CHAPTER V

THE DENSITY OF STATES

In previous chapter an approximate expression for the averaged propagator was obtained. In this chapter we will use the result of the previous chapter to calculate the density of states. Particular attention is given to considering the behaviour of the density of states with the finite correlation length L as one adjustable parameter and comparing our results with the direct measurements of Kukushin and Timofeev [15].

The Density of States

If we have a function N(E) which is the total number of states at a given energy E of an electron-atom system, then a function which is called the density of states is defined by

$$n(E) = \frac{d\,N(E)}{dE} \tag{5.1}$$

or, equivalently

$$n(E) = \frac{1}{V}\sum_{n=1}^{\infty}\delta(E - E_n), \tag{5.2}$$

when E_n is the energy of the nth eigenstate, V is the volume of the system. If the system is disordered, we must average (5.2) over the statistical ensemble for the random potential. It is convenient to consider the density of states in the form of (5.2),

so that in order to apply the path integral method to (5.2), one converts the right hand side into an integral form to get [38],

$$n(E) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \exp\left[(i/\hbar) Et \right] \mathrm{Tr}\, K(\vec{r}, \vec{r}'; t)\, dt \quad (5.3)$$

where the operator Tr denotes the trace of K. The function K is a retarded propagator describing the propagation of an electron from point $\vec{r}$ to point $\vec{r}'$, being the vector positions of the electron in d dimensions. If the propagator K is invariant under translation of $\vec{r}$, then

$$K(\vec{r}, \vec{r}'; t) = K(\vec{r} - \vec{r}'; t) \quad (5.4)$$

so that for finding the density of states, the end point and the initial point must be the same. It, therefore, follows that

$$n(E) = \frac{A}{2\pi\hbar}\int_{-\infty}^{\infty} K(0, 0; t) \exp\left(\frac{i}{\hbar} Et\right) dt, \quad (5.5)$$

where K(0, 0; t) has been evaluated in chapter IV, expression (4.25).

Substituting expression (4.25) into (5.5) we get

$$n(E) = (A/\pi\hbar)\, \mathrm{Re} \int_{0}^{\infty} \exp\left[\frac{i}{\hbar} \{ (E - E_n) t + f(t) \} \right] dt \quad (5.6)$$

where $E_n = (n + \frac{1}{2})\hbar\omega_c$ are the electron energies for the LL's

and

$$f(t) = -\frac{\xi_L t}{2\hbar^2}\int_0^t \left\{ 1 + 8i\frac{E_L}{E_\omega}\sin\left(\frac{\omega}{2}(\tau - y)\right)\frac{\sin\frac{\omega y}{2}}{\sin\frac{\omega t}{2}} \right\}^{-1} dy .$$

The DOS in (5.6) cannot be evaluated analytically due to the complicated part in the exponential term of K(0, 0; t) in (4.27). But we can consider the behaviour of the DOS by making a large-time approximation where (5.6) has an analytic form

$$n(E) = n_0\hbar\omega\left(2\pi\Gamma^2\right)^{-\frac{1}{2}}\sum_{n=0}^{\infty}\exp\left[-(E - E_n)^2/2\Gamma^2\right] \qquad (5.7)$$

where n_0 is a constant, $n_0 = \frac{m}{\pi\hbar^2}$ and the width parameter is

$$\Gamma^2 = \xi_L\frac{x}{4 + x} . \qquad (5.8)$$

The n(E) in (5.7) is clearly a sum of Gaussians centered at the LL energies E_n. The width of the Gaussian Γ is a function of magnetic field, through $x = \hbar\omega/E_L = (2e/\hbar c)BL^2$, and of W(L) and L through $\xi_L = W(L)/\pi L^2$. Clearly as $\Gamma \to 0$, n(E) reduces to a sum of delta functions, $n(E) = n_0\hbar\omega_c\sum_n \delta(E - E_n)$. Typically observed [7-15] values of Γ are $\Gamma \approx 1$ meV or $\Gamma \approx 2$ meV at B = 5T (see Fig. 10 in chapter IV)

The limits of Γ are interesting. For low B or short L, $x \leq 4$, $\Gamma^2 \rightarrow \xi_L x/4$ and Γ is approximately proportional to $B^{1/2}$, as observed. Since $\xi_L x$ is independent of L, the magnitude of Γ is determined chiefly by the magnitude of the potential fluctuations W(L) at moderate B. For large B and long L where $x >> 4$, $\Gamma^2 \rightarrow \xi_L$ and Γ becomes independent of B. The white-noise limit is

$$\Gamma^2_{WN}(B,0) = \lim_{L \to 0} \Gamma^2(B,L) = \xi_L \frac{x}{4} = \frac{1}{2} n_0 \hbar\omega W(0) \tag{5.9}$$

As was shown in Ref. [28, 31, 32], Γ_{WN} is proportional to $B^{1/2}$ and to W(0). In this limit n(E) is also a sum of Gaussians.

