returning to (E.6), we now consider the orders of the integrals

$\iiiint$  $dt_1 ds_1 dt_2 ds_2 = \iint$  $dt_1 dt_2 \sim t^{-1}$, E.9

$\iiiint$  $dt_1 ds_1 dt_2 ds_2 \sim \left\{\iint\right.$  $\left. dt_1 dt_2\right\}^2 \sim t^{-2}$, E.10

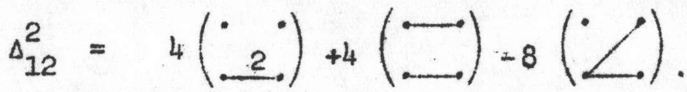
$\iiiint$  $dt_1 ds_1 dt_2 ds_2 \sim t^{-2}$. E.11

We emphasize here that the integrals which yield the results of the order of t^{-1} come only from the integral of a single line type shown in(E.9). According to (E.8), we can write (C.21) in the symbolized form as



E.11

Because of the symmetry of J_{2n}, (E.11) has an equivalent form



E.12

The expression (E.12) implies that the leading term of J_2 is of the order of t^{-1}. Similarly one can prove in general that the leading term of J_{2n} is also of the order of t^{-1}. It means that in the leading term approximation we are look at I_{2n} instead of J_{2n}; thus, we have

$$J_{2n} \rightarrow 4I_{2n} \ . \qquad \text{E.13}$$

APPENDIX F

LLOYD-BEST VARIATIONAL PRINCIPLE

Lloyd and Best[24] formulate an exact variational principle for calculating the density of states over an entire energy range. They showed that it is not $\rho(E)$ or $\ln \rho(E)$ which must be maximized, but the functional

$$P(E) = \int_{-\infty}^{E} dE' \int_{-\infty}^{E'} dE'' \rho(E''). \qquad F.1$$

The functional (F.1) is a pressure of a hypothetical free-fermion system, and has a fascinating analytic relationship to Boltzmann's H-functional.

Recently Sa-yakanit[11] showed in his work that the pressure (F.1) can be simplified by taking an integration by parts

$$P(E) = E' \int_{-\infty}^{E'} dE'' \rho(E'') \Bigg|_{E'=-\infty}^{E'=E} - \int_{-\infty}^{E} dE' E' \rho(E'), \qquad F.2$$

and using the boundary condition that

$$\rho(-\infty) = 0 . \qquad F.3$$

It then follows that

$$P(E,\omega) = \int_{-\infty}^{E} dE'(E - E')\rho(E',\omega). \qquad F.4$$

The result (F.4) is obtained by replacing $P(E)$ and $\rho(E)$ by $P(E,\omega)$ and $\rho(E,\omega)$ respectively for special emphasis on the variational parameter ω .

According to Section 4.2, if we formally set

$$\frac{\alpha^2}{4\beta\xi} = \frac{x^2}{p} , \qquad \text{F.5}$$

where
$$x = \frac{E_\omega}{4} - E , \qquad \text{F.6}$$

and
$$p \sim \omega^{1/2} , \qquad \text{F.7}$$

then we get

$$\rho(x',\omega) \sim \omega^{1/2}(x')^{1/2}\exp\{-(x')^2/p\} . \qquad \text{F.8}$$

By means of (F.6), we now write (F.4) as

$$P(x',\omega) = \int_x^\infty dx'(x' - x)\rho(x',\omega). \qquad \text{F.9}$$

To perform the variational principle, we use the transformation

$$(x')^2 = pz' , \qquad \text{F.10}$$

and then the maximization of the pressure leads us to

$$0 = \frac{d}{d\omega}\omega^{9/8}\int_z^\infty dz' e^{-z'}\{(z')^{1/4} - (z')^{-1/4} . z^{1/2}\}. \qquad \text{F.11}$$

Each integral in (F.11) is an incomplete gamma function[27] which is defined by

$$\Gamma(\alpha, y) \equiv \int_y^\infty dt\ e^{-t}\ t^{\alpha - 1} . \qquad \text{F.12}$$

By using (F.12), (F.11) becomes

$$0 = \frac{d}{d\omega}\ \omega^{9/8}\{\Gamma(\tfrac{5}{4}, z) - z^{1/2}\Gamma(\tfrac{3}{4}, z)\} . \qquad \text{F.13}$$

If one performs the differentiation in (F.13), and uses the identity[27]

$$\frac{d}{dy}\left\{\Gamma(\alpha\ ,y)\right\} = -y^{\alpha-1}\ e^{-y}, \qquad \text{F.14}$$

then

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

Using the asymptotic expansion of the incomplete gamma function[23]

$$\Gamma(\alpha,y) \underset{y \to +\infty}{\simeq} y^{\alpha-1}\ e^{-y}\ , \qquad \text{F.16}$$

one can show that in the case $z \to \infty$

$$\Gamma\ (\tfrac{5}{4}, z) - z^{1/2}\ \Gamma\ (\tfrac{3}{4}, z) = 0. \qquad \text{F.17}$$

Returning to (F.5) and (F.10), we find that z is the exponent of the exponential in the density of states

$$z = \frac{\alpha^2}{4\beta\xi} . \qquad \text{F.18}$$

With (F.18) in the limit $\xi \to 0$, and using (F.17); (F.15) reduces to the familiar minimization of the exponent

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

We thus get the usual variational equation

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

Next we consider the discussion on the end of Section 4.3. When the corrections are included in the density of states, we find the Lloyd-Best variational principle[24] by expanding the exponential of the corrections in series and going beyond the previous steps. This procedure leads us to

$$\rho_n(x',\omega) \quad \sim \quad F_n(\omega)(x')^n(x')^{1/2} \exp\{-(x')^2/p\}, \qquad \text{F.21}$$

where $\rho_n(x',\omega)$ is the n th term of the density of states in power of x', and $F_n(\omega)$ is the function of ω corresponding to $\rho_n(x',\omega)$. Using pressure $P_n(x',\omega)$ defined for (F.21), and we find $P_n'(x',\omega)$ as

$$\frac{d}{d\omega} P_n(x',\omega) \quad = \quad \frac{d}{d\omega} E_n(\omega)\{\Gamma(\frac{5+2n}{4},z) - z^{1/2}\ \Gamma(\frac{3+2n}{4},z)\}$$

$$-E_n(\omega)\{\frac{1}{2\sqrt{z}}\ \Gamma(\frac{3+2n}{4}\ ,z)\}\ \frac{dz}{d\omega}\ , \qquad \text{F.22}$$

where $E_n(\omega)$ is the function of ω corresponding to $F_n(\omega)$. According to (F.16), we see that the two terms in the first parenthesis {} in (F.22) cancel each other in the limit $z \to \infty$, or equivalently $\xi \to o$. Moreover, we find the maximization of the pressure $P(x',\omega)$ is in the form

$$0 \quad = \quad \frac{d}{d\omega} P(x',\omega) \quad = \quad \sum_{n=1}^{\infty} C_n \frac{d}{d\omega} P_n(x',\omega), \qquad \text{F.23}$$

where C_n is the constant of (F.21), and is explicitly independent of ω. In the limit of small ξ , (F.22) implies that (F.23) has a common factor $\frac{dz}{d\omega}$. It means that (F.19) is held, and (F.20) is also true.

Finally we should emphasize that (F.21) and (F.22) are also true even if the n in $(x')^n$ and $\Gamma(\alpha,y)$ is a fraction. This occurs when we include the effect of changing dimension of the white noise model in n . It implies that our proof is valid for all dimensionalities of the white noise model.