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An average propagator of a disordered system

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Abstract. The path integral of an average propagator which arose from Edwards' model of an electron in a random system, is investigated using a technique employed by Feynman for the purpose of handling a polaron problem. The method consists of writing the average propagator as an expectation of the exponential of a correlation function. By expanding the exponential in a power series of the correlation function and considering the nth order moment, it is possible to evaluate the path integral involved analytically. The method is valid for general forms of correlation functions.

An application of the resulting expression to a gaussian correlation function is made. In this case, an approximate result for the diagonal part of the average propagator is obtained explicitly. A discussion is given of an exponential correlation function and the possible implication to extended states is also mentioned.

1. Introduction

Edwards and Gulyaev (1964) first pointed out that by using the Feynman path integral formalism, it is possible to express the average propagator of a completely random system in a closed form (see also Lukes 1965, 1966). The advantage of using such a formalism is that the ensemble average can be carried out at the beginning. This is in contrast with the standard perturbation of the Green function where the ensemble average has to be carried out term by term. Also in this formalism, the fluctuating potential which plays an important role in disordered systems, is automatically built into the formalism.

For a model of an electron moving in a completely random system containing dense and weak scatterers, the average propagator can be expressed as (Edwards 1970)

$$G(\boldsymbol{r}, \boldsymbol{r}'; t) = N \int D(\text{path}) \exp\left\{\frac{\mathrm{i}}{\hbar}\frac{m}{2}\int_0^t \dot{\boldsymbol{r}}^2(\tau)\,\mathrm{d}\tau - \frac{\rho}{2\hbar^2}\int_0^t\int_0^t W(\boldsymbol{r}(\tau)-\boldsymbol{r}(\tau'))\,\mathrm{d}\tau\,\mathrm{d}\tau'\right\} \tag{1}$$

where ρ is the density of the scatterers and W is the correlation function of the potential. Here the averaged potential energy is chosen to be zero. This model is, in fact, equivalent to that of Zittartz and Langer (1966) who considered an electron in a gaussian random potential. The equivalence was also pointed out by Halperin and Lax (1966) as a consequence of the central limit theorem.

The correlation W, which characterizes the statistical properties of disordered systems, generally contains arguments defined at two different times. Formally W could be interpreted as a two-body interaction in the sense of many-body theory. Similar interpretation may also be given in the thermodynamic Green function formalism of disordered systems (Fischbeck 1972).

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The actual form of W, in principle, must be determined from the potential V. For instance, if V is a screened Coulomb potential then W will be an exponential function. However, other forms of W may also be assumed such as a gaussian function (Burke and Lebowitz 1968, Bezak 1970).

The average propagator given in equation (1) can be used to discuss many physical properties of disordered systems such as the density of states which is just the Fourier transform of its diagonal part, the localization problem (Freed 1972, Abram and Edwards 1972) and wave propagation in random media (Chow 1972).

Starting from expression (1), a number of different methods of evaluating the path integral have been published. Edwards and Gulyaev (1964) considered a model in which W is quadratic in coordinates, but local in time. This enabled them to evaluate the path integral exactly. Bezak (1970, 1971), on the other hand, retained all the non-local behaviour of the quadratic correlation function and thus was led to solving an integro-differential equation. Burke and Lebowitz (1968) assumed a gaussian correlation function from the outset and then applied the Feynman variational principle, obtaining a result which is essentially the first cumulant. Finally, Jones and Lukes (1969) showed that the path integral can be represented quite generally as a cumulant series.

The purpose of the present paper is to investigate the path integral of expression (1) without assuming the specific form of W. The method consists of writing the average propagator as an expectation of the exponential of a correlation function and then expanding the exponential in a power series of W. Assuming that the Fourier transform of W exists and employing a technique invented by Feynman (1955) for the purpose of handling a polaron problem, the path integral involved in the calculation can be evaluated analytically.

Since the first application to polarons, this technique has only recently been applied to other problems, such as the diamagnetism of conduction electrons (Papadopoulos and Jones 1971) and the Coulomb potential problem (Goovaerts and Devreese 1972). Therefore, it is of interest to try and apply the technique to Edwards' model. In § 2 a general method of evaluating the path integral of expression (1) is given. In § 3 an application of the resulting expression to a gaussian correlation function is made, and in § 4 a discussion of the results is given.