The present n(E) in (5.8) can display a substantial DOS between LL's depending upon the values of W(L). The value of L depends upon the origin of the disorder. If it is due to screened, charged impurities, L will be approximately equal to the screening length. The role of L here is to set the energy scale via $E_L = \hbar^2/2mL^2$. For $L = 100$ Å, $E_L = 0.4$ meV. Let us assume, just to set scales, that $E_L = 1$ meV. It is convenient to represent n(E) in dimensionless units with all energies scaled by E_L, i.e., we define

$$\xi_L' = \frac{\xi_L}{E_L^2}, \quad \nu = \frac{E}{E_L}, \quad \Gamma'^2 = \frac{\xi_L'}{1 + \frac{4}{x}} = \frac{\xi_L}{E_L^2} \tag{5.10}$$

so that

$$n(\nu) = \left(\frac{1}{2\pi\Gamma'^2}\right)^{1/2} \sum_{n=0}^{\infty} \exp\left(\frac{-1}{2} \frac{\left(\nu - \left(n + \frac{1}{2}\right)x\right)^2}{\Gamma'^2} \right). \tag{5.11}$$

The dependence of the DOS for adjacent LL's on x for $\xi_L' = 1$ is shown in Fig. 11. The DOS between LL's is essentially zero at x = 4 but increases substantially as x decreases to 2 (B ≈ 1.5 T). Basically, as the spacing between LL's decreases a significant DOS between LL's develops. In Fig. 12 we show the dependence of n(E) on ξ_L' for x = 5. As ξ_L' increases from 1 to 5, a substantial DOS between the LL's develops.

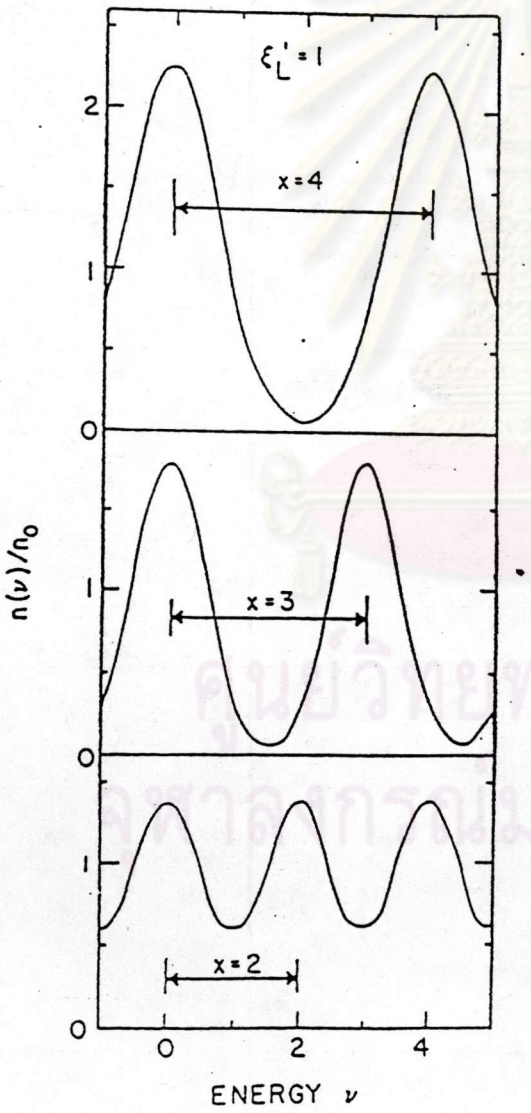

Fig. 11 DOS from eq. (5.11) for $\xi_L' = 1$ and $2 \le x \le 4$.

