森公式の closed-form 解とその応用

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射影演算子を用いて運動方程式を厳密に変形して得られる、一般化された Langevin 方程式を森公式と名付ける。導出された揺動力は元の運動方程式とは異なった時間発展をする。森公式の記憶関数に対する closed-form 解 (CFS) の導出法 (射影演算子展開法) [2]を紹介し、CFS の応用例を報告する。

(1) 久保公式に基づく輸送係数の森公式による厳密な表現を示すと共に、遅延応答関数間の恒等式を用いて、輸送係数の新たな一般表式を示す。また、記憶関数を force-force correlation function で代用する近似 (ここでは MFA と略記) における低振動数極限の固定点を、電気抵抗や一般化された Drude 解析における光学質量において示す。

(2) 緩和現象の森公式による応用として、バンド幅 W_B、バンドギャップ Δ である2－バンドブロッホ電子系における電流演算子について CFS を計算する。その揺らぎは $T=0$ で記憶関数が t^{-1} の包絡線で特徴づけられ、自発的に強く色付いていることを示す[3]。また、$\Delta << W_B$ のパラメータ領域では、高振動数極限で厳密な MFA が $\Delta \lesssim \omega \leq \Delta + 2W_B$ の有限振動数領域で有効であることをも示す。このとき、解析的な記憶関数を得る。

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[2]CFS はこの展開法によらず導出出来る。J. Phys. Soc. Jpn. **66** (1997) 2218

[3]時間スケールが一つしか存在しないため、この揺らぎは通常の Langevin force とは異なる。

Closed-Form Solution to the Mori Formula and its Application

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The derivation of the closed-form solution to the generalized Langevin equation (Mori formula) is reviewed. We derive rigorous constraints for transport coefficients in the limit of low frequency and those obtained in the memory functional approach to the closed-form solution. We calculate the closed-form solution for the relaxation functions of the fluctuating force in a free two-band model to find a long-time tail of t^{-1} and the strongly colored quantum noise at $T = 0$.

KEYWORDS: generalized Langevin equation, Mori formula, closed-form solution, Kubo formula, transport phenomena, relaxation phenomena, quantum noise

§1. Introduction

The Mori formula[1] is itself a formalism where we can derive the generalized Langevin equation (GLE) from the Heisenberg equation of motion by introducing the projection operator, however, we refer to the GLE as the Mori formula for convenience. Since the GLE was deduced and the linear response theory (Kubo formula)[2] was then reformulated,[3] the GLE has been of great interest in statistical physics and solid state physics. The continued fraction solution[3] to the GLE has been mainly used in the memory functional approaches (MFA)[11-17] for application to relaxation and transport phenomena. The GLE was also deduced by the equation of motion for retarded two-time Green's functions[4] and by the recurrence relations for orthogonal operators with the continued fraction solution.[5,6] Some years later than the derivation of the GLE, a long-time tail for velocity autocorrelation functions was reported by the computer simulations[7] and the existence of a long-time tail has been studied so far.[8-10]

In §2, we review the derivation of the closed-form solution to the GLE by Okada *et al.*[18] with the proof of the identity between the GLE and the Kubo formula.[20] In §3, we apply the identity to transport phenomena in the limit of low frequency within the linear response theory and deduce rigorous constraints for transport coefficients and those obtained in the MFA to the closed-form solution. In §4, we take the closed-form solution to investigate relaxation phenomena and quantum noise. We show that the relaxation functions of the fluctuating force in a free two-band model have a long-time tail of t^{-1} at $T = 0$ irrespective of its parameters and dimensionality and that the fluctuating force in the model is the strongly colored quantum noise at $T = 0$. We also present a model where the MFA to the closed-form solution are practically valid. Concluding remarks are given in §5.

§2. The Mori Formula with the Closed-Form Solution

We revisit the GLE (Mori formula)[1] and review the derivation of the closed-form solution to the GLE by Okada *et al.*[18] with the proof of the identity between the GLE and the Kubo formula.[20]

2.1 The GLE and the Kubo formula

We introduce an operator P projecting any operator O on a current operator J in the system described by the Hamiltonian H as

$$PO \equiv \frac{(O, J^{\dagger})}{(J, J^{\dagger})}\, J, \tag{2.1}$$

where the inner product is defined by the canonical correlation function

$$(A(t), B) \;\equiv\; \frac{1}{\beta}\int_0^{\beta} \mathrm{Tr}\,[\rho A(t - \mathrm{i}\hbar\lambda)B]\;\mathrm{d}\lambda, \tag{2.2}$$

with the density operator $\rho \equiv \mathrm{e}^{-\beta H}/\mathrm{Tr}[\mathrm{e}^{-\beta H}]$ and the inverse temperature $\beta \equiv T^{-1}$. Using the formalism in terms of the projection operator P, the GLE for a current operator $J(t) = \mathrm{e}^{\mathrm{i}Ht/\hbar} J \mathrm{e}^{-\mathrm{i}Ht/\hbar}$ is given by[1] for $t > 0$

$$\frac{\mathrm{d}}{\mathrm{d}t}J(t) \equiv \mathrm{i}LJ(t) = [\ \mathrm{e}^{\mathrm{i}Lt}\dot{J} - f(t)\ ] \;+\; f(t), \tag{2.3}$$

$$= -\int_0^t \varphi(t-s)\; J(s)\;\mathrm{d}s \;+\; f(t), \tag{2.4}$$

$$f(t) \equiv \mathrm{e}^{(1-P)\ \mathrm{i}Lt} f, \qquad f = \dot{J}, \tag{2.5}$$

$$\varphi(t) \equiv \frac{(f(t), f^{\dagger})}{(J, J^{\dagger})}. \tag{2.6}$$

We have introduced the quantum Liouville operator $\mathrm{i}LJ \equiv (\mathrm{i}/\hbar)[H, J]_- \equiv \dot{J}$. The expectation value of $f(t)$ in eq. (2.5) vanishes, i.e., $\langle f(t)\rangle = 0$ resulting from $\langle \mathrm{i}LO\rangle = 0$ with $\langle O\rangle = \mathrm{Tr}[\rho O]$. Equation (2.6) is nothing but the fluctuation-dissipation theorem. Therefore $f(t)$ is in general identified with the fluctuating force.

Since the projection operator P is defined by the canonical correlation function, the linear response theory (Kubo formula)[2] is then reformulated as follows:[3] Operating P on the left of both sides of eq. (2.4) and noting $Pf(t) = 0$, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\Xi(t) = -\int_0^t \Xi(t-s)\;\varphi(s)\;\mathrm{d}s, \tag{2.7}$$

$$\Xi(t) \equiv \frac{(J(t), J^{\dagger})}{(J, J^{\dagger})}. \tag{2.8}$$

Taking the Laplace transform of eq. (2.7) yields

$$\Xi(z) \equiv \int_0^\infty dt\ e^{-zt}\ \Xi(t) = \frac{1}{z+\overline{\varphi}(z)},\ \mathrm{Re}\ z > 0. \tag{2.9}$$

On the other hand, the optical conductivity $\sigma(\omega)$ of the system under the external field $\propto e^{-i\omega^+ t}$ with $\omega^+ \equiv \lim_{\epsilon\to 0}\ [\omega + i\epsilon]$ is written in the linear response theory as

$$\sigma(\omega) = \frac{1}{V}\int_0^\infty dt\ e^{i\omega^+ t}\ \beta\ (J(t), J^\dagger) \tag{2.10}$$

with the system volume V. By using eq. (2.9), eq. (2.10) is rewritten[1] as

$$\sigma_M(\omega) = \frac{[W]}{-i\omega^+ + \overline{\varphi}(-i\omega^+)}, \tag{2.11}$$

$$\overline{\varphi}(-i\omega^+) = \int_0^\infty dt\ e^{i\omega^+ t}\ \varphi(t), \tag{2.12}$$

with the conductivity weight tensor $[W] \equiv \beta(J, J^\dagger)/V$.

The term $i\omega_0 J(t)$ which we should include in the r.h.s of eq. (2.4) or $-i\omega_0$ in the dominator in the r.h.s of eqs. (2.9) and (2.11) vanishes. This is because $i\omega_0 \equiv (\dot{J}.J^\dagger)/(J, J^\dagger) = 0$, i.e., $P\dot{J} \equiv 0$ for the self-adjoint operator $J^\dagger = J$, which is derived from the identity $[J, e^{-\beta H}]_- = -i\hbar e^{-\beta H}\int_0^\beta \dot{J}(-i\hbar\lambda)d\lambda$.