2. General method

Equation (1) may be considered as an expectation of some time ordering functional,

$$G(\boldsymbol{r}, \boldsymbol{r}'; t) = G_0(\boldsymbol{r}, \boldsymbol{r}'; t)\left\langle \exp\left(-\frac{\rho}{2\hbar^2} \int_0^t \int_0^t W(\boldsymbol{r}(\tau) - \boldsymbol{r}(\tau'))\, \mathrm{d}\tau\, \mathrm{d}\tau' \right) \right\rangle, \tag{2}$$

where G_0 is the free particle propagator. The symbol $\langle\ \rangle$ denoted the expectation, is defined by

$$\langle \exp(F[\boldsymbol{r}(\tau)]) \rangle = \frac{\int D(\text{path}) \exp(\frac{1}{2} i m \hbar^{-1} \int_0^t \dot{\boldsymbol{r}}^2(\tau)\, \mathrm{d}\tau) \exp(F[\boldsymbol{r}(\tau)])}{\int D(\text{path}) \exp(\frac{1}{2} i m \hbar^{-1} \int_0^t \dot{\boldsymbol{r}}^2(\tau)\, \mathrm{d}\tau)}, \tag{3}$$

where $F[\boldsymbol{r}(\tau)]$ denotes a functional corresponding to

$$-\frac{\rho}{2\hbar^2} \int_0^t \int_0^t W(\boldsymbol{r}(\tau) - \boldsymbol{r}(\tau'))\, \mathrm{d}\tau\, \mathrm{d}\tau'.$$

Thus equation (3) defines the moment generating function which generates all the moments:

$$\langle \exp(F[\boldsymbol{r}(\tau)]) \rangle = \left\langle \sum_{n=0}^{\infty} T \frac{F[\boldsymbol{r}(\tau)]}{n!} \right\rangle = \sum_{n=0}^{\infty} \frac{\mu_n}{n!}, \tag{4}$$

where T is the time ordering operator and μ_n is the nth order moment.

This series may be rewritten as a series in the exponent (Kubo 1962)

$$\langle \exp(F[\boldsymbol{r}(\tau)]) \rangle = \exp\left(\sum_{n=1}^{\infty} \frac{\kappa_n}{n!} \right) \tag{5}$$

where κ_n is the nth order cumulant. Generally a cumulant of order n may be expressed in terms of moments of orders less than or equal to n. The relation between cumulants and moments is given by Kubo,

$$\kappa_n = \sum_{\substack{\{n_i\} \\ (\Sigma_i i n_i = n)}} (-1)^{\Sigma_i n_i - 1} \left(\sum_i n_i - 1 \right)! \prod_i \left\{ \frac{1}{n!} \left(\frac{\mu_i}{i!} \right)^{n_i} \right\}. \tag{6}$$

The meaning of the restriction is that the sum over all sets of number $\{n_i\}$ must satisfy $\Sigma_i i n_i = n$.

To evaluate the average propagator it is convenient to consider the nth order moment which may be written as

$$\mu_n = T\left(-\frac{\rho}{2\hbar^2} \right)^n \int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_1' \ldots \int_0^t \mathrm{d}\tau_n \int_0^t \mathrm{d}\tau_n' \int D(\text{path}) W(\boldsymbol{r}(\tau_1) - \boldsymbol{r}(\tau_1')) \ldots$$
$$\times W(\boldsymbol{r}(\tau_n) - \boldsymbol{r}(\tau_n')) \exp\left(\frac{\mathrm{i}}{\hbar} \frac{m}{2} \int_0^t \dot{\boldsymbol{r}}^2(\tau)\, \mathrm{d}\tau \right) \left\{ \int D(\text{path}) \exp\left(\frac{\mathrm{i}}{\hbar} \frac{m}{2} \int_0^t \dot{\boldsymbol{r}}^2(\tau)\, \mathrm{d}\tau \right) \right\}^{-1}. \tag{7}$$