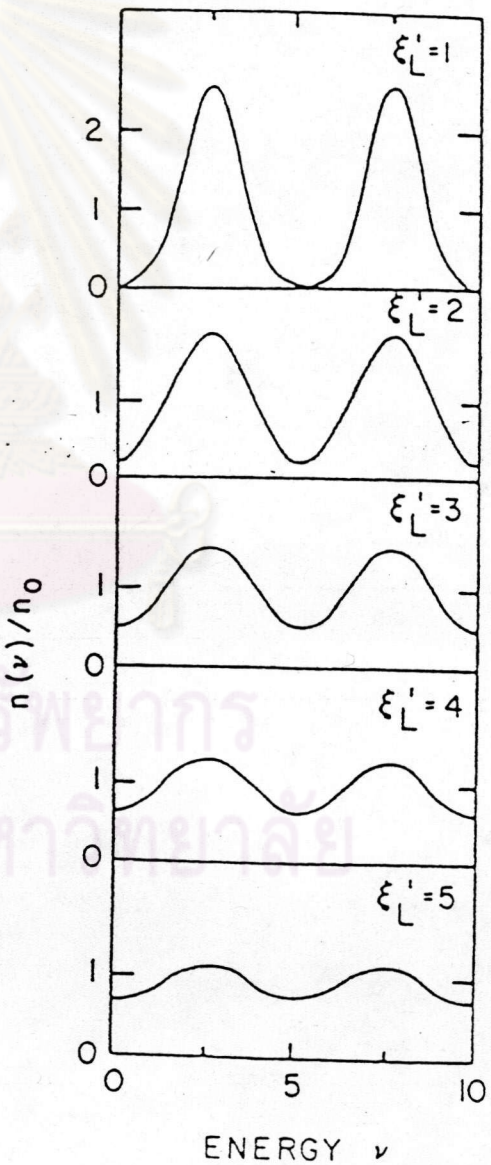

Fig. 12 DOS from eq. (5.11) for x = 5 and $1 \le \xi_L' \le 5$.

We may make comparison with experiment by noting that the DOS in Fig. 12 for $\xi_L' = 4$ and $x = 5$ is very similar to that extracted from a de Haas-van Alphen measurement by Eisenstein et al. [14] shown in Fig. 10. That is, our DOS for $\xi_L' = 4$ and $x = 5$ reproduces the observes value [14] for which $\Gamma = 2.2$ meV at $B = 5T$ ($\hbar\omega = 8.7$ meV). We may use these values in $\Gamma^2 = E_L^2 \xi_L^2 / (1 + 4/x)$ to obtain E_L, giving $E_L = 1.5$ meV. This corresponds to a correlation length $L \approx 50$ Å and $\xi_L' = 10$ meV. A substantial DOS between LL's therefore follows readily from (5.8) or (5.11), for reasonable values of L and ξ_L'.

However, the width Γ of every LL is equal which seems to contradict the direct measurement of Kukushkin and Timofeev using radiative recombination spectra of two-dimensional electrons in a MOS inversion layer [15]. It is certainly a result of using the long-time limit that we obtain a value Γ which is independent of the Landau index. To avoid such an approximation, numerical integration can be used to evaluate the integral in (5.6) exactly and then comparison with experiments can be done to justify our expression for n(E). It is known that optical spectroscopy of two-dimensional electrons makes it possible to study the entire n(E) dependence and yield $n(E_F)$. In all other experiments, one determines only the thermodynamic DOS, i.e. the quantity dn/dE_F, which is in general not equal to $n(E_F)$. So it is more reasonable to compare our numerical results with the magneto-optic experiments.

To calculate the density of states from (5.6), we write

$$n(E) = n_0 (2/\pi) \sum_{n=0}^{\infty} \int_0^{\infty} dt \, \mathrm{Re} \exp\left\{ 2i\left[v/x - (n + \tfrac{1}{2}) \right] t + f'(t) \right\} \tag{5.12}$$

where

$$f'(t) = \frac{-t \sin t}{2ix} \xi_L' \int_0^t dy \frac{1}{[(x/4i)\sin t - \cos t + \cos y]}. \quad (5.13)$$

The integration in (5.13) can be performed analytically. We take $\omega t/2 = N\pi + \theta$, where $N = 0, 1, 2, \ldots$ and $-\pi/2 \le \theta \le \pi/2$, so that (5.12) becomes

$$n(E) = n_0 \sum_{n=0}^{\infty} K\left((\nu - x(n + \tfrac{1}{2})) \right), \quad (5.14)$$

where

$$K(\nu) = (2/\pi) \int_0^{\infty} dt \, \mathrm{Re} \exp\left(2i\nu/x + f'(t) \right) \quad (5.15)$$

with

$$f'(t) = -(N\pi + \theta)\xi' \frac{\sin\theta}{2ix\sqrt{a^2 - 1}} \left[N\pi + 2\tan^{-1}\left(\frac{\sqrt{a-1}}{\sqrt{a+1}} \tan(\theta/2) \right) \right] \quad (5.16)$$

and $a = (x/4i)\sin\theta - \cos\theta, \quad |a - \sqrt{a^2 - 1}| < 1. \quad (5.17)$

The time integral is then performed by using Gaussian quadrature. Figure 13 shows the DOS and its energy dependence from the radiation spectra obtained from the MOS structure for $n = 2.7 \times 10^{12}$ cm^{-2} at T = 1.6 K in a magnetic field B = 0 (figure 13, spectrum 1) and B = 7 T perpendicular to the two-dimensional layer (figure 13, spectrum 2, $\nu = 16$, $N \le 4$). From our expression in (5.14) by choosing an

appropriate ξ_L = 6.8 meV^2 with L = 97 Å corresponding to $E_L = \hbar^2/2mL^2$ = 2 meV (using m = 0.2 m_e as in the experiments), our numerical results for the DOS can fit the experiments very well as shown in Fig. 13 (broken curve). Although our results for the DOS between LL' s seem to be a little lower than those obtained in experiments by the magneto-optic method, they are acceptable because of the tendency of peak-height increasing and peak-width decreasing as the Landau index increases, and are in good agreement.