Hereafter we use the notation for a complex function $G(\omega) \equiv G'(\omega) + iG''(\omega)$ where $G'(\omega)$ and $G''(\omega)$ are real. The Fourier transform of $G(\omega)$ is written from the analyticity as

$$\begin{aligned} G(t) &= \frac{1}{2\pi}\int_{-\infty}^\infty d\omega e^{-i\omega^+ t} G(\omega) \\ &= \frac{1}{\pi}\int_0^\infty d\omega \cos\omega t\ G'(\omega) + \frac{1}{2\pi}\int_{-\infty}^\infty d\omega(\frac{-}{\pi})^2\int_{-\infty}^\infty dx\ \frac{\cos xt}{x-\omega}\int_{-\infty}^\infty dy\ \frac{G'(y)}{y-\omega} \\ &= \frac{2}{\pi}\int_0^\infty d\omega \cos\omega t\ G'(\omega). \end{aligned} \tag{2.13}$$

The integrand of the last term in eq. (2.13) can be replaced by $\sin\omega t\ G''(\omega)$ for the easy performance of integration.

2.2 The closed-form solution

Since the time evolution of the fluctuating force $f(t)$ in eq. (2.5) is governed by the complex projected Liouville operator, i.e.,

$$\frac{d}{dt}f(t) = (1-P)iLf(t), \tag{2.14}$$

eq. (2.12) was then formulated in terms of continued fraction representation.[3] The continued fraction solution is originated in the same procedure where we deduce the generalized fluctuating force $f_1(t)$ from the equation of motion for $f(t)$, which is governed by the generalized Liouville operator $iL_1 \equiv (1-P)iL$, as we have done $f(t)$ from the Heisenberg equation of motion for $J(t)$, eq. (2.3).

First, from the analogy of Feynman's perturbation expansion for the density matrix, we set the projected Liouville operator in eq. (2.5), as follows:[18)]

$$\mathrm{e}^{(1-P)\,\mathrm{i}Lt} \equiv \mathrm{e}^{\mathrm{i}Lt} B(t). \tag{2.15}$$

Since both P and L are time-independent, the time derivative of Eq. (2.15) yields

$$\frac{\mathrm{d}}{\mathrm{d}t}B(t) \;=\; -F(t)B(t), \qquad F(t) \equiv \mathrm{e}^{-\mathrm{i}Lt}\; P\mathrm{i}L\; \mathrm{e}^{\mathrm{i}Lt}. \tag{2.16}$$

Eq. (2.16) can be formally integrated and then solved iteratively to yield for $t > 0$

$$B(t) \;=\; 1 \;+\; \sum_{n=1}^{\infty}(-)^n \int_0^t \mathrm{d}\tau_1 \cdots \int_0^{\tau_{n-1}} \mathrm{d}\tau_n \; F(\tau_1)\cdots F(\tau_n). \tag{2.17}$$

Here we must recall how the definition of P in eq. (2.1) is and note that $F(t)$ in eq. (2.16) includes the term $P\mathrm{i}L$ lined in this order. Since $\dot{J}$ generates $f(t) = \mathrm{e}^{\mathrm{i}Lt}B(t)\dot{J}$, $f(t)$ rotates in the space spanned by J, $\dot{J}$, and $\ddot{J}$. Substituting these results into eq. (2.5), eq. (2.12) is expanded in terms of time convolutions as

$$\overline{\varphi}(-\mathrm{i}\omega^+) \;=\; \int_0^\infty \mathrm{d}t\; \mathrm{e}^{\mathrm{i}\omega^+ t}\, \frac{(\mathrm{e}^{\mathrm{i}Lt}B(t)\dot{J}, \dot{J}^\dagger)}{(J, J^\dagger)} \;\equiv\; \sum_{n=0}^{\infty} \overline{\varphi}^{(n)}(-\mathrm{i}\omega^+), \tag{2.18}$$

where

$$\overline{\varphi}^{(0)}(-\mathrm{i}\omega^+) = \int_0^\infty \mathrm{d}t\; \mathrm{e}^{\mathrm{i}\omega^+ t}\, \frac{(\dot{J}(t), \dot{J}^\dagger)}{(J, J^\dagger)}, \tag{2.19}$$

$$\overline{\varphi}^{(1)}(-\mathrm{i}\omega^+) = \int_0^\infty \mathrm{d}t\; \mathrm{e}^{\mathrm{i}\omega^+ t}(-) \int_0^t \mathrm{d}\tau_1 \frac{(\ddot{J}(\tau_1), J^\dagger)}{(J, J^\dagger)} \frac{(J(t-\tau_1), \dot{J}^\dagger)}{(J, J^\dagger)}, \tag{2.20}$$

$$\begin{aligned} \overline{\varphi}^{(n)}(-\mathrm{i}\omega^+) = {}& \int_0^\infty \mathrm{d}t\; \mathrm{e}^{\mathrm{i}\omega^+ t}(-)^n \int_0^t \mathrm{d}\tau_1 \cdots \int_0^{\tau_{n-1}} \mathrm{d}\tau_n \\ & \times \frac{(\ddot{J}(\tau_n), J^\dagger)}{(J, J^\dagger)} \frac{(\dot{J}(\tau_{n-1}-\tau_n), J^\dagger)}{(J, J^\dagger)} \cdots \frac{(\dot{J}(\tau_1-\tau_2), J^\dagger)}{(J, J^\dagger)} \frac{(J(t-\tau_1), \dot{J}^\dagger)}{(J, J^\dagger)}. \end{aligned} \tag{2.21}$$

Next, by introducing the Laplace transforms as

$$\overline{\psi}_{\dot{J}}(z) = \int_0^\infty \mathrm{d}t\; \mathrm{e}^{-zt}\, \frac{(\ddot{J}(t), J^\dagger)}{(J, J^\dagger)} \;=\; \int_0^\infty \mathrm{d}t\; \mathrm{e}^{-zt}(-)\frac{(\dot{J}(t), \dot{J}^\dagger)}{(J, J^\dagger)}, \tag{2.22}$$

$$\overline{\psi}_{J}(z) = \int_0^\infty \mathrm{d}t\; \mathrm{e}^{-zt}\, \frac{(J(t), \dot{J}^\dagger)}{(J, J^\dagger)} \;=\; \int_0^\infty \mathrm{d}t\; \mathrm{e}^{-zt}(-)\frac{(\dot{J}(t), J^\dagger)}{(J, J^\dagger)}, \tag{2.23}$$

Eqs. (2.19), (2.20) and (2.21) are simplified respectively as

$$\overline{\varphi}^{(0)}(-\mathrm{i}\omega^+) = -\;\overline{\psi}_{\dot{J}}(-\mathrm{i}\omega^+), \tag{2.24}$$

$$\overline{\varphi}^{(1)}(-\mathrm{i}\omega^+) = -\;\overline{\psi}_{\dot{J}}(-\mathrm{i}\omega^+)\;\overline{\psi}_{J}(-\mathrm{i}\omega^+), \tag{2.25}$$

$$\overline{\varphi}^{(n)}(-\mathrm{i}\omega^+) = (-)^n\,\overline{\psi}_{\dot{J}}(-\mathrm{i}\omega^+)\;\Big(-\;\overline{\psi}_{J}(-\mathrm{i}\omega^+)\Big)^{n-1}\;\overline{\psi}_{J}(-\mathrm{i}\omega^+). \tag{2.26}$$

Then eq. (2.18) is rewritten in the closed-form as

$$\overline{\varphi}(-\mathrm{i}\omega^+) \;=\; -\;\overline{\psi}_{\dot{J}}(-\mathrm{i}\omega^+)\sum_{n=0}^{\infty}\Big(\overline{\psi}_{J}(-\mathrm{i}\omega^+)\Big)^n \;=\; \frac{-\;\overline{\psi}_{\dot{J}}(-\mathrm{i}\omega^+)}{1\;-\;\overline{\psi}_{J}(-\mathrm{i}\omega^+)}. \tag{2.27}$$

As is well-known, $\overline{\psi}_{\dot{J}}(-\mathrm{i}\omega^+)$ is written in terms of the retarded $\dot{J}$-$\dot{J}$ response function $\chi_{\dot{J}\dot{J}}(\omega^+)$ as

$$\overline{\psi}_{\dot{J}}(-\mathrm{i}\omega^+) = -\int_0^\infty \mathrm{d}t\ \mathrm{e}^{\mathrm{i}\omega^+ t}\Lambda(t) = -[W]^{-1}\ \frac{\chi_{\dot{J}\dot{J}}(\omega^+)\ -\ \chi_{\dot{J}\dot{J}}(0^+)}{-\mathrm{i}\omega}, \tag{2.28}$$

$$\Lambda(t) \equiv \frac{(\dot{J}(t), \dot{J}^\dagger)}{(J, J^\dagger)}. \tag{2.29}$$

Similarly, $\overline{\psi}_J(-\mathrm{i}\omega^+)$ is written in terms of the retarded J-J response function $\chi_{JJ}(\omega^+)$ as

$$\overline{\psi}_J(-\mathrm{i}\omega^+) = -\int_0^\infty \mathrm{d}t\,\mathrm{e}^{\mathrm{i}\omega^+ t}\Pi(t) = -[W]^{-1}\ \chi_{JJ}(\omega^+), \tag{2.30}$$

$$\Pi(t) \equiv \frac{(\dot{J}(t), J^\dagger)}{(J, J^\dagger)}. \tag{2.31}$$

The retarded A-A response function $\chi_{AA}(\omega^+)$ is given by the analytic continuation of the temperature Green's function,

$$\chi_{AA}(\mathrm{i}\omega_n) \ = \ \frac{1}{\mathrm{V}}\int_0^\beta \mathrm{d}\tau\ \mathrm{e}^{\mathrm{i}\omega_n\tau}(-)\langle \mathrm{T}_\tau A^\dagger(\tau)\ A(0)\rangle, \tag{2.32}$$

where $\omega_n = 2n\pi T$ is the Matsubara frequency with an integer n.

