

A SELF-CONSISTENT MODE-COUPLING THEORY FOR THE ANDERSON LOCALIZATION

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ABSTRACT

Self consistent equations for the density response and the electrical conductivity of a fluid in a random potential are derived using projection operator techniques. The equations depend on the static density response function $\chi_0(q)$, the strength of the random potential U_k and the space dimensionality d , and are formally similar for classical and quantum fluids. The present formalism allows us to analyze directly the transport properties of the system without going into the fine details of its structure (i.e. the exact nature of the wavefunction in the quantum case).

I. INTRODUCTION

The motion of an electron gas in a random potential has drawn considerable theoretical attention in recent years since the pioneering works of Anderson and Mott.¹⁻⁵ Many theoretical efforts have been focussed on trying to understand the nature of the wavefunction (under what conditions is it localized or extended). The relevant experimental quantities are however the transport coefficients of the system such as the density response function or the electrical conductivity. One of the most intriguing and controversial aspects of the problem is the existence of a "mobility edge" as a function of the randomness and the spatial dimensionality, i.e. whether the DC conductivity undergoes a sharp phase transition.

In the present paper the problem will be attacked using a mode coupling approach, as is done in nonlinear hydrodynamics.⁶⁻⁸ Our basic goal will be to derive a set of equations whose solution will directly lead to the quantities of interest, i.e. the electrical conductivity and the density response function, without having to go through a detailed analysis regarding the nature of the wavefunction. This paper is based on the mode-coupling formulation of Kawasaki⁶ and Kadanoff and Swift⁷ and we use the exact static density response function $\chi_0(p)$ as an input to the mode coupling calculations. This enables us to use various microscopic diagrammatic techniques to study the static properties of the system, or even treat them phenomenologically, and then the present equations may be used to calculate the dynamical response functions of interest. The present equations enable us to discuss in a convenient and unified way effects of randomness, energy, temperature and dimensionality. They also allow for a simple comparison of classical and quantum fluids.^{9,10} In Section II we introduce the basic formal definitions to be used in this paper and in Section II we define the transport properties of interest and relate all of them to the kubo transformed density response function, $\hat{\chi}_{\rho\rho}(q,\omega)$. In Section IV we define the self consistent equations for the density and current response functions. Section V presents another set of equations derived using a different time-ordering scheme and finally, in Section VI we discuss our results and analyze their limiting behavior.

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II. CORRELATION FUNCTIONS, RESPONSE FUNCTIONS AND KUBO TRANSFORMS

In this section we shall introduce the basic definitions and notation to be used later.¹¹ We consider a fluid consisting of N identical particles in a volume Ω . The coordinates and momenta of the j particle will be denoted r_j, p_j respectively and the set $\{r_j, p_j\}$ form a $6N$ dimensional phase space. Let A_j, B_j etc. be a set of single particle operators which depend on the j particle only. We then define in q space

$$A_q \equiv \frac{1}{2} \sum_j [\exp(iq \cdot r_j) A_j + A_j \exp(iq \cdot r_j)]. \quad (1)$$

Similarly we define B_q, C_q etc. We note that since A_j are Hermitian, then

$$A_q^\dagger = A_{-q} \quad (1a)$$

where A_q^\dagger is the Hermitian conjugate of A_q .

We define the correlation function of A and $B, C_{AB}(q, \tau)$ as follows:

$$C_{AB}(q, \tau) \equiv \langle A_q(\tau) | B_q(0) \rangle \equiv \text{Tr}(A_{-q}(\tau) B_q(0) \rho_{eq}), \quad (2)$$

where

$$A_q(\tau) \equiv \exp(iL\tau) A_q \equiv \exp(iH\tau) A_q \exp(-iH\tau), \quad (3)$$

and

$$\rho_{eq} \equiv \exp(-H/kT) / \text{Tr} \exp(-H/kT). \quad (4)$$

Here H is the Hamiltonian of the system, L is the Liouville operator $L \equiv [H, \]$ and ρ_{eq} is the Canonical distribution function at temperature T . The linear response function (susceptibility) which measures the expectation value of A_q given an external field that couples B_q is¹¹

$$\chi_{AB}(q, \tau) \equiv \langle [A_q(\tau), B_q] \rangle \equiv \langle A_q(\tau) | B_q(0) \rangle - \langle B_q(0) | A_q(\tau) \rangle. \quad (5)$$

The Kubo transform of A and B is defined as:

$$\begin{aligned} \hat{\chi}_{AB}(q, \tau) &\equiv \langle \langle A_q(\tau) | B_q \rangle \rangle \equiv \int_0^{1/kT} d\lambda \langle A_q(\tau - i\lambda) | B_q \rangle \\ &\equiv \int_0^{1/kT} d\lambda \text{Tr}[\exp(\lambda H) A_q(\tau) \exp(-\lambda H) B_q \rho_{eq}]. \end{aligned} \quad (6)$$

In ω space we define the one sided (advanced) Fourier transform:

$$C_{AB}(q, \omega) = -i \int_0^\infty d\tau \exp(i\omega\tau) C_{AB}(q, \tau). \quad (7a)$$

and similarly for $\chi_{AB}(q, \omega)$ and $\hat{\chi}_{AB}(q, \omega)$. The inversion of (7a) is:

$$C_{AB}(q, \tau) = \frac{i}{2\pi} \int_{-\infty}^{\infty} d\omega \exp(-i\omega\tau) C_{AB}(q, \omega). \quad (7b)$$