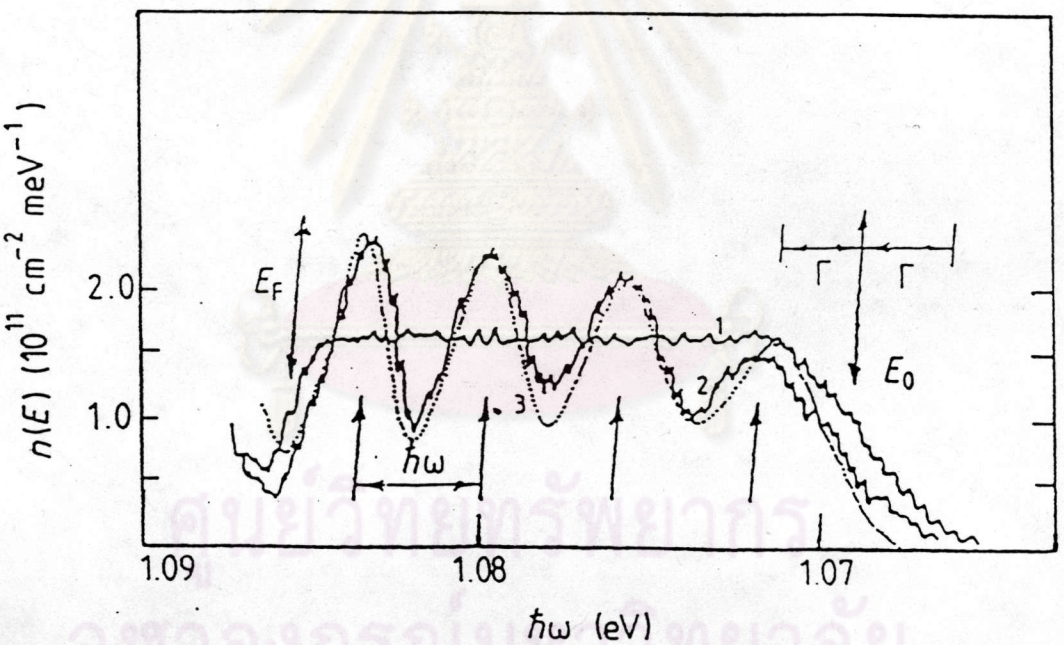

Fig. 13 Curves 1 and 2 show the emission spectra of 2D electrons found for T = 1.6 K with B = 0 (spectrum 1) and B = 7 T, $\hbar\omega$ = 4 meV (spectrum 2). Curve 3 (broken curve) shows the numerical result for the DOS using ξ_L = 6.8 meV^2 with L = 97 Å. The magnitude of the DOS at B = 0, $n_0 = 1.6 \times 10^{11}$ cm^{-2} meV^{-1}, was found by equating the integrated emission intensity in spectra 1 and 2.

Although the first cumulant approximation is sufficient to obtain an appropriate DOS which compares very well with experiment [15], some results for the first cumulant approximation as shown in Fig. 14 suggest that the approximate DOS can take on negative values when the energies of the electron are higher, which is unphysical. To overcome this, we could consider going beyond the first-order cumulant approximation.

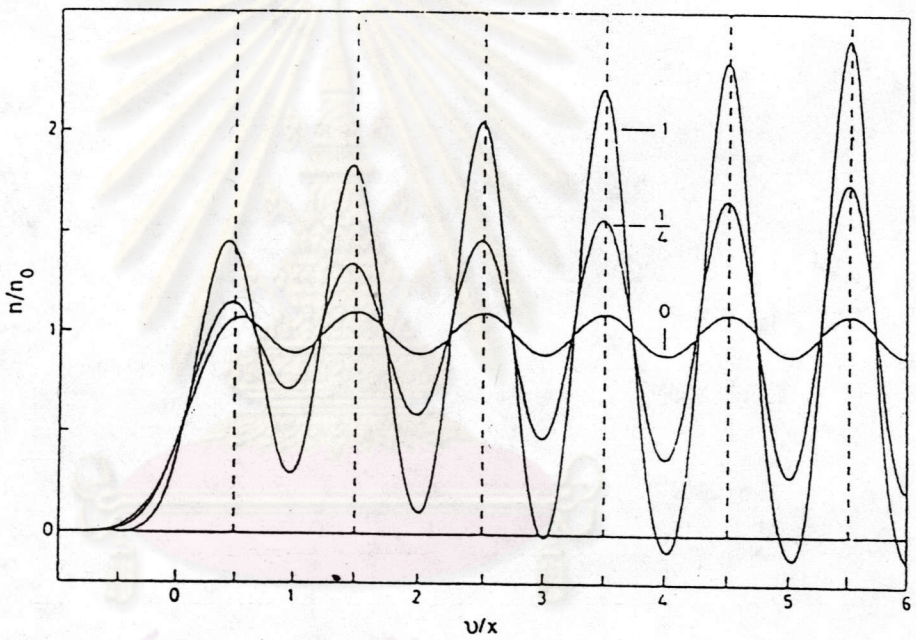

Fig. 14 Plot of the approximate density of states, n, coming from (5.6) as a function of the energy v/x for three different values of the correlation function length L and a fixed variance ξ_L. Numbers attached to the curve are values of 1/x. Here the units are chosen such that m = 1, e = 1.