We note that the Kubo formula for $\sigma(\omega)$ given in eq. (2.10) is rewritten as

$$\sigma_{\mathrm{K}}(\omega) \ = \ \frac{\chi_{JJ}(\omega^+)\ -\ \chi_{JJ}(0^+)}{-\mathrm{i}\omega^+}. \tag{2.33}$$

Equation (2.10) is also rewritten as

$$\frac{1}{2}\left(f(t+0) + f(t-0)\right) = \frac{1}{2\pi}\int_{-\infty}^\infty \mathrm{d}\omega\ \mathrm{e}^{-\mathrm{i}\omega^+ t}\ \sigma(\omega) \tag{2.34}$$

with $f(t) \equiv \theta(t)\ \beta\ (J(t), J^\dagger)/\mathrm{V}$. Using eq. (2.34) with $t = 0$, we obtain

$$[W] \ = \ \frac{1}{\pi}\int_{-\infty}^\infty \mathrm{d}\omega\ \sigma'_{\mathrm{K}}(\omega) \ = \ -\chi'_{JJ}(0^+). \tag{2.35}$$

Thus, substituting eq. (2.27) into eq. (2.11), a rigorous expression for eq. (2.6) or (2.11) in terms of the retarded response functions is obtained.

A clue to the GLE lies in the derivation of $f(t) = \mathrm{e}^{(1-P)\ \mathrm{i}Lt}\dot{J}$ from the general solution to the Heisenberg equation of motion as in eq. (2.3). Here we note that the inner product of $g(t) = \mathrm{e}^{\mathrm{i}L(1-P)}\dot{J}$ instead of $f(t)$ coincides with the closed-form solution, i.e., $(g(t), g^\dagger)/(J, J^\dagger) = \overline{\varphi}(-\mathrm{i}\omega^+)$ with $g^\dagger = f^\dagger$. This is because $\dot{J}[\,\mathrm{i}L, 1-P\,]_-\dot{J} = 0$ resulting from $P\dot{J} \equiv 0$, however, the substitution of $g(t)$ for $f(t)$ does not deduce the GLE in vain.

2.3 Proof of the identity between the GLE and the Kubo formula

First, using eq. (2.35), eq. (2.11) with eq. (2.27) is rewritten as

$$\sigma_{\mathrm{M}}(\omega) \ = \ \frac{-\ \chi_{JJ}(0^+)}{-\mathrm{i}\omega^+ + \dfrac{\chi_{\dot{J}\dot{J}}(\omega^+)\ -\ \chi_{\dot{J}\dot{J}}(0^+)}{-\mathrm{i}\omega^+}\ \dfrac{1}{\chi_{JJ}(\omega^+)\ -\ \chi_{JJ}(0^+)}}. \tag{2.36}$$

The retarded response function $\chi_{jj}(\omega^+)$ is defined as

$$\chi_{jj}(\omega^+) \equiv \frac{1}{\mathrm{V}}\int_{-\infty}^{\infty} \mathrm{d}t\ \mathrm{e}^{\mathrm{i}\omega^+ t}\ (-)\frac{\mathrm{i}}{\hbar}\ \theta(t)\ \langle\ [\dot{J}^\dagger(t), \dot{J}(0)]_-\ \rangle, \tag{2.37}$$

$$= \frac{1}{\mathrm{V}}\int_{0}^{\infty} \mathrm{d}t\ \mathrm{e}^{\mathrm{i}\omega^+ t}\ (-)\frac{\mathrm{i}}{\hbar}\ \langle\ [\frac{\mathrm{d}}{\mathrm{d}t}J^\dagger(t), \dot{J}(0)]_-\ \rangle. \tag{2.38}$$

Noting that there exists no correlation between $t = 0$ and $t = \infty$, eq. (2.38) can be integrated by parts to yield

$$\chi_{jj}(\omega^+) = \frac{1}{\mathrm{V}}\frac{\mathrm{i}}{\hbar}\ \langle\ [J^\dagger(0), \dot{J}(0)]_-\ \rangle\ -\ \mathrm{i}\omega^+\ \frac{1}{\mathrm{V}}\int_{0}^{\infty} \mathrm{d}t\ \mathrm{e}^{\mathrm{i}\omega^+ t}\ (-)\frac{\mathrm{i}}{\hbar}\ \langle\ [J^\dagger(t), \dot{J}(0)]_-\ \rangle. \tag{2.39}$$

Using the relations, $(-\mathrm{i}/\hbar)\langle\ [A(0), B^\dagger(0)]_-\ \rangle = \beta(B(0), \dot{A}^\dagger(0))$ with $A = J^\dagger$ and $B^\dagger = \dot{J}$, and $\langle\ [J^\dagger(t), \dot{J}(0)]_-\ \rangle = -\langle\ [(\mathrm{d}/\mathrm{d}t)J^\dagger(t), J(0)]_-\ \rangle$, eq. (2.39) is rewritten as

$$\chi_{jj}(\omega^+) = -\frac{\beta}{\mathrm{V}}(\dot{J}(0), \dot{J}^\dagger(0))\ +\ \mathrm{i}\omega^+\ \frac{1}{\mathrm{V}}\int_{0}^{\infty} \mathrm{d}t\ \mathrm{e}^{\mathrm{i}\omega^+ t}\ (-)\frac{\mathrm{i}}{\hbar}\ \langle\ [\frac{\mathrm{d}}{\mathrm{d}t}J^\dagger(t), J(0)]_-\ \rangle. \tag{2.40}$$

Using the sum rule as in eq. (2.35) and integrating the second term in the r.h.s. of eq. (2.40) by parts once again, we obtain an identity[20]

$$\chi_{jj}(\omega^+) = \chi_{jj}(0^+)\ -\ (\mathrm{i}\omega^+)^2\chi_{JJ}(\omega^+) \tag{2.41}$$

between eq. (2.37) and the retarded response function

$$\chi_{JJ}(\omega^+) \equiv \frac{1}{\mathrm{V}}\int_{-\infty}^{\infty} \mathrm{d}t\ \mathrm{e}^{\mathrm{i}\omega^+ t}\ (-)\frac{\mathrm{i}}{\hbar}\ \theta(t)\ \langle\ [J^\dagger(t), J(0)]_-\ \rangle. \tag{2.42}$$

Finally, inserting eq. (2.41) into eq. (2.36), eq. (2.11) with eq. (2.27) is proved to be identical to eq. (2.33), i.e., $\sigma_{\mathrm{M}}(\omega) = \sigma_{\mathrm{K}}(\omega)$.

§3. Transport Phenomena

Here we present rigorous constraints in the limit of low frequency derived from eq. (2.41) on the transport coefficients within the linear response theory (Kubo formula)[2] and the memory functional approaches (MFA)[11,12,14-17] to the closed-form solution.[20]

3.1 Drude weight and dc-resistivity

The conductivity weight tensor $[W]$ is obtained by evaluating the second derivative at $\omega = 0$ of $\chi'_{jj}(\omega^+)$,

$$\begin{aligned}\chi'_{jj}(\omega^+) &= \chi'_{jj}(0^+) + \omega^2\chi'_{JJ}(\omega^+)\\ &\simeq (-)\frac{\beta}{\mathrm{V}}(\dot{J}(0), \dot{J}^\dagger(0))\ +\ a'_J\omega^2, \quad a'_J \equiv -[W] < 0.\end{aligned} \tag{3.1}$$

If there exists finite dc-resistivity in the system, i.e.,

$$\sigma'(\omega) = \frac{\chi''_{JJ}(\omega^+)}{-\omega} \simeq \frac{a''_J\omega}{-\omega}, \quad \rho \equiv \lim_{\omega\to 0}\sigma'(\omega)^{-1} = \frac{(-)}{a''_J} > 0, \tag{3.2}$$

then $\chi''_{jj}(\omega^+)$ behaves around $\omega = 0$ as

$$\chi''_{jj}(\omega^+) \simeq a''_J\omega^3, \quad a''_J < 0. \tag{3.3}$$

Successive application of eq. (2.41) leads to

$$\lim_{\omega\to 0}\left[\frac{\chi''_{J^nJ^n}(\omega^+)}{-\omega^{2n+1}}\right]^{-1} = \rho, \tag{3.4}$$

where $\chi_{J^nJ^n}(\omega^+)$ is the retarded J^n-J^n response function with $J^n = (\mathrm{i}L)^n J$.