Denoting the eigenstates of our Hamiltonian H (without the external field) by α and β with eigenvalues E_α and E_β and using Eqs. (2), (5), (6) and (7a) we have:

$$C_{AB}(q, \omega) = \sum_{\alpha, \beta} P(\alpha) \frac{(A_{-q})_{\alpha\beta} (B_q)_{\beta\alpha}}{\omega - \omega_{\beta\alpha} + i\epsilon} \quad (8a)$$

$$\chi_{AB}(q, \omega) = \frac{1}{\hbar} \sum_{\alpha, \beta} [P(\alpha) - P(\beta)] \frac{(A_{-q})_{\alpha\beta} (B_q)_{\beta\alpha}}{\omega - \omega_{\beta\alpha} + i\epsilon}, \quad (8b)$$

and

$$\hat{\chi}_{AB}(q, \omega) = \sum_{\alpha, \beta} \frac{P(\alpha) - P(\beta)}{\hbar \omega_{\beta\alpha}} \cdot \frac{(A_{-q})_{\alpha\beta} (B_q)_{\beta\alpha}}{\omega - \omega_{\beta\alpha} + i\epsilon}, \quad (8c)$$

where $P(\alpha) \equiv \langle \alpha | \rho_{eq} | \alpha \rangle$, and

$$\omega_{\beta\alpha} = E_\beta - E_\alpha. \quad (8d)$$

Eqs. (8) are very useful for demonstrating the formal analytical properties of C , χ and $\hat{\chi}$, as well as for establishing various relations between them (see Eqs. (9)-(13)). However, the usage of Eqs. (8) for the actual evaluation of the correlation functions is quite limited since they contain the complicated many-body eigenstates α, β etc. of the total Hamiltonian, which are rarely known. The common methods for the evaluation of Eqs. (8) are diagrammatic techniques¹² or reduced equations of motion.¹³⁻¹⁵ We further note that the three types of correlation functions defined here are not independent and any one of them determines the others,¹¹⁻¹⁶ however, for certain types of manipulations it is more convenient to adopt one of these definitions. As is clearly seen from Eqs. (8) we have:

$$\hbar \chi_{AB}(q, \omega) = C_{AB}(q, \omega) + C_{AB}^*(-q, -\omega), \quad (9)$$

and

$$\hat{\chi}_{AB}(q, \omega) = \frac{1}{\omega} [\chi_{AB}(q, \omega) - \chi_{AB}(q, 0)]. \quad (10)$$

The correlation functions may be decomposed into their real and imaginary parts as follows:

$$\Psi \equiv \Psi' - i \Psi'' \quad \Psi = C, \hat{X}, \hat{X} \text{ etc.} \quad (11)$$

Upon taking the imaginary part of Eq. (9) we get the fluctuation dissipation theorem:

$$\hbar \chi_{AB}''(q, \omega) = [1 - \exp(-\hbar\omega/kT)] C_{AB}''(q, \omega). \quad (12)$$

Another useful relation which may be proved from Eqs. (8) is the Kramers-Kronig relation between the real and the imaginary parts of the correlation functions, i.e.

$$\Psi'(q, \omega) - \frac{1}{\pi} \text{PP} \int d\omega' \frac{\Psi''(\omega')}{\omega' - \omega} \quad \Psi = C, \hat{X}, \hat{X} \text{ .} \quad (13)$$

III. DENSITY AND CURRENT RESPONSE FUNCTIONS OF A FLUID

We consider a fluid of noninteracting particles which are moving in a random external potential. The Hamiltonian is assumed to have the form:

$$H = \sum_j \left[\frac{p_j^2}{2m} + U(r_j) \right] \quad (14)$$

Here U is a random potential defined by its correlation functions:

$$\overline{U(r)} = 0 \quad (14a)$$

$$\overline{U(r)U(r')} = f(r-r') \quad (14b)$$

etc.

We shall now introduce the density and current operators ρ_q and J_q respectively defined as follows:

$$\rho_q = \sum_j \exp(iq \cdot r_j), \quad (15)$$

$$\dot{\rho}_q = \frac{i}{\hbar} [H, \rho_q] \equiv \frac{i}{\hbar} q \cdot J_q \quad (16a)$$

Using Eqs. (14) - (16) we have:

$$J_q = \frac{1}{2m} \sum_j [p_j \exp(iq \cdot r_j) + \exp(iq \cdot r_j) p_j], \quad (16b)$$

where m is the mass of our particles. We shall be interested in the electrical conductivity $\sigma(q, \omega)$ which is given by the Kubo transformed current response function, i.e.¹¹

$$\sigma(q, \omega) = \frac{ie^2}{\hbar\Omega} \hat{\chi}_{JJ}(q, \omega) = \frac{ie^2}{\hbar\Omega\omega} [\chi_{JJ}(q, \omega) - \chi_{JJ}(q, 0)]. \quad (17)$$

Here e is the electrical charge of the particles and Ω is the volume of the system.

An important property of Kubo transforms $\hat{\chi}$ is that like the ordinary correlation functions C , they may be viewed as scalar products of two operators in Liouville space, i.e. the quantity $\langle\langle A_q | B_q \rangle\rangle$ defined in Eq. (6) (like $\langle A_q | B_q \rangle$ defined in Eq. (2)) satisfies all the requirements of a scalar product, namely

$$(a) \quad \langle\langle A_q | B_q \rangle\rangle^* = \langle\langle B_q | A_q \rangle\rangle, \quad (18a)$$

$$(b) \quad \text{if } |B_q\rangle\rangle = c_1 |B_q\rangle\rangle + c_2 |\hat{B}_q\rangle\rangle \text{ then,}$$

$$\langle\langle A_q | B_q \rangle\rangle = c_1 \langle\langle A_q | B_q \rangle\rangle + c_2 \langle\langle A_q | \hat{B}_q \rangle\rangle \quad (18b)$$

and

$$(c) \quad \langle\langle A_q | A_q \rangle\rangle > 0 \quad (18c)$$

and the equality sign holds only when $|A_q\rangle\rangle \equiv 0$.

We note in passing that the randomness of the potential in our problem arises from other degrees of freedom and the trace operation in our scalar products involves therefore the averaging over the random potential as well.