Second-Order Cumulant Approximation

Approximating expression (4.19) by using the second cumulant, we have

$$K_1(0,0;t) = K_0(0,0;t)\exp\left[\frac{i}{\hbar}\langle S - S_0\rangle - \frac{1}{2\hbar^2}\left\{\langle (S-S_0)^2\rangle - \langle S - S_0\rangle^2\right\}\right] \tag{5.18}$$

From eq. (4.11) and (4.16) we can write

$$S - S_0 = \frac{i}{2\hbar}\frac{W(L)}{\pi L^2}\int_0^t d\tau \int_0^t d\sigma \exp\left[-(\vec{r}(\tau)-\vec{r}(\sigma))^2/L^2\right]$$

$$= \frac{i}{2\hbar}W(L)\int_0^t d\tau\int_0^t d\sigma\int_0^t \frac{d\vec{k}}{(2\pi)^2}\exp\left[-\frac{k^2L^2}{4} + i\vec{k}\cdot(\vec{r}(\tau)-\vec{r}(\sigma))\right] \tag{5.19}$$

then we have

$$\langle S - S_0\rangle = \frac{i}{2\hbar}\frac{W(L)}{\pi L^2}\int_0^t d\tau\int_0^t d\sigma \frac{1}{1+\frac{4i\hbar}{L^2}\frac{\sin\frac{\omega}{2}(t-|\tau-\sigma|)\sin\frac{\omega}{2}|\tau-\sigma|}{m\omega\sin\frac{\omega t}{2}}} \tag{5.20}$$

also

$$(S-S_0)^2 = -\frac{1}{4\hbar^2}\{W(L)\}^2\int_0^t d\tau\int_0^t d\sigma\int_0^t\frac{d\vec{k}}{(2\pi)^2}\exp\left(-\frac{k^2L^2}{4}\right)$$

$$\cdot\int_0^t d\tau'\int_0^t d\sigma'\int_0^t\frac{d\vec{k}'}{(2\pi)^2}\exp\left(-\frac{k'^2L^2}{4}\right)$$

$$\cdot \exp\left[\, i\vec{k}\cdot\left(\vec{r}(\tau)-\vec{r}(\sigma)\right)+ i\vec{k}'\cdot\left(\vec{r}(\tau')-\vec{r}(\sigma')\right)\right]$$

$$= -\frac{1}{4\hbar^2}\{W(L)\}^2\int_0^t d\tau\int_0^t d\sigma\int_0^t d\tau'\int_0^t d\sigma'\int_0^t\frac{d\vec{k}}{(2\pi)^2}\int_0^t\frac{d\vec{k}'}{(2\pi)^2}$$

$$\cdot\ \exp\left\{-\frac{(k^2+k'^2)L^2}{4}\right\}\cdot\ \exp\left\{\frac{i}{\hbar}\int_0^t d\xi\,\vec{f}\,(\xi)\cdot\vec{r}\,(\xi)\right\} \tag{5.21}$$

where $\vec{f}\,(\xi) = \hbar\vec{k}\left[\delta(\xi-\tau)-\delta(\xi-\sigma)\right]+\hbar\vec{k}'\left[\delta(\xi-\tau')-\delta(\xi-\sigma')\right]$ is the generating function. From Feynman and Hibbs (1965, p.184) the characteristic functional can be expressed as

$$\left\langle \exp\left\{\frac{i}{\hbar}\int_0^t d\xi\,\vec{f}\,(\xi)\cdot\vec{r}(\xi)\right\}\right\rangle$$

$$= \exp\left\{-\frac{i}{\hbar}\frac{1}{m\omega\sin\frac{\omega t}{2}}\int_0^t d\xi\int_0^t d\xi'\,\vec{f}^{\,\dagger}(\xi)\,g(\xi,\xi')\,\vec{f}(\xi')\right\} \tag{5.22}$$

where

$$g(\xi,\xi') = \left\{\sin\frac{\omega\xi}{2}\sin\frac{\omega}{2}(t-\xi')\,H(\xi'-\xi)\right.$$

$$\left.+\ \sin\frac{\omega}{2}(t-\xi)\sin\frac{\omega\xi'}{2}\,H(\xi-\xi')\right\}\cdot\exp\left\{-\frac{\omega}{2}J(\xi-\xi')\right\}$$

$$= \frac{1}{2}\left\{\cos\frac{\omega}{2}\left(t-\left(\xi+\xi'\right)\right)-\cos\frac{\omega}{2}\left(t-\left|\xi-\xi'\right|\right)\right\}$$

$$\cdot\left(\cos\frac{\omega}{2}(\xi-\xi')-J\sin\frac{\omega}{2}(\xi-\xi')\right). \tag{5.23}$$

