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Theoretical Solid-State Physics, Herbstsemester 2011

Blatt 7

Abgabe: 8. November, 12:00H (Treppenhaus 4. Stock)
Tutor: Dr. Gerson J. Ferreira Zi.: 4.7b

(1) **Properties of thermal two-time correlation functions** (5 Points)
The goal of this problem is to demonstrate some properties of the (thermal) two-time correlation functions $\langle A(t)B(t')\rangle$, where

$$\langle\ldots\rangle \equiv \frac{\mathrm{Tr}(\ldots e^{-\beta H})}{\mathrm{Tr}(e^{-\beta H})} \tag{1}$$

denotes the thermal average with respect to the Hamiltonian H [$\beta \equiv (k_{\mathrm{B}}T)^{-1}$], and $A(t) \equiv e^{iHt/\hbar}A(0)e^{-iHt/\hbar}$ is an operator in the Heisenberg picture.

(a) Demonstrate the following "time-homogeneity" property of these two-time correlation functions:

$$\langle A(t)B(t')\rangle = \langle A(t-t')B(0)\rangle = \langle A(0)B(t'-t)\rangle \,. \tag{2}$$

(b) Prove the Kubo-Martin-Schwinger identity:

$$\langle A(t)B(0)\rangle = \langle B(0)A(t+i\hbar\beta)\rangle \,.$$

(c) Using the results of (a) and (b) show that

$$(C_{\mathrm{S}})_\omega = \coth\left(\frac{\beta\hbar\omega}{2}\right)(C_{\mathrm{A}})_\omega \,,$$

where $(C_{\mathrm{S}})_\omega$ and $(C_{\mathrm{A}})_\omega$ are the Fourier transforms of the symmetric $C_{\mathrm{S}}(t) \equiv \langle\{A(t),A(0)\}\rangle$ and antisymmetric $C_{\mathrm{A}}(t) \equiv \langle[A(t),A(0)]\rangle$ autocorrelation functions of A, respectively.

(2) **Quantum diffusion formalism and optical conductivity** (5 Points)
The quantum diffusion formalism offers a theoretical framework for description of charge-carrier transport, even under conditions in which the Boltzmann-equation approach is inapplicable. The central quantity in this formalism is the quantum-mechanical spread

$$\Delta X^2(t) \equiv \langle[X(t)-X(0)]^2\rangle \,,$$

where $X(t) \equiv e^{iHt/\hbar}X(0)e^{-iHt/\hbar}$ is the Heisenberg representation of the total position operator and $\langle\ldots\rangle$ stands for the thermal average with respect to the Hamiltonian H.

(a) Show that

$$\frac{d}{dt}\Delta X^2(t) = \int_0^t C_{\mathrm{S}}^V(t')dt' \,,$$

where $C_{\mathrm{S}}^V(t) \equiv \langle V_X(t)V_X(0) + V_X(0)V_X(t)\rangle$ is the symmetric autocorrelation function of the velocity operator $V_X(t) \equiv dX(t)/dt$.

(b) The dissipative part of the optical (dynamic) conductivity at $\omega \neq 0$ is given by

$$\sigma(\omega) = \frac{e^2}{\hbar\nu\omega}\,\mathrm{Re}\int_0^\infty e^{i\omega t}\langle[V_X(t), V_X(0)]\rangle dt \,,$$

where ν is the system volume. Using the properties of Fourier transforms, derive the following relation between the quantum spread and the optical conductivity:

$$\sigma(\omega) = -\frac{e^2\omega^2}{\nu}\,\frac{\tanh(\beta\hbar\omega/2)}{\hbar\omega}\,\mathrm{Re}\int_0^\infty e^{i\omega t}\Delta X^2(t)dt \,.$$