Making use of Eqs. (18) we may define a Mori projection operator

$$\hat{P} \equiv |\rho_q\rangle\rangle \langle\langle \rho_q | \chi_\rho(q) \rangle\rangle^{-1}, \quad (19a)$$

and the complementary projection

$$\hat{Q} \equiv 1 - \hat{P}. \quad (19b)$$

Here:

$$\chi_\rho(q) \equiv \langle\langle \rho_q | \rho_q \rangle\rangle \equiv \sum_{\alpha, \beta} \frac{P(\alpha) - P(\beta)}{\hbar\omega_{\beta\alpha}} |(\rho_q)_{\alpha\beta}|^2 \quad (20)$$

The significance of \hat{P} is that when it operates on some arbitrary operator $|C\rangle\rangle$ is projects it onto $|\rho_q\rangle\rangle$, i.e.

$$\hat{P}|C\rangle\rangle \equiv |\rho_q\rangle\rangle \langle\langle \rho_q | C \rangle\rangle \cdot \chi_\rho^{-1}(q) \quad (21)$$

$\chi_p(q)^{-1}$ is a normalization factor introduced to make sure that $\hat{P}^2 = \hat{P}$.
Another quantity that we introduce is the tetradic T matrix :17,18

$$\Upsilon(\omega) \equiv L + L \frac{1}{\omega - L + i\epsilon} L, \quad (22)$$

which may be alternatively written as

$$\Upsilon(\omega) = \omega^2 \left[\frac{1}{\omega - L + i\epsilon} - \frac{1}{\omega + i\epsilon} \right]. \quad (23)$$

The equivalence of Eqs. (22) and (23) may be easily shown as follows. (hereafter we shall omit the $+i\epsilon$ factor and throughout this paper ω should be understood as $\omega + i\epsilon$).

$$\begin{aligned} \Upsilon(\omega) &\equiv L + L \frac{1}{\omega - L} L = L + [(L - \omega) + \omega] \frac{1}{\omega - L} [(L - \omega) + \omega] = L - (L - \omega) + \omega^2 \frac{1}{\omega - L} - 2\omega \\ &= \omega^2 \left(\frac{1}{\omega - L} - \frac{1}{\omega} \right) \end{aligned} \quad (24)$$

Upon multiplying Eq. (23) by a projection operator \hat{P} from right and left we get:

$$\hat{P} \Upsilon \hat{P} = \omega^2 \left[\hat{P} \frac{1}{\omega - L} \hat{P} - \frac{1}{\omega} \hat{P} \right] \quad (25)$$

when using the specific projection \hat{P} (Eq. (19)) in Eq. (25) we get:

$$\hat{\chi}_{JJ} = \frac{\omega^2}{q^2} \left[\hat{\chi}_{\rho\rho} - \frac{1}{\omega} \chi_p(q) \right], \quad (26)$$

Eqs. (26) and (17) immediately result in:

$$\sigma(q, \omega) = \frac{ie^2 \omega^2}{\hbar \Omega q^2} \left[\hat{\chi}_{\rho\rho}(q, \omega) - \frac{1}{\omega} \chi_p(q) \right]. \quad (27a)$$

We have now accomplished our goal to express $\sigma(q, \omega)$ in terms of $\hat{\chi}_{\rho\rho}(q, \omega)$. Other quantities of interest are the density response function $\chi_{\rho\rho}(q, \omega)$, the dielectric response function $\epsilon(q, \omega)$ and the dynamic structure factor $S(q, \omega)$. They may all be expressed in terms of $\chi_{\rho\rho}$,¹⁹ i.e.

$$\chi_{\rho\rho}(q, \omega) = \omega \hat{\chi}_{\rho\rho}(q, \omega) + \chi_p(q) \quad (27b)$$

$$\frac{1}{\epsilon(q, \omega)} = 1 + V_q X_{\rho\rho} = 1 + \frac{4\pi e^2}{q^2} [\omega \hat{X}_{\rho\rho}(q, \omega) + X_{\rho}(q)] \quad (27c)$$

$$S(q, \omega) \equiv C_{\rho\rho}''(q, \omega) = \hbar [1 - \exp(\hbar\omega/kT)]^{-1} X_{\rho\rho}'' \quad (27d)$$

Here V_q is the q component of the interparticle interaction and is equal to $4\pi e^2/q^2$ for a coulomb force.²⁰ In the next section we shall develop a theory for $\hat{X}_{\rho\rho}$ which together with Eqs. (27) will yield $\sigma, X_{\rho\rho}, \epsilon$ and S . We should note that $X_{\rho}(q) \equiv X_{\rho\rho}(q, \omega=0)$ but is not necessarily equal to the low frequency limit of $X_{\rho\rho}$ (See Eqs. (83b) and (87b)).

IV. THE SELF CONSISTENT EQUATIONS FOR THE DENSITY AND CURRENT RESPONSE FUNCTIONS

In this section we shall derive the self consistent equations for the transport coefficients of our fluid. This will be done in two stages: we first consider the Kubo transformed density and current response functions $X_{\rho\rho}$ and X_{JJ} and introduce reduced equations of motion (REM) which express them in terms of appropriate relaxation kernels R_{ρ} and R_J respectively (Eqs. (31) and (36)). We then derive a closed set of self consistent equations for these kernels in the long wavelength ($q \rightarrow 0$) limit. All the relevant transport properties ($\sigma, X_{\rho\rho}, \epsilon$ and S) may then be expressed in terms of R_{ρ} . Two comments of clarification should now be made:

1) The reason that we choose $\hat{X}_{\rho\rho}$ and \hat{X}_{JJ} (and not $X_{\rho\rho}$ and X_{JJ}) as our variables is that, as was shown in the previous section, the former (and not the latter) are scalar products in Liouville space and enable us to use standard projection operator techniques.

