CHATER III

FEYNMAN PATH INTEGRALS APPROACH TO QUANTUM TRANSPORT PROBLEMS

Introduction

The starting point for the transport phenomena is to calculate the expectation value of the velocity,

$$\vec{v} = <\hat{\vec{v}}> = \lim_{t->\infty} \mathrm{Tr}(\hat{\dot{\vec{r}}}\hat{\rho}_t) \tag{78}$$

where $\hat{\rho}$ is the density matrix of the system. $\hat{\rho}_t$ must be known very accurately in order to get a sensible result. At zero temperature, as in the case of a random potential, the system is in a well defined state at all times, then the expectation value can be determined from its wave function,

$$\vec{v} = <\hat{\vec{v}}> = \lim_{t->\infty} \int \Psi^*(\vec{r},t)\hat{\dot{\vec{r}}}\Psi(\vec{r},t)d\vec{r}, \tag{79}$$

where $\Psi(\vec{r},t)$ is the wave function of the system. In both cases, either the density matrix or the state wave functions must be known very accurately. It is quite difficult to get such information from a system with imperfections or having interactions with its environment. Feynman's path integrals methods can be used to cure these problems[4, 19]. The trick is that we first eliminate the dynamical variables of the environment[5], such as the oscillation modes, results in the influence functional or average the density matrix over all interaction energies with imperfections [18], results to the impurity influence functional[6].

In next section we will show how we can write down the equation for momentum and energy conservations and in the following section we will show how we can determine the expectation value of the velocity at steady state, calculated by using Feynman's path integrals. We also discuss the effectiveness of this method on the study of the non-linear property of transport problems, or the so-called strong-field case. In the last section we will discuss the weak field case, also called the linear transport problem. We will also discuss the transport of an electron in two-dimensional system in the presence of magnetic field.

Conservation Laws and Constants of Motion

Two of the most useful expressions in the transport theory are equations expressing the conservation of momentum and conservation of energy. These, as well as most other relations of a similar nature, can be derived in the path integral representation as follows [11]. Consider the identity

$$\int\int \mathcal{D}[x_t]\mathcal{D}[x'_t]\exp(S[x,x']) \;=\; \int\int \mathcal{D}[y_t]\mathcal{D}[y'_t]\exp(S[y,y']) \qquad (80)$$

in which (x_t, x'_t) and (y_t, y'_t) are equivalent pairs of integration variables. $S[x,x']$ is any function in (x_t, x'_t). If now we let $y_t = x_t + \lambda r_t$, where $\lambda << 1$, r_t is function of time, and $\mathcal{D}[x_t] = \mathcal{D}[y_t]$. Inserting this into the left hand side above and expanding to the lowest order in λ, we obtain

$$0 \;=\; \int d\tau \int\int \mathcal{D}[x_t]\mathcal{D}[x'_t]\exp(S[x_t,x'_t])\left(\frac{\delta S}{\delta x_\tau}\right) r_t \qquad (81)$$

If we let $r_\tau = \hat{n}(\tau - t_2)$, then we recover the equation for the conservation of momentum in the direction $\hat{n}$ at time t_2. This is the same as replacing the path x_t by the path $x_t + \lambda\hat{n}\delta(\tau - t_2)$, which in classical mechanics leads to Lagrange's equation of motion. Letting $r_\tau = \hat{n}u(\tau - t_2)$ leads to a constant of the motion analogous to the momentum in the direction $\hat{n}$.

Time invariance lies at the root of energy conservation. Thus, replacing y_t by $x(t+\lambda\eta(t)) = x(t)+\lambda\eta(t)\dot{x}_t$ implies that letting $r_\tau = \eta(\tau)\dot{x}_\tau$ in eq.(81) will yield the equation for energy conservation at t_2 if $\eta(t) = \delta(t - t_2)$. For $\eta(t) = u(t - t_2)$ one obtains the constant of the motion corresponding to energy. Equivalenty, one could replace each path x_t in the original path integral by $x(t+\lambda\eta(t))$. The change of variables $\tau = t + \lambda\eta(t)$ can be used to avoid the functional differentiations; however, care must be taken to take any $x(t - t')$ into

$$\begin{aligned} x(t - t' + \lambda\eta(t - t')) &= x(t + \lambda\eta(t) - t' - \lambda\eta(t') \\ &\quad +\lambda\eta(t - t') - \lambda\eta(t')) \\ dt = d\tau(1 - \lambda\dot{\eta}(\tau)) \text{ and } & \; d/dt = (1 + \lambda\dot{\eta}(\tau))d/d\tau \end{aligned}$$

the latter two being valid to first order in λ.

