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A model of dynamical disorder in a uniform time-dependent electric field

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Abstract. The Gaussian white noise (GWN) model immersed in a time-dependent electric field permits an exact evaluation of the retarded/advanced Green functions. The (quantum) kinetic equation can be written down with the aid of the Baym-Kadanoff formalism, and the response to a step-like electric field has been analysed in two recent papers. Both papers report exact solutions which, however, are different. The discrepancy is traced to different (but plausible) ways of treating the thermal instability inherent in the GWN. It is shown how the derived kinetic equation can be used to extract other transport properties as well.

1. Introduction

Quantum kinetic equations have, apart from their conceptual interest, become a topic of active research in the light of recent advances in the fabrication of microstructures, where transport takes place under conditions not compatible with the assumptions implicit in the traditional Boltzmann equation approach. For realistic scattering mechanisms the quantum kinetic equations are extremely complicated and therefore it is of significant interest to examine simplistic interactions in order to understand better the mathematical structure of these equations. The Gaussian white noise model (GWN) (see below for the definitions used in this work) provides a good candidate for such a 'testing laboratory of the theory' because of the particularly manageable mathematics related to it. Indeed, two recent publications (Hänsch and Mahan 1983, to be referred to as HM, Jauho 1985a, to be referred to as J) have developed quantum transport equations based on the Baym-Kadanoff formalism (see these two papers for additional references), and then applied these to the GWN to analyse its transient dynamics. However, the final results of these two papers are different, and the main purpose of this paper is to re-examine the various assumptions underlying the two calculations and to point out where the differences arise. In addition, we complete the calculation whose initial step was described briefly in J, and give some alternate derivations to previously presented results. Finally, since the HM result agrees with the Kubo formula, and J with the Boltzmann equation, our analysis sheds some light on the different assumptions behind the two approaches.

The key point is that GWN possesses an inherent thermal instability (as already pointed out by HM): GWN does not maintain thermal equilibrium. The question is then: can one calculate the response of GWN to an external perturbation using a transport equation that does not maintain thermal equilibrium, or does one have to modify it in some sense? The first approach is that of J while HM follow the second route.

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2. Determination of the retarded Green function

Before turning to the kinetic equations we must first solve the dynamics, i.e. determine the disorder-averaged retarded Green function for GWN in an external electric field. We choose the following form of the field-free Hamiltonian (see Jayannavar and Kumar 1982, Girvin and Mahan 1979)†

$$H = \int \mathrm{d}^3x\, \psi^+(\boldsymbol{x})(-\tfrac{1}{2}\nabla^2)\psi(\boldsymbol{x}) + \int \mathrm{d}^3x\, \psi^+(\boldsymbol{x})\, V(x, t)\psi(\boldsymbol{x}). \tag{1}$$

Here the parametric time dependence of the impurity potential reflects the random thermal fluctuations of the environment. The average over disorder is performed with the formula

$$\begin{aligned} &\langle V(\boldsymbol{x}, t)\rangle = 0 \\ &\langle V(\boldsymbol{x}, t_x)\, V(\boldsymbol{y}, t_y)\rangle = v(\boldsymbol{x}-\boldsymbol{y})\delta(t_x - t_y) \end{aligned} \tag{2}$$

and higher even averages are given as a sum of all pairwise averages. Standard diagrammatic techniques lead to the self-energy

$$\Sigma(\boldsymbol{x}, \boldsymbol{y}, t, t') = v(\boldsymbol{x}-\boldsymbol{y})G(\boldsymbol{x}, \boldsymbol{y}, t, t')\delta(t-t') \tag{3}$$

where G is the full impurity-averaged Green function. In writing (3) we have neglected the so-called crossed diagrams; since our emphasis is not on localisation effects, this should be of no consequence. Further, Girvin and Mahan (1979) have shown in the context of a related phonon model that vertex corrections, in fact, vanish. Adding the external field does not change the diagrammatic structure of the theory, and one ends up with the following Dyson equation for the retarded Green function