To clarify the properties of $\sigma(\omega)$ with the frequency-dependent optical mass $m_{\rm opt}(\omega)$ and the frequency-dependent optical scattering rate $\tau^*_{\rm opt}(\omega)^{-1}$, the following phenomenology known as the generalized Drude analysis[12,14,15,22] is often used as

$$\sigma_{\rm GDA}(\omega) = [W]\,\frac{m_{\rm b}}{m_{\rm opt}(\omega)}\,\frac{1}{\tau^*_{\rm opt}(\omega)^{-1} - \mathrm{i}\omega}, \tag{3.5}$$

where $m_{\rm b}$ is the band mass. Using eq. (2.33) or eq. (2.36), the optical mass in the limit of low frequency is written as

$$\lim_{\omega\to 0}\frac{m_{\rm opt}(\omega)}{m_{\rm b}} = \frac{[W]a'_J}{a''^{\,2}_J}, \tag{3.6}$$

where a'_J is the second derivative at $\omega = 0$ of $\chi'_{JJ}(\omega^+)$. From the requirement of the positive optical mass, we obtain

$$\chi'_{JJ}(\omega^+) \simeq (-)[W] + a'_J\omega^2, \quad a'_J > 0, \tag{3.7}$$

which leads to $\sigma''(\omega) \simeq a'_J\omega$. These relations mean that there exists constraint between the retarded J-regarding response functions and the transport coefficients within the linear response theory.

3.2 Fixed points of the MFA

Next, we present the fixed points in the limit of low frequency of the MFA where eq. (2.27) is replaced by $\overline{\varphi}(-\mathrm{i}\omega^+) \simeq -\overline{\psi}_J(-\mathrm{i}\omega^+)$. In this approximation, using eq. (2.41), $\rho(\omega) = \overline{\varphi}'(-\mathrm{i}\omega^+)/[W]$ is approximated as

$$\rho_{\rm MFA}(\omega) \simeq \frac{-a''_J}{[W]^2}\,\omega^2 \quad \to 0 \quad \text{as} \quad \omega \to 0. \tag{3.8}$$

Using eq. (3.1), the optical mass $m_{\rm opt}(\omega)/m_{\rm b} = 1 - \overline{\varphi}''(-\mathrm{i}\omega^+)/\omega$ is also approximated as

$$\left[\frac{m_{\rm opt}(\omega)}{m_{\rm b}}\right]_{\rm MFA} \simeq 1 - \frac{a'_J\omega}{[W]\omega} \quad \to 2 \quad \text{as} \quad \omega \to 0. \tag{3.9}$$

These relations in the limit of low frequency are in general independent of the model at all. However, we note that the coefficient of ω^2 in eq. (3.8) is described by the dc-resistivity in the system, i.e., eq. (3.2).

§4. Relaxation Phenomena and Quantum Noise

To investigate the long-time tail problem and the fluctuating force $f(t)$ in eq. (2.5), we must consider the system where a dynamical variable such as a current operator J is an unconserved quantity to yield the non-trivial closed-form solution.[19,21] We present a model where the memory functional approaches (MFA)[11-17] to the closed-form solution are practically valid.

4.1 A free two-band model

We study, as an example, the free *d-p* model simulating the electronic system in the CuO_2 plane of the high-T_c superconducting materials,[19,21] which is given in the hole-picture by

$$H = \epsilon_p \sum_{\mathbf{k}\sigma} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \epsilon_d \sum_{i\sigma} d^\dagger_{i\sigma} d_{i\sigma} + N_{\mathrm{L}}^{-\frac{1}{2}} \sum_{i\mathbf{k}\sigma} \Big(\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{R}_i} t_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} d_{i\sigma} + h.c. \Big), \tag{4.1}$$

where $c^\dagger_{\mathbf{k}\sigma}$ and $d^\dagger_{i\sigma}$ are the creation operators for the O-$2p_\sigma$ hole of the bonding orbitals and the Cu $3d_{x^2-y^2}$ Wannier orbitals, respectively. The total number of the unit cells is N_{L}. The atomic energies of the p- and d- holes, ϵ_p and ϵ_d, are measured relative to the chemical potential. The charge transfer gap, $\Delta \equiv \epsilon_p - \epsilon_d$, is found to be the band gap. The transfer energy, $t_{\mathbf{k}} \equiv \sqrt{W(\mathbf{k})}$, is given (explicitly shown later) by the transfer integral between the adjacent Cu and O sites, t_{pd}, and the lattice constant a. Since the current operator J with $\mathbf{q} = \mathbf{0}$ is given as

$$J = \frac{e}{\hbar} N_{\mathrm{L}}^{-\frac{1}{2}} \sum_{i\mathbf{k}\sigma} \Big(\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{R}_i} \nabla_{\mathbf{k}} t_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} d_{i\sigma} + h.c. \Big), \tag{4.2}$$

the unconserved part is then given by

$$\dot{J} = \frac{\Delta}{\hbar} \frac{e}{\hbar} N_{\mathrm{L}}^{-\frac{1}{2}} \sum_{i\mathbf{k}\sigma} \Big(\mathrm{i}\ \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{R}_i} \nabla_{\mathbf{k}} t_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} d_{i\sigma} + h.c. \Big). \tag{4.3}$$

Equation (4.1) is easily diagonalized yielding

$$H = \sum_{\mathbf{k}\sigma} \sum_{\gamma=\pm} E_\gamma(\mathbf{k}) a^\dagger_{\mathbf{k}\sigma\gamma} a_{\mathbf{k}\sigma\gamma}, \tag{4.4}$$

where $E_\gamma(\mathbf{k}) \equiv (1/2)[\epsilon_p + \epsilon_d + \gamma\sqrt{\Delta^2 + 4W(\mathbf{k})}]$ and $a^\dagger_{\mathbf{k}\sigma\gamma} = [(E_\gamma(\mathbf{k}) - \epsilon_d)/\Delta_\gamma(\mathbf{k})] c^\dagger_{\mathbf{k}\sigma} + [t_{\mathbf{k}}/\Delta_\gamma(\mathbf{k})] d^\dagger_{\mathbf{k}\sigma}$ with $d^\dagger_{\mathbf{k}\sigma} = N_{\mathrm{L}}^{-1/2} \sum_i \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{R}_i} d^\dagger_{i\sigma}$ and $\Delta_\gamma(\mathbf{k}) = [\ (E_\gamma(\mathbf{k}) - \epsilon_d)^2 + W(\mathbf{k})\ ]^{1/2}$. The current operator $J \equiv J_{\mathrm{intra}} + J_{\mathrm{inter}}$ is rewritten as

$$J_{\mathrm{intra}} = \frac{e}{\hbar} \sum_{\mathbf{k}\sigma} \sum_{\gamma=\pm} \nabla_{\mathbf{k}} E_\gamma(\mathbf{k}) a^\dagger_{\mathbf{k}\sigma\gamma} a_{\mathbf{k}\sigma\gamma}, \tag{4.5}$$

$$J_{\mathrm{inter}} = \frac{e}{\hbar} \sum_{\mathbf{k}\sigma} \sum_{\gamma=\pm} F(\mathbf{k}) a^\dagger_{\mathbf{k}\sigma-\gamma} a_{\mathbf{k}\sigma\gamma}, \tag{4.6}$$

with $F(\mathbf{k}) = (1/2) \sum_{\gamma=\pm} [\Delta_\gamma(\mathbf{k})/\Delta_{-\gamma}(\mathbf{k})]\ \nabla_{\mathbf{k}} E_\gamma(\mathbf{k})$. Since $[H, J_{\mathrm{intra}}]_- = 0$, $\dot{J}_{\mathrm{intra}} = 0$ and thus eq. (4.3) includes only the interband component, i.e.,

$$\dot{J} = \dot{J}_{\mathrm{inter}} = \frac{e}{\hbar^2} \sum_{\mathbf{k}\sigma} [E_+(\mathbf{k}) - E_-(\mathbf{k})]\ F(\mathbf{k}) \Big(\mathrm{i}\ a^\dagger_{\mathbf{k}\sigma+} a_{\mathbf{k}\sigma-} + h.c. \Big). \tag{4.7}$$