By introducing the Fourier transform of W and rewriting equation (7) as

$$\mu_n = T\left(-\frac{\rho}{2\hbar^2} \right)^n \int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_1' \ldots \int_0^t \mathrm{d}\tau_n \int_0^t \mathrm{d}\tau_n' \int \frac{\mathrm{d}\boldsymbol{k}_1}{(2\pi)^3} V(\boldsymbol{k}_1) \ldots \int \frac{\mathrm{d}\boldsymbol{k}_n}{(2\pi)^3} V(\boldsymbol{k}_n) P_n \tag{8}$$

where $V(\boldsymbol{k})$ represents the Fourier transform of W and P_n, the auxiliary propagator, is defined by

$$P_n = \frac{\int D(\text{path}) \exp\{\mathrm{i}\hbar^{-1} \int_0^t (\frac{1}{2} m \dot{\boldsymbol{r}}^2(\tau) + \boldsymbol{f}_n(\tau) \cdot \boldsymbol{r}(\tau))\, \mathrm{d}\tau\}}{\int D(\text{path}) \exp\{\mathrm{i}\hbar^{-1} \int_0^t (\frac{1}{2} m \dot{\boldsymbol{r}}^2(\tau))\, \mathrm{d}\tau\}}. \tag{9}$$

In obtaining equation (9) we have used the fact that

$$\sum_{i=1}^{n} \boldsymbol{k}_i \cdot (\boldsymbol{r}(\tau_i) - \boldsymbol{r}(\tau_i')) = \frac{1}{\hbar} \int_0^t \boldsymbol{f}_n(\tau) \cdot \boldsymbol{r}(\tau)\, \mathrm{d}\tau, \tag{10}$$

where

$$\boldsymbol{f}_n(\tau) = \sum_{i=1}^{n} \hbar \boldsymbol{k}_i \{ \delta(\tau - \tau_i) - \delta(\tau - \tau_i') \}.$$

Formally, P_n can be expressed in terms of actions as

$$P_n = \int D(\text{path}) \exp\left(\frac{\mathrm{i}}{\hbar} S_n \right) \left\{ \int D(\text{path}) \exp\left(\frac{\mathrm{i}}{\hbar} S_0 \right) \right\}^{-1}$$

where S_n, an action associated with f_n, is defined by

$$S_n = \int_0^t (\tfrac{1}{2}m\dot{r}^2(\tau) + f_n(\tau) \cdot r(\tau))\, d\tau \tag{11}$$

and S_0 is the free-particle action. Because of the potential $f_n \cdot r$, P_n may be interpreted as a free particle acted upon by two sets of impulses with equal amplitude $\hbar k_1, \hbar k_2, \ldots, \hbar k_n$ at two different sets of times $\tau_1, \tau_2, \ldots, \tau_n$ and $\tau'_1, \tau'_2, \ldots, \tau'_n$.

Since the action S_n is linear in the coordinates the path integral can be evaluated exactly (see Feynam and Hibbs 1965, p 60), which after the integration only the classical path remains; the paths which deviate from the classical path are cancelled out in the numerator and denominator. The auxiliary propagator then becomes

$$P_n = \exp\left(\frac{i}{\hbar}(S_{c,n} - S_{c,0})\right), \tag{12}$$

where $S_{c,n}$ and $S_{c,0}$ are the corresponding classical actions.

In order to obtain a classical action, a knowledge of the classical path is required. This can be achieved by making a variation on the action S_n which leads to

$$\ddot{r}_{c,n}(\tau) = \frac{f_n(\tau)}{m}, \tag{13}$$

where $r_{c,n}$ denotes the classical coordinate. On integrating equation (13) twice and assuming boundary conditions as $r_{c,n}(0) = r'$ and $r_{c,n}(t) = r$, a classical path is obtained

$$r_{c,n}(\tau) = \sum_{i=1}^{n} \frac{k_i}{m}\left((\tau - \tau_i)H(\tau - \tau_i) - (\tau - \tau'_i)H(\tau - \tau'_i) + (\tau_i - \tau'_i)\frac{\tau}{t}\right) + (r - r')\frac{\tau}{t} + r', \tag{14}$$

where H denotes the Heaviside step function. Upon partial integration and using equation (13), the classical action can be written as

$$S_{c,n} = \left[\frac{m}{2}\dot{r}_{c,n} \cdot r_{c,n}\right]_0^t + \tfrac{1}{2}\int_0^t f_n(\tau) \cdot r_{c,n}(\tau)\, d\tau. \tag{15}$$