$$G^{\mathrm{r}}(\boldsymbol{p}, t, t') = G^{\mathrm{r}}_A(\boldsymbol{p}, t, t') + \int \mathrm{d}t_1\, G^{\mathrm{r}}_A(\boldsymbol{p}, t, t_1) \sum_{\boldsymbol{q}} \gamma(\boldsymbol{p}-\boldsymbol{q})G^{\mathrm{r}}(q, t_1, t_1)G^{\mathrm{r}}(p, t_1, t') \tag{4}$$

where $\gamma(\boldsymbol{p})$ is the Fourier transform of $v(\boldsymbol{x})$, and

$$G^{\mathrm{r}}_A(\boldsymbol{p}, t, t') = -\mathrm{i}\theta(t-t')\exp\left(-\mathrm{i}\int_{t'}^{t} \mathrm{d}t_1\, \varepsilon(\boldsymbol{p}-\boldsymbol{A}(t_1))\right) \tag{5}$$

is the exact propagator for free particles coupled to an electric field via a vector potential, $\boldsymbol{E}(t) = -\partial/\partial t\, \boldsymbol{A}(t)$ (Jauho and Wilkins 1982, 1984). This non-linear equation for G^{r} is solved with the ansatz

$$\sum_{\boldsymbol{q}} \gamma(\boldsymbol{p}-\boldsymbol{q})G^{\mathrm{r}}(\boldsymbol{q}, t_1, t_1) = -\mathrm{i}\tfrac{1}{2}\gamma_0 \tag{6}$$

where

$$\gamma_0 \equiv \sum_{\boldsymbol{q}} \gamma(\boldsymbol{p}+\boldsymbol{q}). \tag{7}$$

† A lattice version of (1) has been analysed in detail by Ovchinnikov and Erikhman (1974) and Madhukar and Post (1977).

One obtains, in agreement with HM,

$$G^{r}(\boldsymbol{p}, t, t') = -\mathrm{i}\theta(t-t')\exp\left(-\mathrm{i}\int_{t'}^{t} \mathrm{d}t_1\, \varepsilon(\boldsymbol{p}-\boldsymbol{A}(t_1)) - \tfrac{1}{2}\gamma_0(t-t')\right) \tag{8}$$

and it is readily seen that (8) indeed satisfies (4).

3. Kinetic equations

Let us now turn to the kinetic properties of the GWN. Rather than following the integral formulation of transport theory as done by HM and J, we give here an alternate derivation. We employ the Kadanoff-Baym formalism (Kadanoff and Baym 1962, Langreth 1976, Jauho 1983), where the central quantity of interest is the correlation function $G^{<}(\boldsymbol{x}, t, \boldsymbol{x}', t') = \mathrm{i}\langle\psi^{+}(\boldsymbol{x}', t')\psi(\boldsymbol{x}, t)\rangle$ which is the analytic continuation of the (imaginary) time-ordered Green function. To discuss kinetic equations it is convenient to work with the Wigner variables $\boldsymbol{R} = \frac{1}{2}(\boldsymbol{x}+\boldsymbol{x}')$, $\boldsymbol{r} = \boldsymbol{x}-\boldsymbol{x}'$, $T = \frac{1}{2}(t+t')$, and $\tau = (t-t')$. We define the correlation function in the conventional way:

$$G^{<}(\boldsymbol{p}, \omega, \boldsymbol{R}, T) = \int \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}\omega\tau}\int \mathrm{d}^3 r \exp(-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r})\mathrm{i}\langle\psi^{+}(\boldsymbol{R}-\tfrac{1}{2}\boldsymbol{r}, T-\tfrac{1}{2}\tau)\psi(\boldsymbol{R}+\tfrac{1}{2}\boldsymbol{r}, T+\tfrac{1}{2}\tau)\rangle \tag{9}$$

from which the Wigner distribution function can be extracted via

$$f(\boldsymbol{p}, T) = -\mathrm{i}G^{<}(\boldsymbol{p}, \tau=0, T) = -\mathrm{i}\int \frac{\mathrm{d}\omega}{2\pi} G^{<}(\boldsymbol{p}, \omega, T). \tag{10}$$