The temperature Green's functions for eq. (4.2) and (4.3) are then written as

$$\chi_{jj}(\mathrm{i}\omega_n) = \frac{1}{N_\mathrm{L}}\sum_{\mathbf{k}\sigma}(\frac{e}{\hbar}\nabla_\mathbf{k}t_\mathbf{k})^2\sum_{\gamma=\pm}T\sum_{\mathrm{i}\epsilon_n}R^j_\mathrm{inter}(\mathbf{k})\ G_\gamma(\mathbf{k},\mathrm{i}\epsilon_n)G_{-\gamma}(\mathbf{k},\mathrm{i}\omega_n+\mathrm{i}\epsilon_n), \tag{4.8}$$

$$\chi_{JJ}(\mathrm{i}\omega_n) = \frac{1}{N_\mathrm{L}}\sum_{\mathbf{k}\sigma}(\frac{e}{\hbar}\nabla_\mathbf{k}t_\mathbf{k})^2\sum_{\gamma=\pm}T\sum_{\mathrm{i}\epsilon_n}$$
$$\times\Big[\ R^J_\mathrm{inter}(\mathbf{k})\ G_\gamma(\mathbf{k},\mathrm{i}\epsilon_n)G_{-\gamma}(\mathbf{k},\mathrm{i}\omega_n+\mathrm{i}\epsilon_n)+R^J_\mathrm{intra}(\mathbf{k})\ G_\gamma(\mathbf{k},\mathrm{i}\epsilon_n)G_\gamma(\mathbf{k},\mathrm{i}\omega_n+\mathrm{i}\epsilon_n)\ \Big], \tag{4.9}$$

with $R^j_\mathrm{inter}(\mathbf{k}) = (\Delta/\hbar)^2$, $R^J_\mathrm{inter}(\mathbf{k}) = \Delta^2/[\Delta^2+4W(\mathbf{k})]$, $R^J_\mathrm{intra}(\mathbf{k}) = 4W(\mathbf{k})/[\Delta^2+4W(\mathbf{k})]$, and $G_\gamma(\mathbf{k},\mathrm{i}\epsilon_n) = [\mathrm{i}\epsilon_n - E_\gamma(\mathbf{k})]^{-1}$. The intraband component of $\chi_{JJ}(\omega^+)$ obtained from the analytic continuation of eq. (4.9) vanishes as shown in appendix. We rewrite the $\mathbf{k}$-summation as

$$\frac{1}{N_\mathrm{L}}\sum_\mathbf{k}E(W(\mathbf{k})) = \int_0^{d(2t_{pd})^2}\mathrm{d}w E(w)R(w), \quad R(w)\equiv\frac{1}{N_\mathrm{L}}\sum_\mathbf{k}\delta(w-W(\mathbf{k})). \tag{4.10}$$

Here we control the band filling concentration such as $n = {N_\mathrm{L}}^{-1}\sum_{\mathbf{k}\sigma}\theta(-E_-(\mathbf{k})) \equiv 2-\delta^2/2d$ with dimensionality, d, and a parameter $0<\delta<2\sqrt{d}$ that the chemical potential at $T=0$ lies in the band $E_-(\mathbf{k})$ and $W(\mathbf{k}_\mathrm{F}) = \epsilon_p\epsilon_d = (2t_{pd}\delta)^2/4$. Since the interband particle-hole transition with $\mathbf{q}=\mathbf{0}$ is vertical in the $\mathbf{k}$-space, the characteristic energy are between $\omega_-\equiv E_+(\mathbf{k}_\mathrm{F}) = \epsilon_p+\epsilon_d = \sqrt{\Delta^2+(2t_{pd}\delta)^2}$ and $\omega_+\equiv E_+^\mathrm{top}-E_-^\mathrm{bot} = \sqrt{\Delta^2+4d(2t_{pd})^2}$. The band width is written as $W_\mathrm{B} = (\omega_+-\Delta)/2$. The band scheme at $T=0$ is shown in fig. 1. Hereafter we employ units so that $2t_{pd} = \hbar = \epsilon = a = 1$, which are explicitly shown if necessary.

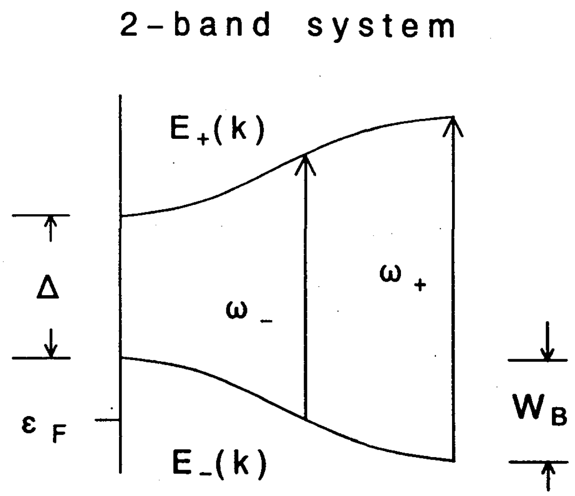


Fig. 1. The band scheme of a free two-band model at $T=0$ with its characteristic parameters and energies

4.2 2D model at $T = 0$

In the 2D model, eq. (4.1) must include the non-bonding term $\epsilon_p \sum_{\mathbf{k}\sigma} c^{\dagger 0}_{\mathbf{k}\sigma} c^0_{\mathbf{k}\sigma}$, however, which specifies only the chemical potential at finite temperatures. We consider the isotropic model with $t_{\mathbf{k}} = 2t_{pd}a[(k_x{}^2 + k_y{}^2)/2\pi]^{1/2}$ instead of $t_{\mathbf{k}} = 2t_{pd}[1 - (\cos k_x a + \cos k_y a)/2]^{1/2}$. This corresponds to taking $R(w) = 1/d$ with $d = 2$ instead of $R(w)$ in eq. (4.10) with van Hove singularity around $w = 1$. The functioin $\chi_{jj}(\omega^+)$ obtained from the analytic continuation of eq. (4.8) is evaluated at $T = 0$ to yield[19]

$$\chi_{jj}(\omega^+) = -A\Big[\ \frac{\omega F(\omega)}{\pi} + \frac{2}{\pi}(\omega_+ - \omega_-) + \mathrm{i}\ \omega\Theta(|\omega|)\ \Big], \tag{4.11}$$

where $A \equiv \Delta^2/8$, $F(\omega) \equiv \log[(\omega_+ - \omega)(\omega_- + \omega)/(\omega_+ + \omega)(\omega_- - \omega)]$ and $\Theta(|\omega|) \equiv \theta(|\omega| - \omega_-)\theta(\omega_+ - |\omega|)$. Equations (2.11), (2.28) and (2.30) are also calculated to yield

$$\sigma(\omega) = \Big[\ W_{\mathrm{D}}\pi\delta(\omega) + \frac{A}{\omega^2}\Theta(|\omega|)\ \Big] + \mathrm{i}\ \Big[\ W\frac{1}{\omega}\ -\ \frac{1}{\pi}\frac{A}{\omega^2}F(\omega)\ \Big], \tag{4.12}$$

$$-\ \overline{\psi}_j(-\mathrm{i}\omega^+) = \frac{A}{W}\Big[\ \Theta(|\omega|) - \mathrm{i}\ \frac{F(\omega)}{\pi}\ \Big], \tag{4.13}$$

$$\overline{\psi}_J(-\mathrm{i}\omega^+) = \frac{A}{W}\Big[\ \frac{F(\omega)}{\pi\omega} + \mathrm{i}\ \frac{1}{\omega}\Theta(|\omega|)\ \Big], \tag{4.14}$$

with $W = W_{\mathrm{D}} + W_{\mathrm{inter}}$ written as $W_{\mathrm{D}} \equiv \epsilon_p\epsilon_d/\pi\omega_-$ and $W_{\mathrm{inter}} \equiv (2A/\pi)(\omega_-^{-1} - \omega_+^{-1})$. The Drude term $\propto \delta(\omega)$ is evaluated from eq. (2.11) noting an infinitesimal number, ϵ, in the dominator of the r.h.s on setting $\omega = 0$, however, the Drude weight W_{D} is evaluated from eq. (2.33) as shown in the appendix. The terms in each of the r.h.s. of eqs. (4.11)-(4.14) are related with each other through the Kramers-Krönig relations and hold the parity. Equation (2.41) holds in the model as it should for eqs. (4.11) and (4.14). The canonical correlations, eqs. (2.8), (2.29) and (2.31), are then calculated from eqs. (4.12)-(4.14) to yield[21]

$$\Xi(t) = 1 + \frac{2A}{\pi W}\Big[\ \frac{\cos\omega_- t - 1}{\omega_-} - \frac{\cos\omega_+ t - 1}{\omega_+} +\ t\ [\mathrm{S_i}(\omega_- t) - \mathrm{S_i}(\omega_+ t)]\ \Big], \tag{4.15}$$

$$\Lambda(t) = \frac{2A}{\pi W}\ \frac{\sin\omega_+ t - \sin\omega_- t}{t}, \tag{4.16}$$

$$\Pi(t) = -\ \frac{2A}{\pi W}\ [\mathrm{S_i}(\omega_+ t) - \mathrm{S_i}(\omega_- t)]. \tag{4.17}$$