We employ the 2x2 matrices introduced by Papadopoulos [39] in his work on the magnetization of harmonically bound charges

$$J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{5.24}$$

which obey the relation $J^2 = -I$, and $e^{\pm J\varphi}$ has the property

$$e^{\pm J\varphi} = I\cos\varphi \pm J\sin\varphi \tag{5.25}$$

If we would like to expand the cumulant until the n order of approximation, then we can write the generating function in general form as

$$\vec{f}(\xi) = \hbar \sum_{i=1}^{n} \vec{k}_i \left[\delta(\xi - \tau_i) - \delta(\xi - \sigma_i) \right] \tag{5.26}$$

So we have

$$\int_0^t d\xi \int_0^t d\xi' \vec{f}^{\,\dagger}(\xi)\, g(\xi - \xi')\, \vec{f}(\xi')$$

$$= \hbar^2 \sum_{ij} \vec{k}_i^{\,\dagger} \left[g(\tau_i - \tau_j) - g(\tau_i - \sigma_j) - g(\sigma_i - \tau_j) + g(\sigma_i - \sigma_j) \right] \vec{k}_j \tag{5.27}$$

in general form. Next, we define

$$B_{ij} = \frac{L^2}{4}\delta_{ij} - \frac{i\hbar}{2m\omega \sin\frac{\omega t}{2}} \left[g(\tau_i - \tau_j) - g(\tau_i - \sigma_j) - g(\sigma_i - \tau_j) + g(\sigma_i - \sigma_j) \right]$$

as a 2x2 matrix. Then $\langle (S - S_0)^n \rangle$ can be written as

$$\langle (S - S_0)^n \rangle = \left(\frac{iW(L)}{2\hbar} \right)^n \prod_i \int_0^t d\tau_i \int_0^t d\sigma_i \frac{1}{(2\pi)^n} \frac{\pi^n}{(\det B)^{1/2}} \tag{5.28}$$

Here we consider only the second cumulant and define

$$\langle S - S_0 \rangle_2 = \langle (S - S_0)^2 \rangle - \langle S - S_0 \rangle^2$$

$$\langle (S - S_0)^2 \rangle = \left(\frac{\hbar \xi'_L t^2 \sin t}{2x} \right)^2 \int_0^1 d\tau_1 \int_0^1 d\sigma_1 \int_0^1 d\tau_2 \int_0^1 d\sigma_2 \frac{1}{B_{11} B_{22} - |B_{12}|^2}$$

$$\langle S - S_0 \rangle = \frac{\hbar \xi'_L t^2 \sin t}{2x} \int_0^1 d\tau_1 \int_0^1 d\sigma_1 \frac{1}{B_{11}}$$

$$\langle S - S_0 \rangle^2 = \left(\frac{\hbar \xi'_L t^2 \sin t}{2x} \right)^2 \int_0^1 d\tau_1 \int_0^1 d\sigma_1 \int_0^1 d\tau_2 \int_0^1 d\sigma_2 \frac{1}{B_{11} B_{22}}$$

where $B_{ij} = \frac{x}{4i} \sin t \delta_{ij} - [g(\tau_i - \tau_j) - g(\tau_i - \sigma_j) - g(\sigma_i - \tau_j) + g(\sigma_i - \sigma_j)]$

and $g(y) = \cos t (1 - |y|) e^{ity}$.

So we can write the second cumulant as

$$\langle S - S_0 \rangle_2 = \left(\frac{\hbar \xi'_L t^2 \sin t}{2x} \right)^2 \int_0^1 d\tau_1 \int_0^1 d\sigma_1 \int_0^1 d\tau_2 \int_0^1 d\sigma_2$$

$$\cdot \left(\frac{1}{B_{11}\, B_{22} - |B_{12}|^2} - \frac{1}{B_{11}\, B_{22}} \right). \qquad (5.29)$$

From expression (5.18), The averaged propagator can be written as

$$K_1(0, 0; t) = K_0(0, 0; t) \exp\left[\frac{i\xi'_L t^2 \sin t}{2x} \int_0^1 d\tau_1 \int_0^1 d\sigma_1 \frac{1}{B_{11}} \right.$$

$$- \frac{\xi'^2_L t^4 \sin^2 t}{8x^2} \int_0^1 d\tau_1 \int_0^1 d\sigma_1 \int_0^1 d\tau_2 \int_0^1 d\sigma_2$$

$$\left. \cdot \left(\frac{1}{B_{11}\, B_{22} - |B_{12}|^2} - \frac{1}{B_{11}\, B_{22}} \right) \right]. \qquad (5.30)$$