We first consider the following simple example. If the classical action S_c is given by

$$S_c = \int dt\mathcal{L}(x_t, \dot{x}_t, t) \tag{82}$$

then the path variation $y_t = x_t + \lambda\eta(t)\dot{x}_t$, which results in

$$\delta S_c = \lambda \int dt\eta(t)\dot{x}_t(\delta\mathcal{L}/\delta x_t) = 0 \tag{83}$$

would yield, upon letting $\tau = t + \lambda\eta(t)$,

$$S_c = \int d\tau(1 - \lambda\dot{\eta}(\tau))\mathcal{L}(x_\tau, \dot{x}_\tau(1 + \lambda\dot{\eta}(\tau)), \tau - \lambda\eta(\tau)) \tag{84}$$

so that

$$\delta S_c = \lambda \int d\tau\eta(\tau)\left(\frac{d\mathcal{L}}{d\tau} - \frac{d(\dot{x}_\tau\partial\mathcal{L}/\partial\dot{x}_\tau)}{d\tau} - \frac{\partial\mathcal{L}}{\partial x}\right) = 0. \tag{85}$$

Hence

$$\frac{d\mathcal{H}}{dt} = \frac{d(\dot{x}\partial\mathcal{L}/\partial\dot{x})}{dt} - \frac{d\mathcal{L}}{dt} = -\frac{\partial\mathcal{L}}{\partial t} = \frac{\partial\mathcal{H}}{\partial t} \tag{86}$$

the usual expression for conservation of energy in classical mechanics. (Note that $\dot{x}\delta\mathcal{L}/\delta x = d\mathcal{L}/dx - d(\dot{x}\partial\mathcal{L}/\partial\dot{x})/dt - \partial\mathcal{L}/\partial t$)

Applying the above method to our influence functional $S_d[x, x']$, as expressed in eq.(76), we obtain for the conservation of momentum the expression

$$f_t + \frac{eB}{c}\epsilon < \dot{x} >_t - m < \ddot{x} >_t = \left\langle \frac{\partial\Phi(x, x')}{\partial x} \right\rangle_t \tag{87}$$

where $\Phi(x, x')$ is the impurities influence functional;

$$\Phi(x, x') = \frac{i}{2\hbar}\int_0^t ds' \left(W(x_s - x_{s'}) - 2W(x_s - x'_{s'}) + W(x'_s - x'_{s'})\right). \tag{88}$$

To calculate the invariant corresponding to momentum, one integrates eq.(87) between some initial time and some final time t, and obtain

$$m < \dot{x} >_t + \frac{e}{c}\partial < A >_t + \int^t dt' \left\langle \frac{\partial\Phi(x, x')}{\partial x} \right\rangle_{t'} = \text{constant of the motion} \tag{89}$$

Here A is the vector potential for the constant magnetic field $B, A = \frac{1}{2}B \times x$. For A independent of x, $< m\dot{x}\frac{e}{c}A >$ is a constant of the motion for a free particle ($< p >$). (Recall that the kinetic momentum is usually defined to be $m\dot{x} = p - \frac{e}{c}A$.) However, for uniform magnetic fields, the invariant for a free particle is $< m\dot{x} + \frac{e}{c}2A >$ as long as A independent of time. The remaining terms in eq.(89) express the residual between momentum gained from the applied field and that loss to the medium and to the Hall current.

The principle utility of quantities such as eq.(89) is that constant of the motion represent invariants which can be used to label basis states in an expansion. For example, in writing out evolution equations (Liouville's equations) for the density matrix of the system, it is customary to use as a basis the momentum state of either free or uniformly accelerating carriers corresponding to zero-order Hamiltonians for non-interacting particles. The interactions then drive the evolution of the system. Such an approach is adequate when indeed the state of the carrier is well characterized by one of these basis states at any given time. However, when the scattering becomes sufficiently strong that the particles cannot be described, either theoretically or experimentally, as occupying a well-defined momentum state at any time (i.e., the drift time in a given state is so small that the state is unacceptably broadened), then the utility of this basis and the applicability of expansions in such a basis are called into serious question. In the absence of dissipation the concept of quasiparticles is sometimes adequate to handle self-energy renormalizations. But in the presence of the applied fields

and dissipation, where energy and momentum are continually acquired from the applied fields and transferred to the medium at nonnegligible rates, quasiparticle bases are inadequate for the reasons given.

In sharp contrast to bases of particles or quasiparticles behaving ballistically between collisions, the representation developed below in the context of an approximate influence functional describes carriers whose motion mimics that of the carriers under the actual conditions of the problem. For particles in these states, constants of the motion such as eq.(89) are preserved between scatterings characterized by scattering rate reflecting differences between the actual evolution of the system and its stimulated evolution. In this manner such invariants of an approximate influence functional can serve as an adequate basis for working out evolution equations.