Since the sine integral is asymptotically expanded as

$$\mathrm{S_i}(x) \equiv \int_0^x \mathrm{d}u\frac{\sin u}{u} = \frac{\pi}{2} - \alpha(x)\cos x - \beta(x)\sin x,$$
$$\alpha(x) \simeq \frac{1}{x}\Big(1 - \frac{2!}{x^2} + \frac{4!}{x^4} - \cdots\Big), \quad \beta(x) \simeq \frac{1}{x^2}\Big(1 - \frac{3!}{x^2} + \frac{5!}{x^4} - \cdots\Big), \tag{4.18}$$

eqs. (4.15)-(4.17) are shown to have a long-time tail of t^{-1} for $t >> \omega_+^{-1}$ and $\Xi(t) - 1 \propto -t^2$, $\Lambda(t) - \Lambda(0) \propto -t^2$ and $\Pi(t) \propto -t$ for $t \lesssim \omega_+^{-1}$ irrespective of the model parameters, δ and Δ. Using eqs. (2.13) and (2.27), eq. (2.6) is written as

$$\varphi(t) = \frac{2}{\pi}\int_{\omega_-}^{\omega_+} \mathrm{d}\omega \cos\omega t\ \overline{\varphi}'(-\mathrm{i}\omega^+), \tag{4.19}$$

$$\overline{\varphi}'(-\mathrm{i}\omega^+) = \frac{AW\omega^2}{[\,W\omega - (A/\pi)F(\omega)\,]^2 + A^2}\,\Theta(|\omega|). \tag{4.20}$$

We show the numerical calculation of eq. (4.19) with eq. (4.20) for the half-filled band case with

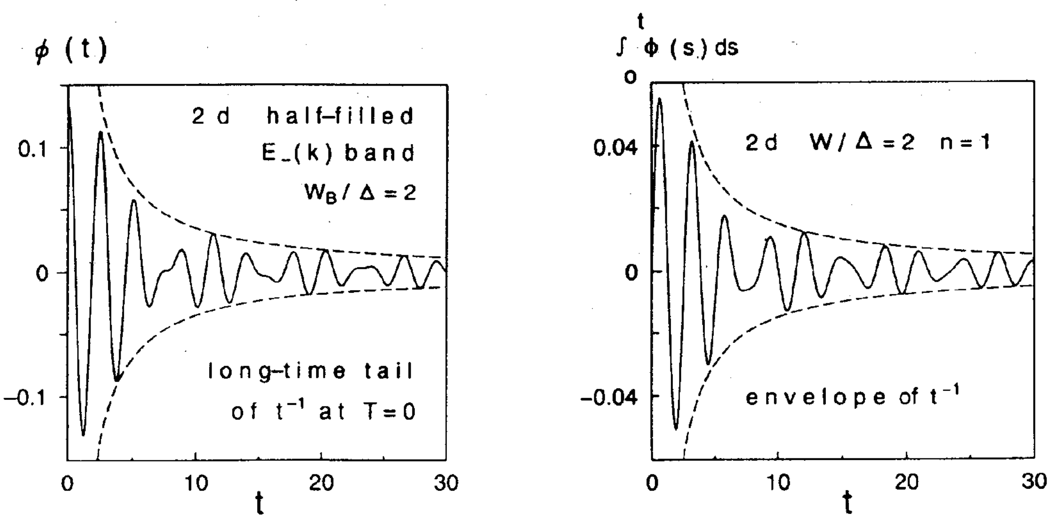


Fig. 2. (a) A long-time tail of t^{-1} for the envelope of $\varphi(t)$ with wave packets in the 2D model at $T = 0$. The parameters are $n = 1$ and $W_{\mathrm{B}}/\Delta = 2$ with $\Delta = 0.577$ and thus the characteristic time is $\omega_+^{-1} = 0.346$. (b) The integrated intensity of $\varphi(s)$ up to t with the envelope of t^{-1}

$\delta = 2$, i.e., $n = 1$ and $W_{\mathrm{B}}/\Delta = 2$ in fig. 2(a).[21] The characteristic time is $\omega_+^{-1} = 0.346$ from $\Delta = 0.577$. For $t \lesssim \omega_+^{-1}$, $\varphi(t) - \varphi(0) \propto -t^2$. A long-time tail of t^{-1} for $t >> \omega_+^{-1}$ is clearly seen for the envelope of the wave packets. Equation (4.15) with $t = \infty$ is $\Xi(t = \infty) = 1 - W_{\mathrm{inter}}/W = 0.978$ with $W = 0.156$. This means that the fluctuating force $f(t)$ for the current operator in the model is the strongly colored quantum noise at $T = 0$. The terminology of *noise* is specified only under the condition that $\Xi(t)$ is $O(1)$ and $\varphi(t)/\varphi(0)$ vanishes as $t \to \infty$ with $\varphi(0) < 1$. The integrated intensity of $\varphi(s)$ up to t does not show the logarithmic divergence but the envelope of t^{-1} as shown in fig. 2(b), which converges to $\overline{\varphi}'(-\mathrm{i}\omega^+)|_{\omega=0} = 0$ as it should from eqs. (2.12) and (4.20). Rewriting eq. (2.11) as $\sigma(\omega) \equiv \rho(\omega)^{-1}$ with the frequency-dependent resistivity $\rho(\omega)$, the integrated intensity to $t = \infty$ corresponds to the dc-resistivity $\rho(0) = 0$ in the model.

When the band gap is much smaller than the band width, $\Delta << W_{\mathrm{B}}$, noting that $A \equiv \Delta^2/8$, we can approximate eq. (4.20) as $\overline{\varphi}'(-\mathrm{i}\omega^+) \simeq (A/W)\Theta(|\omega|)$ with $W \simeq \omega_-/4\pi$ and $\omega_- = \sqrt{\Delta^2 + \delta^2}$. This means that the MFA where eq. (2.27) is replaced by $\overline{\varphi}(-\mathrm{i}\omega^+) \simeq -\overline{\psi}_{\dot{J}}(-\mathrm{i}\omega^+)$, i.e., $f(t)$ in eq. (2.5) is replaced by $\dot{J}(t)$, are practically valid to investigate the system with $\Delta << W_{\mathrm{B}}$. Therefore eq. (4.19) is given by eq. (4.16) as

$$\varphi(t)/\varphi(0) = \frac{1}{\omega_+ - \omega_-}\,\frac{\sin\omega_+ t - \sin\omega_- t}{t}, \tag{4.21}$$

with $\varphi(0) = \Delta^2(\omega_+ - \omega_-)/\omega_- < 1$ and $\omega_+ = 2\sqrt{2}$. Equation (4.15) with $t = \infty$ is written as

$$\Xi(t = \infty) = \frac{\delta^2}{\omega_-^2} + \frac{\Delta^2}{\omega_-\omega_+}. \tag{4.22}$$

We note that δ is the band filling parameter. In the limit of $n \to 0$ with $\Delta << \delta \lesssim 2\sqrt{2}$ and thus $\omega_- \lesssim 2\sqrt{2}$, eq. (4.21) oscillates with almost no damping because of the vanishing dominator in the r.h.s. and eq. (4.22) behaves as $\Xi(t = \infty) \simeq 1 - O(\Delta^2)$. For the intermediate case with $\Delta << \delta \lesssim O(1)$, eq. (4.21) has a tail of t^{-1} with wave packets as shown in fig. 2(a) with $n = 1$ and eq. (4.22) still behaves as $\Xi(t = \infty) \simeq 1 - O(\Delta^2)$. For the case with $\delta \gtrsim 0$ and thus $\omega_- \simeq \Delta$, eq. (4.21) has a tail of t^{-1} with weak oscillations, however, eq. (4.22) crossovers $O(1)$ for $\delta \simeq \Delta$ to $(\delta/\Delta)^2 + \Delta/\omega_+$ for $\delta << \Delta$. Therefore in the limit of $n \to 0$ and $n \to 2$ for the model with $\Delta << W_B$, the fluctuating force $f(t)$ is not identified as noise because the case violates the criterion of *noise* respectively.

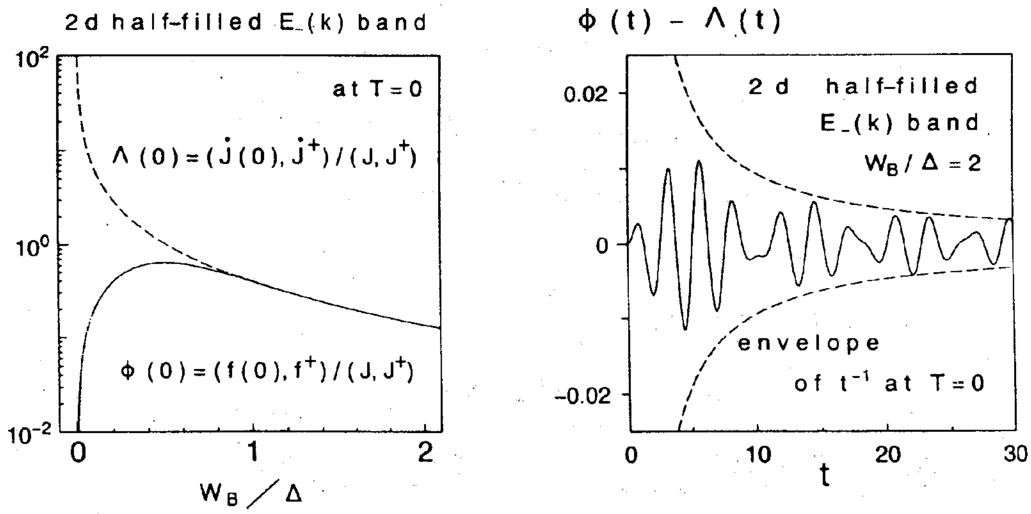


Fig. 3. (a) $\varphi(0)$ and $\Lambda(0)$ as functions of W_B/Δ for the case with $n = 1$ at $T = 0$. When $\Delta >> W_B$, the Born approximation completely break down. (b) Deviation of $\Lambda(t)$ from $\varphi(t)$ for finite time.