2) The usage of the kernels R_{ρ} and R_J instead of the response functions $X_{\rho\rho}$ and X_{JJ} provides a partial resummation of the appropriate series, i.e. a low order approximation to the kernels in some expansion parameter automatically yields an approximation for the response functions which contain certain types of terms to infinite order. The standard REM which $\hat{X}_{\rho\rho}$ satisfies is¹³⁻¹⁵

$$\frac{d\hat{X}_{\rho\rho}(q, t)}{dt} = -q^2 \int_0^t d\tau R_{\rho}(q, t-\tau) \hat{X}_{\rho\rho}(q, \tau) \quad (28)$$

where

$$R_{\rho}(q, \omega) = \langle\langle \rho_q | \hat{L}Q \frac{1}{\omega - LQ} L | \rho_q \rangle\rangle / [X_{\rho}(q) q^2] = \langle\langle J_q | \hat{Q} \frac{1}{\omega - LQ} | J_q \rangle\rangle / X_{\rho}(q) \quad (29)$$

We shall denote the REM of the type (28), which involve a convolution in time as corresponding to the COP (chronological time ordering prescription). In Section V we shall consider another type of REM based on a different time ordering scheme.^{16,21} Eq. (28) should be solved with the initial condition

$$\hat{x}_{\rho\rho}(q, t=0) \equiv x_{\rho}(q) \quad (30)$$

The solution (in ω space) is:

$$\hat{x}_{\rho\rho}(q, \omega) = \frac{1}{\omega - q^2 R_{\rho}(q, \omega)} x_{\rho}(q), \quad (31)$$

In a similar way we may define another projection operator onto the current operator $|J_q\rangle\rangle$ (Eq. (16)):

$$\tilde{P} \equiv |J_q\rangle\rangle\langle\langle J_q| x_J^{-1}(q), \quad (32a)$$

and its complementary projection

$$\tilde{Q} \equiv 1 - \tilde{P}. \quad (32b)$$

where

$$x_J(q) = \langle\langle J_q | J_q \rangle\rangle = \sum_{\alpha, \beta} [P(\alpha) - P(\beta)] \frac{|(J_q)_{\alpha\beta}|^2}{\omega_{\alpha\beta}}. \quad (33)$$

Using the relation:

$$iq(J_q)_{\alpha\beta} = (\rho_q)_{\alpha\beta} = i\omega_{\alpha\beta}(\rho_q)_{\alpha\beta}, \quad (34)$$

we get

$$x_J \equiv x_J(q) = \frac{2}{q^2} \sum_{\alpha\beta} P(\alpha) |(\rho_q)_{\alpha\beta}|^2 \omega_{\alpha\beta} = \frac{N}{m}. \quad (35)$$

This is the exact f sum rule.¹⁹ Proceeding along the same lines of Eqs. (28) - (31) but this time with the new projection (32), we have

$$\hat{x}_{JJ}(q, \omega) = \frac{1}{\omega - R_J(q, \omega)} \cdot x_J, \quad (36)$$

where

$$R_J(q, \omega) = \langle\langle J_q | L \tilde{Q} \frac{1}{\omega - LQ} L | J_q \rangle\rangle / x_J. \quad (37)$$

Eqs. (31) and (36) relate the response functions $\hat{x}_{\rho\rho}$ and \hat{x}_{JJ} to the corresponding kernels R_{ρ} and R_J respectively. Our goal now is to derive a set of self consistent equations for these two kernels. Once these are found we immediately have all our relevant quantities upon the substitution of Eq. (31) in Eqs. (27):

$$\sigma(q, \omega) = \frac{ie^2\omega}{\hbar\Omega} \frac{R_\rho(q, \omega)}{\omega - q^2 R_\rho(q, \omega)} \cdot x_\rho(q) \quad , \quad (38a)$$

$$x_{\rho\rho}(q, \omega) = \frac{R_\rho(q, \omega)q^2}{\omega - R_\rho(q, \omega)q^2} x_\rho(q) \quad , \quad (38b)$$

$$\frac{1}{\epsilon(q, \omega)} = 1 + \frac{4\pi e^2}{q^2} \cdot \frac{R_\rho(q, \omega)q^2}{\omega - R_\rho(q, \omega)q^2} x_\rho(q) \quad , \quad (38c)$$

and

$$S(q, \omega) = \hbar [1 - \exp(-\hbar\omega/kT)]^{-1} \text{Im} \frac{q^2 R_\rho(q, \omega)}{\omega - q^2 R_\rho(q, \omega)} x_\rho(q) \quad . \quad (38d)$$

One relation between R_ρ and R_J is an exact relation which arises immediately by the substitution of Eqs. (31) and (36) in Eq. (26), i.e.

$$\frac{1}{\omega - R_J(q, \omega)} \cdot x_J = \frac{\omega}{q^2} \frac{R_\rho(q, \omega)q^2}{\omega - R_\rho(q, \omega)q^2} x_\rho(q) \quad . \quad (39)$$

We shall now derive a second approximate relation between R_ρ and R_J which together with Eq. (39) will result in a closed set of nonlinear equations for these quantities. We start with Eq. (37) which may be written in the form:

$$R_J(q, \omega) \equiv \langle\langle \dot{J}_q | \dot{Q} \frac{1}{\omega - L\dot{Q}} | \dot{J}_q \rangle\rangle / x_J \quad , \quad (40)$$

where

$$m\dot{J}_q = \frac{im}{\hbar} [H, J_q] = \sum_k U(q-k)(q-k)\rho_k + \frac{iq}{2} E_q + \frac{q^2}{2} J_q \quad , \quad (41)$$

and where

$$E_q = \frac{1}{2m} \sum_j [\exp(iqr_j) p_j^2 + p_j^2 \exp(iqr_j)] \quad , \quad (42)$$

is the kinetic energy density. Hereafter we shall use units where $m=1$.

We shall now introduce three major approximations which allow us to express R_J (Eq. (40)) in terms of R_ρ .

(i) Long wavelength limit ($q \rightarrow 0$)

We are interested in the long wavelength limit of R_ρ and R_J . To that end we define

$$D(\omega) \equiv \lim_{q \rightarrow 0} R_\rho(q, \omega) , \quad (43a)$$

and

$$M(\omega) \equiv \lim_{q \rightarrow 0} R_J(q, \omega) . \quad (43b)$$

Using Eq. (41) we note that for $q \rightarrow 0$ we have:

$$\dot{J}_q \equiv \sum_k U(k) k \rho_k . \quad (44)$$

Substitution of Eq. (44) in Eq. (40) yields:

$$M(\omega) \equiv \sum_{kk'} k k' \langle \langle \rho_k U_k | \frac{1}{\omega - QL} \hat{Q} | U_{k'} \rho_{k'} \rangle \rangle / X_J \quad (45)$$

We recall that the scalar product $\langle \langle \dots \rangle \rangle$ also includes averaging over the random potential.

