Chapter VI

DISCUSSION

What has been achieved in the course of this research is the developing of a method for determining the averaged Green function of disordered systems. When this expression is known it permits the determination of the density of states of disordered systems,the values of which are of great interest in connection with many physical properties of disordered systems.

The present research commenced with the study of the original papers setting out the problem of determining the averaged Green function of disordered systems. These earlier papers were concerned with the method of expanding the averaged Green function of disordered systems as a perturbation expansion of the free electron Green function. In this method the problem of obtaining the averaged Green function of disordered systems is reduced to that of finding the two-body correlation function and the Fourier transform of the potential. Since in this method the exponential tail, which is the important characteristic of the density of states of disordered systems, cannot be obtained, the method used in later papers, that of applying Feynman's path integral formalism to the finding of the averaged Green function of disordered systems,must be employed.

In studying the Feynman's path integral, it is necessary to study how the Feynman expression can be formulated and how to evaluated the path integral. In dealing with disordered systems using Feynman's path integral, we have paid particular attention to the model introduced by Edwards and Gulyaev and by Bezák. The explicit formula for the averaged Green function has been obtained by Bezák, but his expression contains an inherent restriction which makes the calculation of the averaged Green function unduly complicated.

The present research started with the same model as that of Bezák and attemped to apply the relevant methods of path integrals to disordered systems. The method used was to write the averaged Green function of disordered systems in the form of free electron measure, and then apply the cumulant theory in order to work out the averaged Green function. The result was that the first cumulant could be obtained explicity.

Using only the first cumulant, the expression obtained for the averaged Green function is

$$\langle G(\underline{x},\underline{x}';\beta)\rangle = \exp\left(\frac{\eta^2\beta^2}{2}\right)\left(\frac{m}{2\pi\hbar^2\beta}\right)^{3/2}\exp\left\{-\frac{m(\underline{x}-\underline{x}')^2}{2\hbar^2\beta}\left(1+\frac{\omega_G^2\hbar^2\beta^2}{12}\right)\right\}\exp\left(-\frac{\omega_G^2\hbar^2\beta^2}{24}\right).$$

Comparing this expression with that of Bezák,

$$\langle G(\underline{x},\underline{x}';\beta)\rangle = \exp\left(\frac{\eta^2\beta^2}{2}\right)\left(\frac{m}{2\pi\hbar^2\beta}\right)^{3/2}\exp\left(-\frac{m_G(\underline{x}-\underline{x}')^2}{2\hbar^2\beta}\right)\left(\frac{\gamma}{\sinh\gamma}\right)^{3/2}\prod_{n=1}^{\infty}\left\{\frac{\pi(n-\frac{1}{2})}{(\gamma^2+\xi_n^2)^{1/2}}\right\}^3,$$

where $\omega_G = \frac{\eta}{L}\left(\frac{2\beta}{m}\right)^{\frac{1}{2}}$, $m_G = m\gamma\coth\gamma$, $\beta = \frac{1}{k_B T}$

$\gamma = \frac{1}{2}\beta\hbar\omega_G$ and with the restriction that

$$\left\{ 1+\left(\frac{\xi_n}{\gamma}\right)^2 \right\} \xi_n = \tan \xi_n .$$

It can be seen that these two expressions are nearly of the same form. It will be shown below thatthe factor $m\left(1+\frac{\omega_G^2\hbar^2\beta^2}{12}\right)$ corresponds to the effective mass m_G in the Bezák's expression; and the factor $\exp\left(-\frac{\omega_G^2\hbar^2\beta^2}{24}\right)$ probably corresponds to the factor in his expression resulting from the deviation from the classical path $F_\gamma(\hbar\beta)$.

By changing $\coth\gamma$ in Bezák's expression for m_G into $\frac{\exp(\gamma)+\exp(-\gamma)}{\exp(\gamma)-\exp(-\gamma)}$, expanding the exponential terms, and rearranging the terms, we will obtain a value for m_G in Bezák's expression equals to $1+\frac{\hbar^2\beta^2\omega_G^2}{12}-\frac{\hbar^4\beta^4\omega_G^4}{1152}+ \cdots\cdots$.

Thus our factor $m\left(1+\frac{\hbar^2\beta^2\omega_G^2}{12}\right)$ in our expression appears to be nearly equivalent to the effective mass m_G in Bezák's expression. The next higher terms in the expansion of m_G could not be obtained because at this stage is considered only the first cumulant which is a rather rough approximation. If therefore we consider much higher order cumulants, the contribution from these higher cumulants may be added and we believe that if this is done, this factor in our expression then will correspond to the effective mass m_G of Bezák's expression. We have attempted to relate the factor $\exp\left(-\frac{\omega_G^2\hbar^2\beta^2}{24}\right)$ to the Bezák factor $F_\gamma(\hbar\beta)$ by using the limiting cases, i.e. when β is very high and very low respectively, but we did not succeed because the term ζ_n cannot be obtained explicitly from the transcendental equation.

An evaluation for 2nd cumulant was attempted and the result could again be determined explicitly, so it seems as if all the higher order cumulants may also be determined explicitly. If we could find the n^{th} cumulant, we should obtain an explicit expression for the averaged Green function of disordered systems without restriction. Unfortunately due to the complicated nature of the higher cumulants, this has not been worked out.

Instead of finding the n^{th} cumulant, if we could find a general expression for a cumulant of the n^{th} order, thus would simplify the problem.

There is also another method in which every step in evaluating the averaged Green function of disordered systems is exactly the same as the method used in chapter V, except for the first step, in which instead of writing the averaged Green function in the form of the free electron measure we write it in the form of a harmonic oscillator measure. Using this latter method, and evaluating the first cumulant only, will yield considerable information. But the integral in time in this latter method is quite difficult to calculate.