Substitution of equation (14) in equation (15) gives

$$S_{c,n} = \frac{m(r - r')^2}{2t} + \frac{(r - r')}{t} \cdot \sum_{i=1}^{n} \hbar k_i(\tau_i - \tau'_i) + \tfrac{1}{2}\sum_{ij} \frac{\hbar^2 k_i \cdot k_j}{m}\{(\tau_i - \tau_j)H(\tau_i - \tau_j) - (\tau_i - \tau'_j)H(\tau_i - \tau'_j)$$
$$- (\tau'_i - \tau_j)H(\tau'_i - \tau_j) + (\tau'_i - \tau'_j)H(\tau'_i - \tau'_j) + (\tau_i - \tau'_i)(\tau_j - \tau'_j)/t\}. \tag{16}$$

As the classical action of a free particle is $m(r - r)^2/2t$, upon using equations (12) and (16), the nth order moment finally becomes

$$\mu_n = T\left(-\frac{\rho}{2\hbar^2}\right)^n \int_0^t d\tau_1 \int_0^t d\tau'_1 \ldots \int_0^t d\tau_n \int_0^t d\tau'_n \int \frac{dk_1}{(2\pi)^3} V(k_1) \ldots \int \frac{dk_n}{(2\pi)^3} V(k_n)$$
$$\times \exp\left\{\frac{i}{\hbar}\left(\frac{(r - r')}{t} \cdot \sum_{i=1}^{n} \hbar k_i(\tau_i - \tau'_i) + \sum_{ij} \frac{\hbar^2}{2m} k_i \cdot k_j A_{ij}\right)\right\}, \tag{17}$$

where

$$A_{ij} = \{(\tau_i-\tau_j)H(\tau_i-\tau_j)-(\tau_i-\tau_j')H(\tau_i-\tau_j')-(\tau_i'-\tau_j)H(\tau_i'-\tau_j)+(\tau_i'-\tau_j')H(\tau_i'-\tau_j') + (\tau_i-\tau_i')(\tau_j-\tau_j')/t\}.$$

This result is general and can be applied to any form of correlation functions. We present an application in the next section.

3. Application

We now proceed by applying the above result to the case in which W is a gaussian function. For simplicity, we shall limit ourselves to the density of states calculation since this will bring us to consider only the diagonal part of the average propagator. We take W of the form

$$W(\boldsymbol{r}-\boldsymbol{r}') = (\pi L^2)^{-3/2}\exp\left(-\frac{(\boldsymbol{r}-\boldsymbol{r}')^2}{L^2}\right),$$

where L represents a characteristic correlation length of the disordered system. The Fourier transform of W is

$$V(\boldsymbol{k}) = \exp(-\tfrac{1}{4}L^2\boldsymbol{k}^2).$$

Substitution of $V(\boldsymbol{k})$ into equation (17), yields

$$\mu_n = T\left(-\frac{\rho}{2\hbar^2}\right)^n \int_0^t \mathrm{d}\tau_1 \int_0^t \mathrm{d}\tau_1' \cdots \int_0^t \mathrm{d}\tau_n \int_0^t \mathrm{d}\tau_n' \int \frac{\mathrm{d}\boldsymbol{k}_1}{(2\pi)^3}\cdots\int\frac{\mathrm{d}\boldsymbol{k}_n}{(2\pi)^3} \times \exp\left(\mathrm{i}\frac{(\boldsymbol{r}-\boldsymbol{r}')}{t}\cdot[k_n]^{\mathrm{T}}[T_n]-[k_n]^{\mathrm{T}}\cdot[B_n]\cdot[k_n]\right) \tag{18}$$

where $[k_n]$ and $[T_n]$ are the column matrices defined as

$$[k_n] = \begin{bmatrix}\boldsymbol{k}_1\\ \boldsymbol{k}_2\\ \vdots\\ \boldsymbol{k}_n\end{bmatrix} \qquad \text{and} \qquad [T_n] = \begin{bmatrix}\tau_1-\tau_1'\\ \tau_2-\tau_2'\\ \vdots\\ \tau_n-\tau_n'\end{bmatrix}$$