(ii) Factorization

Since the critical behavior of the system is expected to come from collective long wavelength ($k \rightarrow 0$) modes, we shall split Eq. (45) into a high k part denoted $M_0(\omega)$ which may be evaluated using perturbation theory in U , and a long wavelength part. $M_0(\omega)$ does not undergo any drastic change near the Anderson transition. In the long wavelength part of the summation (45), we shall invoke a factorization approximation and factor out the $U_k U_{k'}$ terms in the averaging over the random potential. We thus get

$$M(\omega) = M_0(\omega) + \sum_k k^2 U_k \langle \langle \rho_k | \frac{1}{\omega - QL} \hat{Q} | \rho_k \rangle \rangle / X_J \quad (46)$$

where the k summation now excludes the high k part included in $M_0(\omega)$. Eq. (46) is the most serious assumption made in the present deviation and it is a mean field type of approximation.

(iii) $\hat{Q} \cong 1$

Since the \hat{P} space (Eq. (21)) is very small and the \hat{Q} space is overwhelmingly bigger, it is reasonable to substitute $\hat{Q} = 1 - \hat{P} \cong 1$ in Eq. (46), resulting in

$$\begin{aligned} M(\omega) &\cong M_0(\omega) + \sum_k k^2 U_k \hat{x}_{\rho\rho}(k, \omega) / X_J \\ &\cong M_0(\omega) + \sum_k k^2 U_k \frac{1}{\omega - k^2 R_\rho(k, \omega)} x_\rho(k) / X_J \end{aligned} \quad (47)$$

We have now accomplished our goal. Upon the substitution of Eqs. (43) in Eq. (47) and in Eq. (39) we get:

$$M(\omega) = M_0(\omega) + \sum_k \frac{k^2 U_k}{\omega - k^2 D(\omega)} \frac{1}{x_\rho(k)/x_J}, \quad (48a)$$

and

$$D(\omega) = \frac{1}{\omega - M(\omega)} \cdot \frac{x_J}{x_\rho(q=0)} \quad (48b)$$

Eqs. (48a) and (48b) are our final self consistent equations for $D(\omega)$ and $M(\omega)$. The input information is U_k and $x_\rho(k)$. Once these are solved, we have, using Eqs. (38) and (43a), for the transport coefficients:

$$\sigma(\omega) \equiv \sigma(q \rightarrow 0, \omega) = \frac{ie^2}{\hbar \Omega} D(\omega) \cdot x_\rho(q=0), \quad (49a)$$

$$x_{\rho\rho}(q, \omega) = \frac{D(\omega)q^2}{\omega - D(\omega)q^2} x_\rho(q), \quad (49b)$$

$$\frac{1}{\epsilon(q, \omega)} = 1 + 4\pi e^2 \frac{D(\omega)}{\omega - D(\omega)q^2} x_\rho(q), \quad (49c)$$

and

$$S(q, \omega) = \frac{1}{\hbar} [1 - \exp(-\hbar\omega/kT)]^{-1} \text{Im} \frac{q^2 D(\omega)}{\omega - q^2 D(\omega)} x_\rho(q). \quad (49d)$$

We should note at this point that for a free Fermi gas we have:

$$\frac{1}{\Omega} x_\rho(q=0) = N(E_F) \quad (50a)$$

whereas for a classical gas with n particles per unit volume

$$\frac{1}{\Omega} x_\rho(q=0) = \frac{n}{kT} \quad (50b)$$

Eqs. (48) together with (50a) were derived recently by Vollhardt and Wolfe^{22, 23} for a Fermi gas at $T=0$.

V. THE SELF CONSISTENT EQUATIONS - REVISITED

In Section IV we have derived REM for R_ρ and R_J using the conventional COP equations (Eq. (28)). We shall now consider an alternative scheme based on different REM denoted POP (partial time-ordering

prescription). A detailed study and comparison of the COP and POP equations was given elsewhere.^{16,21} Suffice it to say here that both types of REM are in principle exact, however once approximations are made they may yield very different results, especially in the non-Markovian limit (when the kernels are frequency dependent). The resulting self consistent equations for the density and current response kernels will be different in the POP scheme. The derivation of the new equations is parallel to that of the previous section, the only difference being the form of the REM. Therefore, we shall not go into the details and merely sketch the main steps of the derivation. The POP formulation is based on a convolutionless reduced equation of motion which is local in time.²¹ Instead of Eq. (28), we write:

$$\frac{d\hat{\chi}_{\rho\rho}(q,t)}{dt} = -q^2 \int_0^t d\tau \tilde{R}_\rho(q,\tau) \cdot \hat{\chi}_{\rho\rho}(q,t), \quad (51)$$

where

$$\tilde{R}_\rho(q,\tau) = \frac{1}{q^2} \frac{d}{d\tau} \langle\langle \rho_q | L \exp(-iL\tau) | \rho_q \rangle\rangle \langle\langle \rho_q | \exp(-iL\tau) | \rho_q \rangle\rangle^{-1}. \quad (52)$$

Using Eq. (16a) we may rearrange Eq. (52) in the form:

$$R(q,\tau) = \left\{ \langle\langle J_q(\tau) | J_q \rangle\rangle \langle\langle \rho_q(\tau) | \rho_q \rangle\rangle - q^2 \left[\int_0^\tau d\tau_1 \langle\langle J_q(\tau_1) | J_q \rangle\rangle \right]^2 \right\} / \left[1 + q^2 \int_0^\tau d\tau_1 (\tau - \tau_1) \langle\langle J_q(\tau_1) | J_q \rangle\rangle \right]^{-1} \chi_\rho^{-1}(q) \quad (53)$$