Note that in the present uniform case we have dropped the spurious spatial variable $\boldsymbol{R}$. The Wigner function obeys the following exact transport equation (see, e.g., Jauho 1985b)

$$\frac{\partial}{\partial T} f(\boldsymbol{p}, T) = -\int_{-\infty}^{\infty} \mathrm{d}u\{\Sigma^{r}G^{<} + \Sigma^{<}G^{a} - G^{r}\Sigma^{<} - G^{<}\Sigma^{a}\} \tag{11}$$

where the time variables in the integrand have the structure

$$AB = A[T-u, \tfrac{1}{2}(u+T)]B[u-T, \tfrac{1}{2}(u+T)]. \tag{12}$$

Note that in general it is not possible to obtain a closed equation for the Wigner function because the right-hand side of (11) involves the full correlation function; however, in the present case the one-point nature of the GWN interaction (as evinced by the δ function in time in equation (3)) allows one to obtain a closed equation for f. To complete the derivation of the kinetic equation the self-energies in (11) must be specified; it is at this juncture where the treatments of HM and J depart. Consider first the calculation of HM. They choose

$$\begin{aligned}
\Sigma^{r}(t, t') &= -\mathrm{i}/2\gamma_0\delta(t-t') = -\Sigma^{a}(t, t') \\
\Sigma^{<}(t, t') &= \mathrm{i}\gamma_0 \int \frac{\mathrm{d}\varepsilon}{2\pi} n_{\mathrm{F}}(\varepsilon)\exp[-\mathrm{i}\varepsilon(t-t')] \\
\Sigma^{>}(t, t') &= -\mathrm{i}\gamma_0 \int \frac{\mathrm{d}\varepsilon}{2\pi} (1-n_{\mathrm{F}}(\varepsilon))\exp[-\mathrm{i}\varepsilon(t-t')].
\end{aligned} \tag{13}$$

Here $\Sigma^{\lessgtr}$ are the analytic continuations of the self-energy Σ, defined analogously with $G^{\lessgtr}$, and $n_F(\varepsilon)$ is the Fermi function. Note that this choice satisfies the consistency check $\Sigma^r - \Sigma^a = \Sigma^> - \Sigma^<$. The expression for Σ^r is exact (it emerges from the self-consistent solution to the Dyson equation as given by equations (6)-(8)), and the expressions for $\Sigma^{\lessgtr}$ imply that the GWN is treated as if it maintained thermal equilibrium. Expressed in other words, the use of $\Sigma^<$ (as given by (13)) in the kinetic equation means that the scattering events increasing the population in a given momentum state $\boldsymbol{p}$ (i.e. the 'scattering-in' term) act as if the particles were emerging from an underlying thermal equilibrium state. As shown by HM, the GWN is never in thermal equilibrium: a particle interacting with GWN heats up (see also below where we make this statement more quantitative). Thus the choice (13) is a natural way of impeding the scattering-induced heating: recall that one is looking for the effects of the applied field and not for some spurious effects caused by the interaction.

With (13), and introducing the kinetic momentum $\boldsymbol{k} = \boldsymbol{p} - \boldsymbol{A}(T)$, equation (11) becomes

$$\left(\frac{\partial}{\partial T} + \boldsymbol{E}(T) \cdot \frac{\partial}{\partial \boldsymbol{k}}\right) f(\boldsymbol{k}, T) = -\gamma_0 [f(\boldsymbol{k}, T) - g(\boldsymbol{k}, T)] \tag{14}$$

where

$$g(\boldsymbol{k}, T) = \int_0^\infty \mathrm{d}\tau \int \frac{\mathrm{d}\varepsilon}{2\pi} n_F(\varepsilon) 2 \cos\left[\tau\varepsilon - \int_{T-\tau}^{T} \mathrm{d}u\, \varepsilon\left(\boldsymbol{k} - \int_u^T \boldsymbol{E}(v)\, \mathrm{d}v\right)\right] \exp(-\tfrac{1}{2}\gamma_0 \tau). \tag{15}$$