Finally, we can calculate the density of states as

$$n(E) = (A/\pi\hbar)\, \mathrm{Re} \int_0^\infty \exp\left[\frac{i}{\hbar} \{ (E - E_n) t + f(t) \} \right] dt \qquad (5.31)$$

where $$f(t) = \frac{i\xi'_L t^2 \sin t}{2x} \int_0^1 d\tau_1 \int_0^1 d\sigma_1 \frac{1}{B_{11}}$$

$$- \frac{\xi'^2_L t^4 \sin^2 t}{8x^2} \int_0^1 d\tau_1 \int_0^1 d\sigma_1 \int_0^1 d\tau_2 \int_0^1 d\sigma_2$$

$$\cdot \left(\frac{1}{B_{11}\, B_{22} - |B_{12}|^2} - \frac{1}{B_{11}\, B_{22}} \right) \Bigg].$$

In expression (5.30), the integrals cannot be performed analytically. To avoid this difficulty, we calculate them numerically. The method of numerical calculation is the *Monte Carlo* method [40]. This is a technique which is best suited to the complicated multidimensional integrals.

Monte Carlo Evaluation of Integrals [40]

The basic idea of the Monte Carlo method is to sample the integral statistically, so that, independently of the dimension of the integral, the sampling errors decrease as $1/\sqrt{N}$ where N is the number of points at which the integrand is sampled. The Monte Carlo method for evaluating an integral is based on the familiar central limit theorem. Consider an integral of the following general form

$$I = \int d^n x \, f(\vec{x}) \, P(\vec{x}) \qquad (5.32)$$

where $\vec{x}$ is a vector in n-dimensions and $P(\vec{x})$ is a probability distribution satisfying the condition

$$P(\vec{x}) \geq 0$$

$$\int d^n x \, P(\vec{x}) = 1 \, .$$

Note that there is an infinite freedom, which we will subsequently exploit, to decompose the integrand of any multidimensional integral in the form of eq. (5.31).

We will now try to approximate I by forming the average of N independent samples of the probability distribution $P(\vec{x})$

$$X = \frac{1}{N} \sum_{\substack{i=1 \\ \vec{x}_i \in P(\vec{x})}}^{N} f(\vec{x}_i) \qquad (5.33)$$

where throughout this chapter, the notation $\vec{x}_i \in P(\vec{x})$ indicates that the variable $\vec{x}_i$ is sampled according to the function $P(\vec{x})$. In order to use such an average as a controlled approximation for I, we need to know the probability distribution for the variable X, and especially how this distribution behaves for large N. To simplify notation, it is convenient to define the mean value of a function $g(\vec{x})$ with respect to the distribution $P(\vec{x})$ as follows

$$\langle g \rangle_P \equiv \int d^n x \; g(\vec{x}) P(\vec{x}) . \qquad (5.34)$$

By definition, $\langle f \rangle_P = I$.

The probability for obtaining a particular value X when each $\vec{x}$ is distributed according to $P(\vec{x})$ may be written as follows:

$$\rho(X) = \int \prod_{i=1}^{N} d^n x_i \, P(\vec{x}_i) \, \delta\left(\frac{1}{N} \sum_{j=1}^{N} f(\vec{x}_j) - X \right) . \qquad (5.35)$$

Using the integral representation for the δ-function, the probability distribution for X may be written

$$\rho(X) = \int \prod_{i=1}^{N} d^n x_i \, P(\vec{x}_i) \cdot \frac{N}{2\pi} \int d\lambda \exp\left(iN\lambda X - i\lambda \sum_{j=1}^{N} f(\vec{x}_j) \right)$$

$$= \frac{N}{2\pi} \int d\lambda \exp\left[iN\lambda X + N \ln\left\{ \int d^n y \, P(\vec{y}) \exp\left(- i\lambda f(\vec{y}) \right) \right\} \right] \tag{5.36a}$$

$$\equiv \frac{N}{2\pi} \int d\lambda \exp\left[NF(\lambda, X) \right]$$

where

$$F(\lambda, X) \equiv i\lambda X + g(\lambda) \tag{5.36b}$$

$$g(\lambda) \equiv \ln\left\{ \int d^n y \, P(\vec{y}) \exp\left(- i\lambda f(\vec{y}) \right) \right\}. \tag{5.36c}$$