The corresponding equation for conservation of energy and the related constant of the motion can be obtained from time invariance as indicated. The result is

$$f < \dot{x} >_t - \frac{1}{2}\frac{d < \dot{x} m \dot{x} >_t}{dt} = \frac{d < \Phi(x, x') >_t}{dt}. \qquad (90)$$

Expression eq.(90) illustrates how the energy absorbed from the applied fields is distributed to the kinetic and interaction energies. From eq.(90), we note that there is an absence of a term in the magnetic field, since a static magnetic field cannot alter the energy of a charged particle.

As with momentum, an integration over time of eq.(90) will give us an energy related invariant in the following form

$$\frac{1}{2} < \dot{x} m \dot{x} >_t \; + \; < \Phi(x, x') >_t - \int^t dt' f < \dot{x} >_{t'}$$
$$= \text{constant of the motion} \qquad (91)$$

Here, as in eq.(87), each term, each expectation value, is represented by its path integration expectation value indicated above.

The primary purpose of expressions eq.(87)-eq.(91) lies not only in their implications for steady state quantities but in that such quantities evaluated for more general models can be used as bases for density matrices in place of free-particle energy and momenta. We turn now to the evaluation of the above expectation values.

Non-linear Transport

To determine the transport problem of our model system, let we consider the equation for the conservation of momentum expressed in eq.(87),

$$f_t + \frac{eB}{c} \epsilon < \dot{\vec{r}} >_t - m < \ddot{\vec{r}} >_t \; = \; \left\langle \frac{\partial \phi(\vec{r}, \vec{r}')}{\partial \vec{r}} \right\rangle_t \qquad (92)$$

where the expectation is made with respect to the density matrix of the system in Feynman path integrals representation,

$$\langle O(\vec{r}) \rangle \; = \; \int d\vec{r}_t \int d\vec{r}'_t \delta(\vec{r}_t - \vec{r}'_t) \int d\vec{r}_0 \int d\vec{r}'_0 \rho(\vec{r}_0, \vec{r}'_0)$$
$$\cdot \int \mathcal{D}[\vec{r}_s] \int \mathcal{D}[\vec{r}'_s] O(\vec{r}_s) \exp\left\{ \frac{i}{\hbar} S[\vec{r}, \vec{r}'] \right\} \qquad (93)$$

where the action fucntion $S[\vec{r},\vec{r}']$ is the short hand notation of the one appear in eq.(76);

$$S[\vec{r},\vec{r}'] = \int_0^T ds \left(\mathcal{L}(\vec{r},\dot{\vec{r}};f) - \mathcal{L}(\vec{r}',\dot{\vec{r}}';f')\right) + \phi(\vec{r},\vec{r}') \tag{94}$$

At steady state of eq.(92), $<\ddot{\vec{r}} = 0$, the rate of momentum gains from the applied fields is balanced to the rate to the momentum lose into the system by scattering with impurities, then eq.(92) reduces to

$$f_t + \frac{eB}{c}\epsilon <\dot{\vec{r}}>_t = \left\langle \frac{\partial\phi(\vec{r},\vec{r}')}{\partial\vec{r}} \right\rangle_t \tag{95}$$

At this steady state condition, we say that an electron will move with constant *drift velocity* v_D.

To consider this equation more explicitly, let us move our problem on to the moving reference frame, R, which moves with the same velocity of an electron, $\dot{R} = v_D$. That is let us make the transformation

$$\begin{aligned} r_t &= R_t + u_t \\ r'_t &= R - t + u'_t \end{aligned} \tag{96}$$

where u and u' are the fluctuations of the electronic paths on the moving frame result from scattering with impurities. In transport problem, the important quantity is the drift velocity of the carriers which is expressed in terms of the applied fields, then we will neglect the equation for the fluctuations on the left hand side of eq.(95) and we will get

$$f_t + \frac{eB}{c}\epsilon v_D = \left\langle \frac{\partial\phi(u,u')}{\partial u} \right\rangle_t . \tag{97}$$

The right hand side of this equation is the task of our calculation in this thesis work. We first simplify them by looking at the expression of the impurity influence functional $\phi(\vec{r},\vec{r}')$, eq.(88), and then write the potential correlation function in terms of its Fourier transformed form

$$W(r_t - r_{t'}) = \frac{1}{A}\sum_k w(k) e^{ik(r_t - r_{t'})} \tag{98}$$

Since in our model system, we will use the gaussian function for the potential correlation function, then its Fourier component will have the property $w(k) = w(-k)$.