Equation (14) has a relaxation time form where the non-equilibrium distribution function relaxes to the time- and field-dependent function g. We observe that before the field is turned on ($T < 0$) the equilibrium momentum distribution

$$f^{\mathrm{eq}}(\boldsymbol{k}) = \int \frac{\mathrm{d}\varepsilon}{2\pi} n_F(\varepsilon) A(\boldsymbol{k}, \varepsilon) \tag{16}$$

where the equilibrium spectral density is given by

$$A(\boldsymbol{k}, \varepsilon) = \frac{\gamma_0}{(\varepsilon - \varepsilon(\boldsymbol{k}))^2 + (\frac{1}{2}\gamma_0)^2} \tag{17}$$

satisfies (14) identically. HM compute the steady state current, and to do this we set $\boldsymbol{E}(t) = \boldsymbol{F}$ (all transients have died away) in (15). The variable T drops out from the problem, and we are led to consider

$$\boldsymbol{F} \cdot \frac{\partial}{\partial \boldsymbol{k}} f(\boldsymbol{k}) = -\gamma_0 f(\boldsymbol{k}) + \gamma_0 \int \frac{\mathrm{d}\varepsilon}{2\pi} n_F(\varepsilon) 2 \int_0^\infty \mathrm{d}u \times \cos\left(u\varepsilon - \int_0^u \mathrm{d}v\, \varepsilon(\boldsymbol{k} - \boldsymbol{F}v)\right) \exp(-\tfrac{1}{2}\gamma_0 u). \tag{18}$$

We now extract the current from (18). We proceed in two steps. First sum over $\boldsymbol{k}$ on both sides of (18). This gives

$$N = \sum_{\boldsymbol{k}} f(\boldsymbol{k}) = \sum_{\boldsymbol{k}} \int \frac{\mathrm{d}\varepsilon}{2\pi} n(\varepsilon) \int_0^\infty \mathrm{d}u\, 2 \cos\left(u\varepsilon - \int_0^u \mathrm{d}v\, \varepsilon(\boldsymbol{k} - \boldsymbol{F}v)\right) \exp(-\tfrac{1}{2}\gamma_0 u). \tag{19}$$

Next, we multiply (18) by $\boldsymbol{k}$, and sum over it. The left-hand side gives $-\boldsymbol{F}N$, and using (19) we obtain the following explicit result for the current ($\boldsymbol{J}=\Sigma_{\boldsymbol{k}}\,\boldsymbol{k}f(\boldsymbol{k})$):

$$\boldsymbol{J}=\sum_{\boldsymbol{k}}\left(\frac{1}{\gamma_0}\boldsymbol{F}+\boldsymbol{k}\right)\int\frac{\mathrm{d}\varepsilon}{2\pi}n_{\mathrm{F}}(\varepsilon)2\int_0^{\infty}\mathrm{d}u\,\cos\left(u\varepsilon-\int_0^u\mathrm{d}v\,\varepsilon(\boldsymbol{k}-\boldsymbol{F}v)\right)\exp(-\tfrac{1}{2}\gamma_0 u). \tag{20}$$

Defining a new variable $\boldsymbol{k}'=\boldsymbol{k}+\boldsymbol{F}/\gamma_0$, and linearising with respect to $\boldsymbol{F}$, gives after some algebra

$$\boldsymbol{J}=\sum_{\boldsymbol{k}}\boldsymbol{k}(\boldsymbol{k}\cdot\boldsymbol{F})\int\frac{\mathrm{d}\varepsilon}{2\pi}(-n_{\mathrm{F}}'(\varepsilon))\frac{1}{2}\left(\frac{\gamma_0}{(\varepsilon-\varepsilon(\boldsymbol{k}))^2+(\frac{1}{2}\gamma_0)^2}\right)^2 \tag{21}$$

in complete agreement with HM and also the Kubo formula result (Girvin and Mahan 1979) (see equations (A14) and (A15) in HM).