When the band gap is much larger than the band width, $\Delta >> W_B$, the MFA completely break down as shown in fig. 3(a) for $\varphi(0)$ and $\Lambda(0)$ for the case with $n = 1$. For the case with $W_B/\Delta = 2$, the MFA seems to be valid for the time $t \lesssim \omega_+^{-1}$, however, we show in fig. 3(b) that $\Lambda(t)$ for finite time deviates with oscillation from $\varphi(t)$ shown in fig. 2(a).

4.3 1D model at $T = 0$

Next we consider the 1D model with $t_k = 2t_{pd}[1 - ka/\pi]^{1/2}$ instead of $t_k = 2t_{pd}\cos(ka/2)$. This corresponds to taking $R(w) = 1/d$ with $d = 1$ instead of $R(w)$ in eq. (4.10) with van Hove singularity around $w = 0, 1$. The function $\chi_{jj}(\omega^+)$ at $T = 0$ is written as

$$\chi_{jj}(\omega^+) = -A(\omega)\Big[\, \omega F(\omega) - \Delta F(\Delta) + \mathrm{i}\ \pi\omega\Theta(|\omega|) \,\Big], \tag{4.23}$$

with $A(\omega) \equiv \Delta^2/[\pi^2(\omega^2 - \Delta^2)]$. Equations (2.11), (2.28) and (2.30) are also calculated to yield

$$\sigma(\omega) = W_{\mathrm{D}}\pi\delta(\omega) + \frac{A(\omega)}{\omega^2}\pi\Theta(|\omega|) + \mathrm{i}\Big[\frac{W_{\mathrm{D}}}{\omega} + \frac{\Delta F(\omega) - \omega F(\Delta)}{\pi^2\Delta(\Delta^2 - \omega^2)} + \frac{F(\omega) - [\mathrm{d}F(0)/\mathrm{d}\omega]\omega}{\pi^2\omega^2}\Big], \tag{4.24}$$

$$-\,\overline{\psi}_j(-\mathrm{i}\omega^+) = \frac{A(\omega)}{W}\Big[\, \pi\Theta(|\omega|) - \mathrm{i}[F(\omega) - \frac{\omega}{\Delta}F(\Delta)] \,\Big], \tag{4.25}$$

$$\overline{\psi}_J(-\mathrm{i}\omega^+) = \frac{A(\omega)}{W}\Big[\, \frac{F(\omega)}{\omega} - \frac{F(\Delta)}{\Delta} + \mathrm{i}\ \frac{\pi}{\omega}\Theta(|\omega|) \,\Big], \tag{4.26}$$

with $W = W_{\mathrm{D}} + W_{\mathrm{inter}}$ written as $W_{\mathrm{D}} \equiv 2/\pi^2\omega_-$ and $W_{\mathrm{inter}} \equiv (2/\pi^2)[F(\Delta)/2\Delta - \omega_-^{-1} + \omega_+^{-1}]$. Equations (4.23)-(4.26) hold the analyticity such as the Kramers-Krönig relations, the parity and the identity of eq. (2.41). The canonical correlations, eqs. (2.8), (2.29) and (2.31), are then calculated from eqs. (4.24)-(4.26) to yield

$$\Xi(t) = 1 + \frac{2}{\pi^2 W}\Big[\, H(\omega_+) - H(\omega_-) - \frac{F(\Delta)}{2\Delta} \,\Big], \tag{4.27}$$

$$\Lambda(t) = \frac{2}{\pi^2 W}\Big[\, I(\omega_+) - I(\omega_-) \,\Big], \tag{4.28}$$

$$\Pi(t) = \frac{2}{\pi^2 W}\Big[\, J(\omega_+) - J(\omega_-) \,\Big], \tag{4.29}$$

where

$$H(x) \equiv \Big[\, \frac{1}{x} - \frac{\beta[(x-\Delta)t] - \beta[(x+\Delta)t]}{2\Delta} - t\alpha(xt) \,\Big]\cos xt + \Big[\, \frac{\alpha[(x-\Delta)t] - \alpha[(x+\Delta)t]}{2\Delta} - t\beta(xt) \,\Big]\sin xt - \frac{1}{x}, \tag{4.30}$$

$$I(x) \equiv \frac{\alpha[(x-\Delta)t] - \alpha[(x+\Delta)t]}{2}\,\Delta\sin xt \;-\; \frac{\beta[(x-\Delta)t] - \beta[(x+\Delta)t]}{2}\,\Delta\cos xt, \tag{4.31}$$

$$J(x) \equiv -\,\frac{\beta[(x+\Delta)t] + \beta[(x-\Delta)t] - 2\beta(xt)}{2}\sin xt \;-\; \frac{\alpha[(x+\Delta)t] + \alpha[(x-\Delta)t] - 2\alpha(xt)}{2}\cos xt. \tag{4.32}$$

Using eq. (4.18) into eqs. (4.30)-(4.32), eq. (4.27) subtracting $\Xi(t = \infty) = 1 - W_{\mathrm{inter}}/W$, eq. (4.28) and eq. (4.29) also show a long-time tail of t^{-1} for $t >> \omega_+^{-1}$ respectively as

$$\Xi(t) \simeq \frac{2}{W}\Big[\, \frac{A(\omega_+)\sin\omega_+ t}{\omega_+{}^2} - \frac{A(\omega_-)\sin\omega_- t}{\omega_-{}^2} \,\Big]\frac{1}{t}, \tag{4.33}$$

$$\Lambda(t) \simeq \frac{2}{W}\Big[\, A(\omega_+)\sin\omega_+ t - A(\omega_-)\sin\omega_- t \,\Big]\frac{1}{t}, \tag{4.34}$$

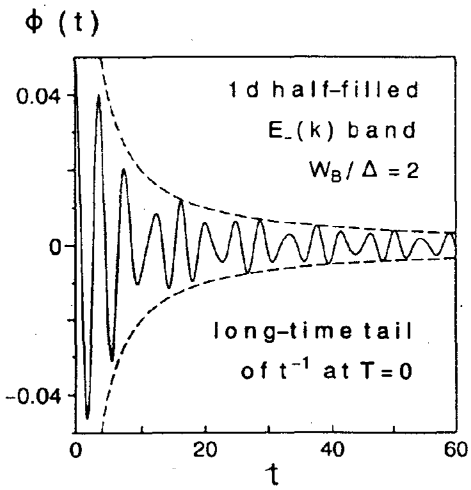
$$\Pi(t) \simeq \frac{2}{W}\Big[\, \frac{A(\omega_-)\cos\omega_- t}{\omega_-} - \frac{A(\omega_+)\cos\omega_+ t}{\omega_+} \,\Big]\frac{1}{t}, \tag{4.35}$$

and $\Xi(t) - 1 \propto -t^2$, $\Lambda(t) - \Lambda(0) \propto -t^2$ and $\Pi(t) \propto -t$ for $t \lesssim \omega_+^{-1}$ irrespective of the model parameters, δ and Δ.

Using eqs. (4.25) and (4.26), we yield

$$\overline{\varphi}'(-\mathrm{i}\omega^+) = \frac{\pi A(\omega) W \omega^2}{B(\omega)^2 + [\ \pi A(\omega)\ ]^2}\ \Theta(|\omega|), \tag{4.36}$$

with $B(\omega) \equiv W\omega - A(\omega)[F(\omega) - \omega F(\Delta)/\Delta]$. We perform the numerical calculation of eq. (4.19) with eq. (4.36) for the half-filled band case with $\delta = \sqrt{2}$, i.e., $n = 1$ and $W_B/\Delta = 2$ to observe a long-time tail of t^{-1} for the envelope of wave packets for $t >> \omega_+^{-1}$ in fig. 4(a) as well for the 2D model. The characteristic time is $\omega_+^{-1} = 0.490$ from $\Delta = 0.408$ and $\Xi(t = \infty) = 0.983$. The integrated intensity of $\varphi(s)$ up to t also shows the envelope of t^{-1} as shown in fig. 4(b), which converges to $\overline{\varphi}'(-\mathrm{i}\omega^+)|_{\omega=0} = 0$ as it should from eqs. (2.12) and (4.36). The fluctuating force $f(t)$ for the current operator in the model is also the strongly colored quantum noise at $T = 0$ as well in the 2D model.