and $[B_n]$ is a square matrix of order n with elements defined by

$$B_{ij} = \frac{L^2}{4}\delta_{ij}-\frac{\mathrm{i}\hbar}{2m}A_{ij}.$$

If the sequences of time ordering are chosen such that $\tau_i > \tau_i' > \tau_j > \tau_j'$, for $i > j$ and $\tau_i < \tau_i' < \tau_j < \tau_j'$, for $i < j$ then the matrix element of $[B_n]$ is simplified to

$$B_{ij} = \left(\frac{L^2}{4}+\frac{\mathrm{i}\hbar}{2m}(\tau_i-\tau_i')-\frac{\mathrm{i}\hbar}{2mt}(\tau_i-\tau_i')^2\right)\delta_{ij}-\left(\frac{\mathrm{i}\hbar}{2mt}(\tau_i-\tau_i')(\tau_j-\tau_j')\right)_{i\neq j}. \tag{19}$$

Since the distribution of the $\boldsymbol{k}_i$ is a gaussian distribution, the $\boldsymbol{k}$ integration can be carried out (see Friedman 1956, p 105), the result being

$$\mu_n = \left(-\frac{\rho}{2\hbar^2}\right)^n 2^n n! \frac{\pi^{3n/2}}{(2\pi)^{3n}} \int_0^t \mathrm{d}\tau_1 \int_0^{\tau_1} \mathrm{d}\tau_1' \ldots \int_0^{\tau_{n-1}'} \mathrm{d}\tau_n \int_0^{\tau_n} \mathrm{d}\tau_n' \times \exp\left(\frac{(\boldsymbol{r}-\boldsymbol{r}')^2}{4\hbar^2 t^2}[T_n]^{\mathrm{T}}[B_n]^{-1}[T_n]\right)(\det B_n)^{-3/2} \tag{20}$$

where $\det B_n$ is the determinant of $[B_n]$.

As mentioned above, the interest of this paper is in the density of states, thus by putting $\boldsymbol{r} = \boldsymbol{r}'$, equation (20) reduces to

$$\mu_n = \left(-\frac{\rho}{8\hbar^2\pi^{3/2}}\right)^n n! \int_0^t \mathrm{d}\tau_1 \int_0^{\tau_1} \mathrm{d}\tau_1' \ldots \int_0^{\tau_{n-1}'} \mathrm{d}\tau_n \int_0^{\tau_n} \mathrm{d}\tau_n' (\det B_n)^{-3/2}. \tag{21}$$

This equation is quite complicated, being a $2n$ fold integration. In order to obtain the main contribution, we assume that the matrix $[B_n]$ can be divided into two parts, the diagonal part $[I_n]$ and the off-diagonal part $[B_n']$. Considering first the diagonal part, we see that the determinant of the matrix $[I_n]$ can be written as a product of n first order determinants, which allows the nth order moment μ_n to be written as a product of n terms. The first order moment μ_1 is given by

$$\mu_1 = -\frac{\rho}{8\hbar^2\pi^{3/2}} \int_0^t \mathrm{d}\tau_1 \int_0^{\tau_1} \mathrm{d}\tau_1' \left(\frac{L^2}{4} + \frac{\mathrm{i}\hbar}{2m}(\tau_1 - \tau_1') - \frac{\mathrm{i}\hbar}{2mt}(\tau_1 - \tau_1')^2\right)^{-3/2}. \tag{22}$$

On carrying out the integration,

$$\mu_1 = \frac{\mathrm{i}\rho}{\hbar^3\pi^{3/2}} mt \left(L - \frac{2m\mathrm{i}}{\hbar t} L^3\right)^{-1} \tag{23}$$

and on summing up all the moments,

$$G(\boldsymbol{r}, \boldsymbol{r}; t) = G_0(\boldsymbol{r}, \boldsymbol{r}; t)\left(1 + \mu_1 + \frac{\mu_1^2}{2!} + \ldots + \frac{\mu_1^n}{n!} + \ldots\right) = G_0(\boldsymbol{r}, \boldsymbol{r}; t)\exp(\mu_1) \tag{24}$$

gives finally the first cumulant for the diagonal part of the average propagator.