Now let us turn to the calculation sketched in J. There the following expression for $\Sigma^<$ is used:

$$\begin{aligned}\Sigma^<(\boldsymbol{p},t,t')&=\sum_{\boldsymbol{q}}\gamma(\boldsymbol{p}-\boldsymbol{q})G^<(\boldsymbol{q},t,t)\delta(t-t')\\&=\mathrm{i}\sum_{\boldsymbol{q}}\gamma(\boldsymbol{p}-\boldsymbol{q})f(\boldsymbol{q},t)\delta(t-t').\end{aligned} \tag{22}$$

The kinetic equation is now

$$\left(\frac{\partial}{\partial T}+\boldsymbol{E}(T)\cdot\frac{\partial}{\partial\boldsymbol{k}}\right)f(\boldsymbol{k},T)=-\gamma_0 f(\boldsymbol{k},t)+\sum_{\boldsymbol{k}'}\gamma(\boldsymbol{k}-\boldsymbol{k}')f(\boldsymbol{k}',T). \tag{23}$$

Ovchinnikov and Erikhman (1974) have given the lattice version of this equation, and its zero-field form appears also in the works of HM and Jayannavar and Kumar (1982). We observe that this equation is identical to the semiclassical Boltzmann equation which one would write for the GWN. Equation (23) resembles also the conventional impurity Boltzmann equation. Observe however (and this is crucial) that the energy-conserving δ function in the collision integral is missing. However, we emphasise that (23) is actually far more general than the Boltzmann equation: it was obtained with an exact sequence of transformations starting from the quantum kinetic equation for the correlation function $G^<$. It is well known that the lowest-order gradient approximation to the quantum kinetic equation in many cases (elastic impurities, electron–phonon interactions) leads to the Boltzmann equation; the GWN is a special interaction in the sense that the quantum kinetic equation coincides with the Boltzmann equation. This property is a consequence of the one-point character of GWN.

The current can be evaluated in a straightforward way starting from (23). As a preliminary, sum (23) over $\boldsymbol{k}$ to get ($N=\Sigma_{\boldsymbol{k}}f(\boldsymbol{k})$)

$$\frac{\partial}{\partial T}N=-\gamma_0 N+\sum_{\boldsymbol{k}\boldsymbol{k}'}\gamma(\boldsymbol{k}-\boldsymbol{k}')f(\boldsymbol{k}',t)=0 \tag{24}$$

or $N=$ constant. Thus the continuity equation is identically satisfied. Note that this is not the case for the model treated by HM: the right-hand side of (14) does not vanish when summed over $\boldsymbol{k}$. Thus, in general, the particle number, equation (19), depends on the field, and the assumed underlying thermal background acts as a source (or sink) of particles. These problems, however, do not occur in *linear* theory, to which the final result (21) applies. In passing, we point out a related problem: the total particle number calculated with the exact equilibrium expression (16)

$$N=\sum_{\boldsymbol{k}}f^{\mathrm{eq}}(\boldsymbol{k})=\int\frac{\mathrm{d}\varepsilon}{2\pi}\sum_{\boldsymbol{k}}n_{\mathrm{F}}(\varepsilon)A(\boldsymbol{k},\varepsilon) \tag{25}$$

diverges. To see this, consider

$$\sum_{\boldsymbol{k}} A(\boldsymbol{k}, \varepsilon) = c\gamma_0 \int_0^{\infty} \frac{\mathrm{d}\varepsilon_k \, \varepsilon_k^{1/2}}{(\varepsilon - \varepsilon_k)^2 + (\frac{1}{2}\gamma_0)^2} = c'\{\varepsilon + [\varepsilon^2 + (\tfrac{1}{2}\gamma_0)^2]^{1/2}\}^{1/2} \tag{26}$$

where we have suppressed unimportant multiplicative constants. The integral over ε in (25) diverges because of the negative energy tail of (26).

Turning back to the evaluation of the current, we multiply (23) by $\boldsymbol{k}$, and sum over it, to obtain

$$\frac{\partial}{\partial T}\boldsymbol{J} - \boldsymbol{F}N = -\gamma_0 \boldsymbol{J} + \sum_{\boldsymbol{k},\boldsymbol{k}'} \boldsymbol{k}\gamma(\boldsymbol{k} - \boldsymbol{k}')f(\boldsymbol{k}') = 0 \tag{27}$$

where we have used (7) and assumed that $\Sigma_{\boldsymbol{k}} \boldsymbol{k}\gamma(\boldsymbol{k}) = 0$ by symmetry (we consider crystals with inversion symmetry). Using the boundary condition $\boldsymbol{J}(T = 0) = 0$ (the field is switched on at $T = 0$), we obtain

$$\boldsymbol{J} = \boldsymbol{F}NT. \tag{28}$$

This is an intriguing result: the interaction with the GWN potential has entirely dropped out.