The solution of Eq. (51) with the initial condition Eq. (30) is:

$$\hat{\chi}_{\rho\rho}(q,t) = \exp\left[-q^2 \int_0^t d\tau (t-\tau) \tilde{R}_\rho(q,\tau)\right] \cdot \chi_\rho(q) \quad (54)$$

Similarly using the POP scheme we have in analogy with (36)

$$\hat{\chi}_{JJ}(q,\tau) = \exp\left[-\int_0^\tau d\tau_1 (\tau - \tau_1) \tilde{R}_J(q,\tau_1)\right] \cdot \chi_J \quad (55)$$

where

$$\tilde{R}_J(q,\tau) = \frac{d}{d\tau} \langle\langle J_q | L \exp(-iL\tau) | J_q \rangle\rangle \langle\langle J_q | \exp(-iL\tau) | J_q \rangle\rangle^{-1}. \quad (56)$$

We reiterate that Eqs. (54) and (55) are exact provided the kernels (52) and (56) are evaluated rigorously.

Upon substitution of Eq. (54) in Eqs. (27) we get:

$$\sigma(q,\omega) = \frac{ie^2}{\hbar\Omega} \frac{\omega^2}{q^2} \int_0^\infty d\tau \exp(i\omega\tau) \{\exp[-q^2 K(q,\tau)] - 1\} \chi_\rho(q), \quad (57a)$$

$$\chi_{\rho\rho}(q, \omega) = i\omega \int_0^{\infty} d\tau \exp(i\omega\tau) \{ \exp[-q^2 K(q, \tau)] - 1 \} \chi_{\rho}(q), \quad (57b)$$

$$\frac{1}{\epsilon(q, \omega)} = 1 + \frac{i4\pi e^2 \omega}{q^2} \int_0^{\infty} d\tau \exp(i\omega\tau) \{ \exp[-q^2 K(q, \tau)] - 1 \} \chi_{\rho}(q), \quad (57c)$$

$$S(q, \omega) = \frac{\hbar}{1 - \exp(-\hbar\omega/kT)} \text{Im} \int_0^{\infty} d\tau \exp(i\omega\tau) \exp[-q^2 K(q, \tau)] \chi_{\rho}(q), \quad (57d)$$

where

$$K(q, \tau) = \int_0^{\tau} dt_1 (\tau - \tau_1) \tilde{R}_{\rho}(q, \tau_1). \quad (58)$$

The POP kernels \tilde{R}_{ρ} and \tilde{R}_J are related by the exact relation obtained by substituting Eqs. (54) and (55) in Eq. (26)

$$\exp\left[-\int_0^{\tau} dt_1 (\tau - \tau_1) \tilde{R}_J(q, \tau_1)\right] = \frac{\omega^2}{q^2} \int_0^{\infty} d\tau \exp(i\omega\tau) \{ \exp[-q^2 \int_0^{\tau} dt_1 (\tau - \tau_1) \tilde{R}_{\rho}(q, \tau_1)] - 1 \} \chi_{\rho}(q) / \chi_J \quad (59)$$

We now, as in Section IV, go to the long wave length limit and define

$$\tilde{M}(\tau) \equiv \lim_{q \rightarrow 0} R_J(q, \tau), \quad (60a)$$

$$\tilde{D}(\tau) = \lim_{q \rightarrow 0} R_{\rho}(q, \tau). \quad (60b)$$

Making assumptions (i) - (iii) of Section IV we finally get the self consistent POP equations:

$$\tilde{M}(\tau) = \tilde{M}_0(\tau) + \sum_k \frac{U_k^2}{k} k^2 \exp[-k^2 \int_0^{\tau} dt_1 (\tau - \tau_1) \tilde{D}(\tau_1)] \chi_{\rho}(q) / \chi_J, \quad (61a)$$

and

$$\tilde{D}(\tau) = \exp\left[-\int_0^{\tau} dt_1 (\tau - \tau_1) \tilde{M}(\tau_1)\right] \cdot \chi_J / \chi_{\rho}(q=0). \quad (61b)$$

where $\tilde{M}_0(\tau)$ is a non-critical (high k) contribution to $\tilde{M}(\tau)$. Eqs. (61) are analogous to Eqs. (48) but in general they may yield different solutions since approximation (i) - (iii) when made within the POP scheme have a different significance. Once $\tilde{M}(\tau)$ and $\tilde{D}(\tau)$ are solved then the transport coefficients are obtained by the substitution of Eq. (54) in Eqs. (57):

$$\sigma(\omega) = \frac{ie^2}{\hbar\Omega} \omega^2 \int_0^\infty d\tau \tilde{K}(\tau) \exp(i\omega\tau) \cdot \chi_\rho(q=0), \quad (62a)$$

$$\chi_{\rho\rho}(q, \omega) = i\omega \int_0^\infty d\tau \exp(i\omega\tau) \{ \exp[-q^2\tilde{K}(\tau)] - 1 \} \chi_\rho(q=0), \quad (62b)$$

$$\frac{1}{\epsilon(q, \omega)} = 1 + i \frac{4\pi e^2 \omega}{q^2} \int_0^\infty d\tau \exp(i\omega\tau) \{ \exp[-q^2\tilde{K}(\tau)] - 1 \} \chi_\rho(q) \quad (62c)$$

$$S(q, \omega) = \frac{\hbar\omega}{[1 - \exp(-\hbar\omega/kT)]}$$

$$\text{Re} \int_0^\infty d\tau \exp(i\omega\tau) \{ \exp[-q^2\tilde{K}(\tau)] - 1 \} \chi_\rho(q) \quad (62d)$$

where

$$\tilde{K}(\tau) = \int_0^\tau d\tau_1 (\tau - \tau_1) \tilde{D}(\tau_1). \quad (62e)$$