Under the transformation of eq.(96), the symmetry property of the $w(k)$ and the condition for the averaging process, we can write the expression for eq.(97) as

$$\begin{aligned} f_t + \frac{eB}{c}\epsilon v_D &= \frac{2}{\hbar}\mathrm{Re}\frac{1}{A}\sum_k w(k)k\int_0^\tau d\sigma e^{ikv_D(\tau-\sigma)} \\ &\quad \cdot \left\langle e^{ik(u_\tau - u_\sigma)}\right\rangle \end{aligned} \tag{99}$$

where the expectation appear on the right hand side of this equation has an expression as

$$\begin{aligned} \left\langle e^{ik(u_\tau - u_\sigma)}\right\rangle &= \int du_T du'_T \delta(u_T - u'_T)\int du_0 \int du'_0 \rho(u_0, u'_0) \\ &\quad \cdot \int \mathcal{D}[u_t]\int \mathcal{D}[u'_t] e^{ik(u_\tau - u_\sigma)} \\ &\quad \cdot \exp\left\{\frac{i}{\hbar}\int_0^T dt(\mathcal{L}(u,\dot{u};f_L) - \mathcal{L}(u',\dot{u}';f_L)) + \frac{i}{\hbar}\phi(u,u')\right\} \end{aligned} \tag{100}$$

where f_L is the Lorentz force which acts on electron on the moving frame. The right hand side of eq.(100) contains all information of the applied fields, $\vec{B}$ and

$\vec{\mathcal{E}}$. If we do not cut any terms or make no approximation about the fields, this equation will cause the non-linear relation of the drift velocity to the applied fields. This is the effectiveness of this technique to look for such a non-linearity in transport problem.

Linear Transport

The expression of the averaging $\exp\{ik(u_\tau - u_\sigma)\}$ is a kind of generating functional, so let define

$$\left\langle e^{ik(u_\tau - u_\sigma)} \right\rangle = g(f_\delta[\tau, \sigma]) \tag{101}$$

where f_δ is defined to be equal to $\hbar k(\delta(t-\tau) - \delta(t-\sigma))$, the delta force. The linear transportation is considered in the case of weak field, then, empirically, we can expand $g(f_\delta)$ into series of the applied fields as

$$g(f_\delta) = g_0 + g_1 + g_2 + \ldots \tag{102}$$

where g_0 is the term which contains no applied fields. g_1 contains term in the first order and so on. In this case, the transport coefficients are considered as the linear term of the applied fields by defining the relaxation time τ_r as, see eq.(99),

$$f_t + \frac{eB}{c}\epsilon v_D - g_1 = m v_D \left(\frac{1}{\tau_r}\right) \tag{103}$$

and from eq.(99) we have

$$\frac{1}{\tau_r} = \frac{2}{\hbar m}\mathrm{Re}\frac{1}{A}\sum_k w(k)k \int_0^\tau d\sigma e^{ikv_D(\tau-\sigma)} g(f_\delta[\tau, \sigma]) \tag{104}$$

From eq.(103), to keep the efect of g_1 term, we rewrite it as

$$f_t + \frac{eB}{c}\epsilon v_D = m v_D \left(\frac{1}{\tau_{eff}}\right) \tag{105}$$

The mobility is defined from the relation

$$v_D = \mu \mathcal{E} \tag{106}$$

which from eq.(105), we get

$$\mu = \frac{(-e)}{m} \begin{pmatrix} 1/\tau_{eff} & -\Omega \\ \Omega & 1/\tau_{eff} \end{pmatrix}^{-1} . \tag{107}$$

Our task of this thesis work is to calculate the mobility of an electron in our model system in the linear transformation regime. And then determine the conductivity σ of an electron from the *Kubo-Greenwood* formula [20], [21];

$$\sigma = \int dE \left(-\frac{\partial f(E)}{\partial E}\right) (-e) n(E) \mu(E) \tag{108}$$

where $n(E)$ is the density of states of an electron in such a system and $\mu(E)$ is the mobility, calculated at absolute zero temperature, eq.(107). If we have applied the electric field in $\hat{x}$- direction , the longtitudinal component of the conductivity will have the expression

$$\sigma_{xx} = \int dE \left(-\frac{\partial f(E)}{\partial E}\right) n(E) \mu_{xx}(E) \tag{109}$$

but for the transverse component, an electron will drift in the transverse direction to the applied electric field by Lorentz force. Also our system was added with some imperfections, then the transverse component of the conductivity should be determined from the expression[20], [21]

$$\sigma_{yx} = \frac{1}{kT} \int dE f(E) n(E) \mu_{yx}(E) \tag{110}$$

These expressions of conductivity have given some sign of quantum Hall conductivity as has been studied by Sa-yakanit[22] in the lowest order of approximation. My work will extend his studies up to the long correlation length limit.