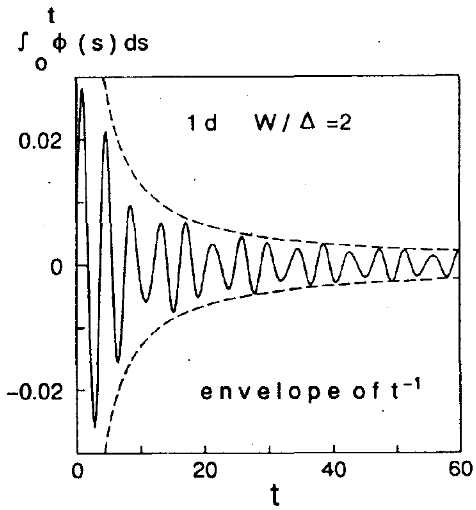


Fig. 4. (a) A long-time tail of t^{-1} for the envelope of $\varphi(t)$ with wave packets in the 1D model at $T = 0$. The parameters are $n = 1$ and $W_B/\Delta = 2$ with $\Delta = 0.408$ and thus the characteristic time is $\omega_+^{-1} = 0.490$. (b) The integrated intensity of $\varphi(s)$ up to t with the envelope of t^{-1}.

The MFA is again valid for the model with $\Delta << W_B$ and eq. (4.19) with eq. (4.36) is given by eq. (4.28) with $\Delta << W_B$ as

$$\varphi(t)/\varphi(0) = \frac{\omega_-\omega_+}{\omega_+ - \omega_-}\ \Big[\ \frac{\cos\omega_- t}{\omega_-} - \frac{\cos\omega_+ t}{\omega_+} + t\ [\mathrm{S_i}(\omega_- t) - \mathrm{S_i}(\omega_+ t)]\ \Big], \tag{4.37}$$

with $\varphi(0) = 2\Delta^2(\omega_+ - \omega_-)/(\pi^2 W) < 1$ and $\omega_+ = 2$. Equation (4.27) with $t = \infty$ is written as

$$\Xi(t = \infty) = \frac{W_D}{W}, \qquad W = \frac{1}{\pi^2\Delta}\ \Big[\ \log[1 + \frac{\Delta}{\omega_-}] - \log[1 - \frac{\Delta}{\omega_-}]\ \Big]. \tag{4.38}$$

We note that $W_D = 2/\pi^2\omega_-$ with $\omega_- = \sqrt{\Delta^2 + \delta^2}$ and that δ is the band filling parameter. In the limit of $n \to 0$ with $\Delta << \delta \lesssim 2$ and thus $\omega_- \lesssim 2$, eq. (4.37) oscillates with almost no damping because of the vanishing dominator in the r.h.s. and eq. (4.38) behaves as $\Xi(t=\infty) \simeq 1 - O(\Delta^2)$. For the intermediate case with $\Delta << \delta \lesssim O(1)$, eq. (4.37) has a tail of t^{-1} with wave packets as shown in fig. 4(a) with $n = 1$ and eq. (4.38) still behaves as $\Xi(t=\infty) \simeq 1 - O(\Delta^2)$. For the case with $\delta \gtrsim 0$ and thus $\omega_- \simeq \Delta$, eq. (4.37) has a tail of t^{-1} with weak oscillations as well eq. (4.15) does, however, eq. (4.38) crossovers $O(1)$ for $\delta \simeq \Delta$ to $1/\log[2\Delta/\delta]$ for $\delta << \Delta$. Therefore in the limit of $n \to 0$ and $n \to 2$ for the model with $\Delta << W_{\rm B}$, the fluctuating force $f(t)$ is not identified as noise because the case violates the criterion of *noise* respectively as well for the 2D model.

The MFA also completely break down for the model with $\Delta >> W_{\rm B}$ as well for the 2D model. The behavior of $\varphi(0)$ and $\Lambda(0)$ for the case with $n = 1$ is much similar to fig. 3(a) and $\Lambda(t)$ for the case deviates with oscillation from $\varphi(t)$ as also observed in fig. 3(b).

§5. Concluding Remarks

In summary, we have reviewed the derivation of the closed-form solution to the GLE (Mori formula) with the proof of the identity between the GLE and the Kubo formula. We have applied the identity to transport phenomena in the limit of low frequency within the linear response theory and deduced rigorous constraints for transport coefficients and those obtained in the MFA (memory functional approach) to the closed-form solution. We have also taken the closed-form solution to investigate relaxation phenomena and quantum noise to find that the relaxation functions of the fluctuating force in a free two-band model have a long-time tail of t^{-1} at $T = 0$ irrespective of its parameters and dimensionality and that the fluctuating force in the model is the strongly colored quantum noise at $T = 0$. We have also presented a model where the MFA to the closed-form solution are practically valid.

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Appendix: The Drude Weight of The Conductivity

The intraband component of the temperature Green's functions for eq. (4.9) is written as

$$\chi_{\rm intra}(\mathrm{i}\omega_n) = \frac{1}{N_{\rm L}} \sum_{\mathbf{k}\sigma} (\frac{e}{\hbar}\nabla_{\mathbf{k}} t_{\mathbf{k}})^2 \, R^J_{\rm intra}(\mathbf{k}) \sum_{\gamma=\pm} K^\gamma_{\rm intra}(\mathrm{i}\omega_n), \tag{A·1}$$

$$\begin{aligned} K^\gamma_{\rm intra}(\mathrm{i}\omega_n) &\equiv T \sum_{\mathrm{i}\epsilon_n} G_\gamma(\mathbf{k}, \mathrm{i}\epsilon_n) G_\gamma(\mathbf{k}, \mathrm{i}\omega_n + \mathrm{i}\epsilon_n), \\ &= \frac{(-)}{\pi} \int_{-\infty}^{\infty} \mathrm{d}x \; f_{\rm F}(x) \Big[G''_\gamma(\mathbf{k}, x^+) G_\gamma(\mathbf{k}, x + \mathrm{i}\omega_n) + G_\gamma(\mathbf{k}, x - \mathrm{i}\omega_n) G''_\gamma(\mathbf{k}, x^+) \Big], \end{aligned} \tag{A·2}$$

with the Fermi distribution function $f_{\mathrm{F}}(x) \equiv [\, \mathrm{e}^{\beta x} + 1\,]^{-1}$. The analytic continuation of eq. (A·1) vanishes because

$$K^{\gamma}_{\mathrm{intra}}(\omega^+) = \int_{-\infty}^{\infty} \mathrm{d}x \; f_{\mathrm{F}}(x)\; \delta(x - E_\gamma(\mathbf{k}))\; \Big[\; G_\gamma(\mathbf{k}, x+\omega^+) + G_\gamma(\mathbf{k}, x-\omega^+)\; \Big],$$

$$= f_{\mathrm{F}}(-E_\gamma)\; \Big[\; P\frac{1}{\omega} - \mathrm{i}\pi\delta(\omega) + P\frac{1}{-\omega} + \mathrm{i}\pi\delta(-\omega)\; \Big] = 0. \qquad \text{(A·3)}$$

However, the Drude conductivity $\sigma_{\mathrm{intra}}(\omega) = -\chi''_{\mathrm{intra}}(\omega^+)/\omega \equiv W_{\mathrm{D}}\delta(\omega)$ is obtained from eq. (2.33) as

$$\frac{-K^{\gamma\,''}_{\mathrm{intra}}(\omega^+)}{\omega} = \pi \int_{-\infty}^{\infty} \mathrm{d}x\; \frac{f_{\mathrm{F}}(x)}{\omega}\; \delta(x - E_\gamma(\mathbf{k}))\; \Big[\; \delta(x+\omega - E_\gamma(\mathbf{k})) - \delta(x - \omega - E_\gamma(\mathbf{k}))\; \Big],$$

$$= \pi \int_{-\infty}^{\infty} \mathrm{d}x\; \frac{f_{\mathrm{F}}(x) - f_{\mathrm{F}}(x+\omega)}{\omega}\; \delta(x - E_\gamma(\mathbf{k}))\; \delta(x+\omega - E_\gamma(\mathbf{k})),$$

$$= \pi \int_{-\infty}^{\infty} \mathrm{d}x\; (-)\; \frac{\mathrm{d}f_{\mathrm{F}}(x)}{\mathrm{d}x}\; \delta(x - E_\gamma(\mathbf{k}))\; \delta(\omega), \qquad \text{(A·4)}$$

$$W_{\mathrm{D}} = \frac{1}{N_{\mathrm{L}}} \sum_{\mathbf{k}\sigma} (\frac{e}{\hbar}\nabla_{\mathbf{k}} t_{\mathbf{k}})^2\; R^{J}_{\mathrm{intra}}(\mathbf{k}) \sum_{\gamma=\pm} \pi \int_{-\infty}^{\infty} \mathrm{d}x\; (-)\; \frac{\mathrm{d}f_{\mathrm{F}}(x)}{\mathrm{d}x}\; \delta(x - E_\gamma(\mathbf{k})). \qquad \text{(A·5)}$$

Equation (A·5) is also obtained by calculating the integrated intensity of the conductivy with a finite half-width artificially attached in the spectra of the Green's function $G_\gamma(\mathbf{k}, \omega^+)$.[22]

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