VI. DISCUSSION

We have derived coupled self consistent equations which enable us to calculate the electrical conductivity, dielectric constant, the density response function and the dynamic structure factor of a fluid in a random potential. All these quantities are expressed in terms of the density response kernel $D(\omega)$ (Eqs. (49)) or $\tilde{D}(\tau)$ (Eqs. (62)). $D(\omega)$ or $\tilde{D}(\tau)$ may be obtained by solving the self consistent equations, Eqs. (48) and Eqs. (61) respectively. It should be noted that the density kernels $D(\omega)$ and $\tilde{D}(\tau)$ are simply related by a Fourier transformation, i.e.

$$D(\omega) = -i \int_0^\infty d\tau \exp(i\omega\tau) \tilde{D}(\tau). \quad (63)$$

This may easily be seen by noting that using Eq. (29) we have:

$$D(\omega) = \lim_{q \rightarrow 0} R_\rho(q, \omega) = \langle\langle J_0 | \frac{1}{\omega - L} | J_0 \rangle\rangle / \chi_J \quad (64a)$$

whereas when using Eq. (53) we get

$$\tilde{D}(\tau) = \lim_{q \rightarrow 0} R_\rho(q, \tau) = \langle\langle J_0 | \exp(-iL\tau) | J_0 \rangle\rangle / \chi_J. \quad (64b)$$

Eqs. (63) immediately follows from Eqs. (64). Despite the simple relation (63), the solutions of the self consistent Eqs. (48) and (61) do not necessarily satisfy Eq. (63). The reason is that the approximations made in the derivation of Eqs. (48) and (61) are different and we may get different results especially when $D(\omega)$ is strongly frequency dependent.^{16,21} Only detailed study may reveal which form is to be preferred. It should be noted however that Eqs. (48) are easier to solve since they may be solved for each frequency independently whereas Eqs. (61) are solved for the entire function $D(\tau)$. At this stage we wish to clarify the connection between $D(\omega)$ and the ordinary diffusion coefficient $D_0(\omega)$. The latter is the kernel of the density correlation function, i.e.

$$C_{\rho\rho}(q, \omega) = \frac{1}{\omega - q^2 D_0(\omega)} S(q) \quad (65)$$

where $S(q)$ is the static structure factor

$$S(q) = \langle \rho_q | \rho_q \rangle = \sum_{\alpha, \beta} P(\alpha) |(\rho_q)_{\alpha\beta}|^2 \quad (66)$$

Using Eqs. (12), (49b) and (65) and taking the $q \rightarrow 0$ limit we have:

$$\frac{D''(\omega)}{D_0''(\omega)} = \frac{1 - \exp(-\hbar\omega/kT)}{\hbar\omega} \cdot \frac{S(q=0)}{\chi_\rho(q=0)} = \frac{kT}{\hbar\omega} [1 - \exp(-\hbar\omega/kT)] \quad (67)$$

In the limit $\omega \rightarrow 0$, $T \rightarrow 0$ but $\hbar\omega \ll kT$ we thus have

$$\frac{D''(\omega)}{D_0''(\omega)} \xrightarrow{\omega \rightarrow 0} 1, \quad (68)$$

and utilizing the Kramers Kronig relation (13), we then have:

$$D(\omega) \cong D_0(\omega) \quad (69)$$

Eq. (69) holds for typical DC experiments in the Anderson localization problem. For $T=1^\circ\text{K}$, e.g. it holds for $\omega < 10^9 \text{ sec}^{-1}$.

We shall now focus on Eqs. (48) and simplify them further. Towards that end let us define the Laplace transform:

$$\hat{D}(s) = \int_0^\infty d\tau \tilde{D}(\tau) \exp(-s\tau) \quad (70)$$

It is clear from Eq. (63) that

$$D(\omega) = -i\hat{D}(-i\omega) \quad (71a)$$

Similarly we define $\hat{M}(s)$ such that

$$M(\omega) = -i\hat{M}(-i\omega) \quad (71b)$$

As is clearly seen from eqs. (64) and (71) D and M are real and this simplifies our analysis.

Upon multiplying Eq. (48a) by $D(s)$ and substituting Eq. (48b), we get:

$$\begin{aligned} \hat{D}(s)M(s) &= \frac{x_J}{x_\rho(q=0)} - \hat{D}(s) \cdot s, \\ &= \hat{M}_0(s)\hat{D}(s) + \sum_k \frac{\overline{U_k^2} k^2 \hat{D}(s)}{k s + k^2 \hat{D}(s)} \frac{x_\rho(k)}{x_J}, \end{aligned} \quad (72)$$

i.e.

$$\frac{\hat{D}(s)}{D_0(s)} = 1 - \frac{x_\rho(q=0)}{x_J} \sum_k \frac{\overline{U_k^2} k^2 \hat{D}(s)}{k s + k^2 \hat{D}(s)} \frac{x_\rho(k)}{x_J}, \quad (73)$$

where

$$\hat{D}_0(s) = \frac{1}{s + M_0(s)} \frac{x_J}{x_\rho(q=0)} \quad (74)$$

is a microscopic non-critical diffusion kernel which does not vary significantly in the vicinity of the transition. Assuming that U_k and $x_\rho(k)$ are weakly dependent on k for small values of k , we then get:

$$\frac{\hat{D}(s)}{D_0(s)} = 1 - \lambda \left(\frac{s}{\hat{D}(s) k_0^2} \right)^{\frac{d}{2}} \int_0^{\sqrt{D k_0^2 / s}} dy \frac{y^{d+1}}{1+y^2} \quad (75)$$

Here we have changed the k summation to an integration

$$\sum_k \rightarrow \frac{\Omega}{(2\pi)^3} \int_0^{k_0} k^{d-1} dk \quad (76)$$

where k_0 is an upper cutoff (of the order of the lattice spacing), and

$$\lambda = \frac{\Omega}{(2\pi)^3} \overline{U_0^2} \frac{x_\rho(q=0)^2}{x_J} k_0^d \quad (77)$$

is a dimensionless coupling strength.

Eq. (75) is our final equation for the diffusion kernel. The input information that enters this equation is the dimensionless coupling strength λ , the microscopic diffusion coefficient $D_0(s)$ and the microscopic cutoff wavevector k_0 .