For a specified value of X, we will perform the λ integral using the stationary phase approximation and denote the stationary value of λ for a given X as $\tilde{\lambda}(X)$. The stationary condition $\left.\frac{\partial F}{\partial \lambda}\right]_{\tilde{\lambda}(X)} = 0$ yields

$$X = ig'(\tilde{\lambda}(X)) = \frac{\int d^n y \, f(\vec{y}) \, P(\vec{y}) \exp\left(- i\tilde{\lambda}(X) f(\vec{y}) \right)}{\int d^n y \, P(\vec{y}) \exp\left(- i\tilde{\lambda}(X) f(\vec{y}) \right)} \tag{5.37}$$

which implicitly defines $\tilde{\lambda}(X)$. Including the quadratic correction $\left.\frac{\partial^2 F}{\partial \lambda^2}\right]_{\tilde{\lambda}(X)} =$ $g''(\tilde{\lambda}(X))$, the probability distribution for large N is

$$\rho(X) = \left[\frac{N}{-g''(\tilde{\lambda}(X))\,2\pi}\right]^{\frac{1}{2}} \exp\left\{ NF(\tilde{\lambda}(X), X)\right\}\left\{1 + O\left(\frac{1}{N}\right)\right\}. \tag{5.38}$$

To display the X-dependence of the exponent explicitly, we first find the extrema

$$\frac{dF(\tilde{\lambda}(X), X)}{dX} = \frac{\partial F}{\partial X} + \frac{\partial F}{\partial \lambda}\frac{d\tilde{\lambda}}{dX} = i\tilde{\lambda}(X) = 0 \tag{5.39}$$

where we have used the stationary condition $\frac{\partial F}{\partial \lambda} = 0$. Note that there is only one solution $\tilde{\lambda}(X) = 0$ for which by eq. (5.37) $X = \langle f \rangle_P$. Expanding to second order around this point

$$\left.\frac{d^2 F\left(\tilde{\lambda}(X), X\right)}{d X^2}\right]_{\tilde{\lambda}=0} = i\left.\frac{d\tilde{\lambda}(X)}{dX}\right]_{\tilde{\lambda}=0}$$

$$= \frac{1}{g''(\tilde{\lambda} = 0)} \tag{5.40}$$

$$= \frac{-1}{\langle f^2 \rangle_P - \langle f \rangle_P^2}$$

where we have differentiated eq. (5.37) with respect to X to evaluate $\frac{d\tilde{\lambda}(X)}{dX}$. Thus $\rho(X)$ has a single maximum at $X = \langle f \rangle_P$ and is monotonically decreasing away from this point with curvature specified by the variance $\langle f^2 \rangle_P - \langle f \rangle_P^2$. No matter what the distribution $P(\vec{x})$, the function $f(\vec{x})$, or the dimension n, for large N the average eq. (5.33) becomes normally distributed about I with standard deviation $\sigma = \frac{1}{\sqrt{N}} \left[\langle f^2 \rangle_P - \langle f \rangle_P^2 \right]^{1/2}$. Thus, a general integral may be approximated

$$\int d^n x \, f(\vec{x}) \, P(\vec{x}) = \frac{1}{N} \sum_{\substack{i = 1 \\ \vec{x}_i \in P(\vec{x})}}^{N} f(\vec{x}_i) \pm \frac{1}{\sqrt{N}} \left[\langle f^2 \rangle_P - \langle f \rangle_P^2 \right]^{1/2} \tag{5.41}$$

and the variance may be evaluated by the usual unbiased estimate

$$\langle f^2 \rangle_P - \langle f \rangle_P^2 \approx \frac{N}{N-1} \left[\frac{1}{N} \sum_i f(\vec{x}_i)^2 - \left(\frac{1}{N} \sum_i f(\vec{x}_i) \right)^2 \right]. \tag{5.42}$$

Note that the factor $\frac{N}{N-1}$ to remove the bias is irrelevant for large N so that one effectively uses eq. (5.41) to evaluate both $\langle f^2 \rangle_P$ and $\langle f \rangle_P^2$.

The great hope is to obtain a result which can be made arbitrarily accurate to within controlled sampling errors. That is, given δ, there exists some N such that

$$\int d^n x \, f(\vec{x}) \, P(\vec{x}) - \frac{1}{N} \sum_{\substack{i = 1 \\ \vec{x}_i \in P(\vec{x})}}^{N} f(\vec{x}_i) < \delta .$$

We must ask at the outset whether the Monte Carlo method is, in fact, as general as this hope suggests. The answer, unfortunately, is no because of two distinct fundamental limitations:

1. The function must be dominantly positive. If the integrals of the positive and negative regions of f are separately much larger in magnitude than their sum, then the stochastic noise will hide the signal for all practical values of N.

2. The probability distribution must be sampled independently over all $\vec{x}$.

From the numerical result (see appendix), we cannot get an important physically. This is because the result from the second-order cumulant expansion can be very large, which is unphysical. These unphysical results do not show us that the Monte Carlo method is not appropriate. However, it shows that the second-order cumulant approximation is not useful. Presumably one would have to calculate all cumulants to get a good physical result. It must be stressed, however, that the first order cumulant approximation is excellent agreement with experiments. We will have some discussion and conclusion in the next chapter.