4. Other transport properties

While the GWN is unable to relax momentum, and hence does not lead to a finite conductivity (this property is related to the absence of diffusion) it does affect the energy balance. Let us calculate the time dependence of the average kinetic energy with the kinetic equation (23). Multiplying (23) with $\frac{1}{2}k^2$, and summing over $\boldsymbol{k}$, we can show that

$$\varepsilon(T) \equiv \sum_{\boldsymbol{k}} \tfrac{1}{2}k^2 f(\boldsymbol{k}) = \varepsilon(T = 0) + \gamma_2 NT + \tfrac{1}{2}NF^2T^2 \tag{29}$$

where

$$\gamma_2 = \sum_{\boldsymbol{k}} \tfrac{1}{2}k^2 \gamma(\boldsymbol{k}). \tag{30}$$

The two time-dependent terms in (29) can be interpreted as follows. The last term corresponds to free particles accelerating under the influence of a uniform electric field. The other term describes heating due to the GWN interaction: thus it is yet another manifestation of the 'self-heating' effect discussed by HM.

The present kinetic approach can also be used to rederive the results of Jayannavar and Kumar (1982) with very little effort. They were concerned with the long-time behaviour of $\langle x^2(t)\rangle$, and they found non-diffusive behaviour, $\langle x^2(t)\rangle \sim t^3$. To calculate $\langle x^2(t)\rangle_{F=0}$ we replace the field driving term $\boldsymbol{F} \cdot \partial/\partial \boldsymbol{k}$ by $\boldsymbol{k} \cdot \nabla_{\boldsymbol{R}}$ (it can be shown that this replacement is exact). We extract

$$\langle x^2(T)\rangle \equiv \int \mathrm{d}\boldsymbol{R}\, R^2 \sum_{\boldsymbol{k}} f(\boldsymbol{k}, \boldsymbol{R}, T)$$

by considering the equations of motion for $\langle x^2\rangle$, $\langle xk\rangle$ and $\langle k^2\rangle$ and obtain

$$\partial^2\langle x^2(T)\rangle/\partial T^2 = \varepsilon(T = 0) + 2\gamma_2 NT \tag{31}$$

which can be integrated to give the long-time behaviour

$$\langle x^2(T)\rangle \to 1/3\gamma_2 NT^3. \tag{32}$$

If one chooses a Gaussian matrix element $\gamma(\boldsymbol{k}) = V_0^2 \exp(-\frac{1}{2}\alpha^2 k^2)$, it is seen that (32) and (30) reproduce exactly the result of Jayannavar and Kumar (see their equation (17)).

5. Discussion

In summary, we have analysed two different approaches to determining the behaviour of GWN in an external field. In a sense, neither of these approaches leads to an entirely satisfactory result: in the approach of HM, where an underlying thermal equilibrium is assumed, problems arise with conservation laws (see discussion below equation (24)), whereas in the approach of J, where the one-point character of the GWN is included also for the 'scattering-in' term in the collision integral, the GWN interaction drops out entirely from the current, and is present only in the expression for the average kinetic energy. This state of matters would seem to indicate that the GWN is too pathological to serve as a testing model for quantum kinetic theories.

Finally we comment on the differences of the kinetic approach and the Kubo formula approach. In general, the Kubo formula gives the linear transport coefficient in terms of a (thermal equilibrium) two-particle Green function. Given the interactions, a theory for this object can be developed, and an explicit expression for the transport coefficient is obtained. For the theory to be consistent, the result should agree with the one obtained from the linearised kinetic equation, and this is indeed the case for, e.g., electron–impurity and electron–phonon scattering (see HM, Jauho 1983). This is *not* the case for the GWN: a linearisation of the GWN kinetic equation is not meaningful because the thermal equilibrium distribution function does not satisfy it. This suggests that the application of the Kubo formula can be tricky: one should first ascertain that the problem under consideration maintains thermal equilibrium and to obtain this information requires an investigation of the corresponding kinetic equation, which may be quite difficult in general.

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