Let us see what do we expect from our kernel $D(s)$ for the Anderson localization. In the metallic side of the transition there is a finite DC conductivity whereas in the insulating side it vanishes like ω^β . Assuming that the polarizability $\alpha(\omega) = \sigma(\omega)/\omega$ remains finite in the insulating phase^{22,23} we have $\beta=1$. We thus get:

$$\sigma(\omega) \xrightarrow{\omega \rightarrow 0} \begin{cases} \text{const.} & \text{conducting phase} \\ \omega & \text{insulating phase} \end{cases} \quad (78)$$

This implies using Eq. (49a):

$$\hat{D}(s) \xrightarrow{s \rightarrow 0} \begin{cases} \text{const.} & \text{conducting phase} \\ \xi^2 s & \text{insulating phase} \end{cases} \quad (79)$$

Making use of a Tauberian theorem,²⁴ which relates the small frequency behavior of $D(s)$ to the long time behavior of its Fourier transform $D(\tau)$, and of Eq. (62e), we get also:

$$\tilde{K}(t) \xrightarrow{t \rightarrow \infty} \begin{cases} t & \text{conducting phase} \\ \xi^2 & \text{insulating phase} \end{cases} \quad (80)$$

The existence of the Anderson transition may thus be investigated using Eq. (75) by looking for a value of $\lambda = \lambda_c$ such that for $\lambda < \lambda_c$ $D(s) \sim \text{const.}$ and for $\lambda > \lambda_c$ $D(s) = \xi^2 s$ at low frequencies. By virtue of Eqs. (63e), (63) and (69) it is clear that $K(t)$ is simply the second moment of a density fluctuation in the medium created initially at $r=0$. Eq. (80) shows that for $\lambda < \lambda_c$ the second moment diverges linearly at long times, whereas for $\lambda > \lambda_c$ the second moment assumes asymptotically a finite value, namely the correlation length ξ . Let us investigate the existence of λ_c in 3d. To that end we rewrite Eq. (75) for $d=3$ as:

$$\frac{\hat{D}(s)}{D_0(s)} = 1 - \frac{1}{3} \lambda + \lambda \frac{s}{\hat{D}_{k_0}^2} - \lambda \left(\frac{s}{\hat{D}_{k_0}^2} \right)^{3/2} \text{arctg} \sqrt{\frac{\hat{D}_{k_0}^2}{s}} \quad (81)$$

A simple inspection of Eq. (80) shows that $\lambda_c=3$ and we have:

$$\hat{D}(s) = \hat{D}_0(s) \left[1 - \frac{1}{3} \lambda \right] \quad s \rightarrow 0 \quad \lambda < 3 \quad (82a)$$

$$\hat{D}(s) = 0 \quad s \rightarrow 0 \quad \lambda > 3 \quad (82b)$$

Vollhardt and Wolfle²³ have recently derived similar equations. However, their derivation is made specifically for a Fermi gas at $T=0$. The present derivation is less restrictive and we show that the general structure of the equations is insensitive to the details of the model (classical or quantum fluid, temperature, space dimensionality, etc.) This enables us to connect the Anderson problem with the classical phenomena of long time tails in nonlinear hydrodynamics.^{6,9,10} After a lengthy diagrammatic calculation Vollhardt and Wolfle got an equation similar to Eq. (75) but with d replaced by $d-2$. They have shown that their equation predicts a phase transition for $d>2$ as it should, whereas the present equation predicts such a phase transition for all $d>0$. This arises due to our mean field approximation (Eq. (46)) which certainly fails for low dimensionalities. It is interesting to note however that the structure of the equation is the same for a classical and a quantum fluid. We also see that for $d>3$ there is no difference between our result and that of Vollhardt and Wolfle.

Using the present derivation we may conclude that some of the features of the Anderson localization in 3d are not at all quantum mechanical and maybe the detailed study of the nature of the wave functions, whether they are localized or extended is superfluous in the sense that the transport coefficients are not so sensitive to these details, and the transition exists also in a classical fluid.¹⁰

Finally let us see what we do predict for the density response function (Eq. (27b)) near the Anderson transition. Upon substituting (79) in (49b) we get:

$$x_{\rho\rho}(q, \omega) = \begin{cases} x_{\rho}(q) & \text{conducting phase} & (83a) \\ \frac{\xi^2 q^2}{1 - \xi^2 q^2} \cdot x_{\rho}(q) & \text{insulating phase} & (83b) \end{cases}$$

since $x_{\rho}(q) \equiv x_{\rho\rho}(q, \omega=0)$ this means that for the insulating phase

$$\lim_{\omega \rightarrow 0} x_{\rho\rho}(q, \omega) \neq x_{\rho\rho}(q, \omega=0) \quad (84)$$

In fact, in r space we have for the insulating phase

$$x_{\rho\rho}(r, \omega=0) = \int x_{\rho}(r-r') F(r') \quad (85)$$

where

$$F(r') = \delta(r') + \exp(-r'/\xi)/(r')^{d/2} \quad (86)$$

is a dynamic contribution to $x_{\rho\rho}$. Eq. (86) was derived recently by Vollhardt and Wolfle.²³ Within the POP formalism, substitution of Eq. (80) in (62b) yields:

$$\lim_{\omega \rightarrow 0} x_{\rho\rho}(q, \omega) = \begin{cases} x_{\rho}(q) & \text{conducting phase} & (87a) \\ [\exp(-\xi^2 q^2) - 1] x_{\rho}(q) & \text{insulating phase} & (87b) \end{cases}$$

So that for the insulating phase we have again Eq. (85) where

$$F(r') = \exp(-r'^2/\xi^2) + \delta(r') \quad (88)$$

We note that in the metallic phase where $D(\omega)=\text{const.}$ and $\bar{K}(t)\sim t$ both formulations(83a) or (87a) yield the same result. This is a general feature of the POP and COP schemes that in the Markovian limit they are identical.^{16,21} However the difference between Eqs. (86) and (88) is a manifestation of the difference in predictions of both formulations in the non-Markovian limit, where $D(\omega)$ is frequency dependent.

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