It is interesting to see the physical meaning of retaining only the diagonal part of $[B_n]$. For this purpose, we consider two limiting cases of L. In the case of large L, as considered by Bezak, equation (23) reduces to

$$\mu_1 = -\frac{\rho t^2}{2\hbar^2\pi^{3/2}L^3}. \tag{25}$$

This result is the same as that obtained by Bezak (1971, equation (48)), if we had defined the gaussian correlation function without the prefactor $(\pi L^2)^{-3/2}$. For small L, equation (23) diverges. This divergence is well known as due to short wavelength potential fluctuations.

To obtain the next contribution, the off-diagonal elements of the $[B_n]$ matrix must be considered. However, in this case the $\det B_n$ is no longer written as a product of lower order determinants in a simple way. Instead of dealing with the determinant, we may use the identity

$$(\det B_n)^{-3/2} = \exp(-\tfrac{3}{2}\,\mathrm{Tr}\,\ln[B_n]).$$

Then by writing

$$[B_n] = [I_n](I + [I_n]^{-1}[B'_n])$$

the trace term becomes

$$\text{Tr} \ln[B_n] = \text{Tr} \ln[I_n] + \text{Tr} \ln(I + [I_n]^{-1}[B'_n]), \tag{26}$$

where I is a unit matrix. The first term on the right hand side gives rise to the first order cumulant as discussed above. The higher corrections come solely from the second term. On expanding the logarithm of the second term in a power series of $[B'_n]$, one finds that the first term of the expansion vanishes identically. The first correction term really comes from the second term of the expansion.

Although, in principle, it is possible to write down all the higher order terms without difficulty, the integrations are very involved and no analytic results have yet been obtained.

4. Discussions

The path integral of a model disordered system introduced by Edwards has been investigated. In order to evaluate the path integral, we employed a technique invented by Feynman. Using this technique, it has been found possible to evaluate analytically the path integral of the nth moment which arose from the expansion of the exponential of a correlation function. The final result which is valid for general forms of correlation function is given in equation (17).

For a gaussian correlation function, it has been shown that the $\boldsymbol{k}_i$ integration can be carried out and that the result depends on only a set of time integrations. It is shown also that for the diagonal part of the nth moment, by selection of the diagonal element of the $[B_n]$ matrix, an explicit result is obtained which leads to the first cumulant in equation (24). The higher corrections can be obtained by considering the off-diagonal matrix $[B'_n]$.

In considering the higher order correction to equation (24), the possibility of expanding the corrections in a power series of $[B'_n]$ was discussed, but because of the time mixing in $[B'_n]$, the full analytic treatment could not be carried through. It is noted that the time mixing term can be eliminated as suggested by Goovaerts and Devreese by considering the integral transform of the average propagator $K = \int \mathrm{d}\boldsymbol{r} G(\boldsymbol{r}, \boldsymbol{r}'; t)$. However, in such a case information relevant to disordered systems will be destroyed.

The procedure used in this paper is very similar in spirit to the works of Papadopoulos and Jones (1971) and Goovaerts and Devreese (1972). The only difference is that in this paper the functional $F[\boldsymbol{r}]$ contains an argument defined at two different times, whereas in the two other papers only a single variable is involved, and thus corresponds to considering local potentials. In this respect the approach in this paper is more closely related to the original work of Feynman on polarons.

The procedure used here has also been applied to the case where W is an exponential. Unfortunately, in this case no explicit result could be obtained for the diagonal part of the nth moment, even considering the diagonal element of $[B_n]$. However, explicit result for limiting cases such as the so-called small-time approximation and large-time approximation of the first cumulant can be obtained. These two limiting cases could be used to obtain the density of states appropriate for band tail or band edge of the heavily doped semiconductors (Lukes and Rogers 1973).

Finally, we note that, the non-diagonal part of the nth moment in equation (20), might be useful for examining the delocalized state of Edwards' model since in this case the symmetry of the system need not be broken (Abram and Edwards 1971).

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