Theoretical Physics V

SS 2014 **9.7.2014**
Assignment XII **Due date 16.7.2014**

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Problem 1 *Mori's inner product*

Show that Mori's scalar product defined by

$$\langle B; A\rangle_\rho = \int_0^1 dx \mathrm{Tr}[B\rho^x A^\dagger \rho^{1-x}] \tag{1}$$

a) is linear in B and antilinear in A, *(0.25 points)*

b) obeys $\langle A; B\rangle_\rho = \langle B; A\rangle_\rho^*$, and *(0.25 points)*

c) satisfies $\langle A; A\rangle_\rho \geq 0$. *(0.75 points)*
Hint: You can use the fact that $\mathrm{Tr}[C_1 C_2] \geq 0$ *when* C_1, C_2 *are positive semidefinite.*

d) Show that $\mathrm{Tr}[C_1 C_2] \geq 0$ when C_1, C_2 are Hermitian and positive semidefinite. *(1.25 points)*
Hint: A positive semidefinite matrix has exactly one positive semidefinite square root.

Above A and B are operators and ρ is a density operator.

Problem 2 *Spin diffusion*

Let us consider a fluid composed of uncharged particles with spin $\frac{1}{2}$ that interact through velocity- and spin-independent forces. This description applies, e.g., in liquid He^3.
The magnetization and magnetization currents are given by

$$\mathbf{M}(\mathbf{r}, t) = \sum_n \gamma s_n(t)\delta(\mathbf{r} - \mathbf{r}_n(t)), \quad \mathbf{j}^M(\mathbf{r}, t) = \sum_n \gamma s_n(t)\left\{\mathbf{p}_n(t), \delta(\mathbf{r} - \mathbf{r}_n(t))/2m\right\}. \tag{2}$$

Here the nth particle has the position $\mathbf{r}_n$, momentum $\mathbf{p}_n$, and spin s_n along the direction of quantization. All the particles have mass m and the gyromagnetic ratio γ.
Magnetization and magnetization current satisfy the continuity equation

$$\frac{\partial}{\partial t}\mathbf{M}(\mathbf{r}, t) + \nabla \cdot \mathbf{j}^M(\mathbf{r}, t) = 0. \tag{3}$$

When the relevant properties of the system vary slowly with $\mathbf{r}$ and t one has

$$\langle \mathbf{j}^M(\mathbf{r}, t)\rangle = -D\nabla\langle \mathbf{M}(\mathbf{r}, t)\rangle, \tag{4}$$

where D is the spin diffusion constant.
Suppose a magnetic field has been adiabatically turned on and is switched off at $t = 0$.

$$\begin{aligned} \mathbf{H}(\mathbf{r}, t) &= \mathbf{H}(\mathbf{r}) e^{\epsilon t}, \qquad && t < 0 \\ &= 0, && t > 0. \end{aligned} \tag{5}$$

Here ϵ is a small positive quantity. The induced magnetization can be written in the form

$$\langle \mathbf{M}(\mathbf{r}) \rangle = \chi \mathbf{H}(\mathbf{r}) \tag{6}$$

where χ is called static spin susceptibility.

a) Show that

$$\mathbf{M}(\mathbf{k}, z) = \frac{\chi \mathbf{H}(\mathbf{k})}{-iz + Dk^2}, \tag{7}$$

where

$$\mathbf{M}(\mathbf{k}, z) = \int d\mathbf{r} e^{-i\mathbf{k}\cdot\mathbf{r}} \int_0^\infty dt e^{izt} \langle \mathbf{M}(\mathbf{r}, t) \rangle \tag{8}$$

denotes Fourier transform in space and Laplace transform in time. *(1.5 points)*
Hint: Start with Eqs. (3) *and* (4). *Carry out the transformation of Eq.* (8) *and integrate by parts. Finally use* (6) *to relate the Fourier transform of* $\langle \mathbf{M}(\mathbf{r}, 0) \rangle$ *to* $\mathbf{H}(\mathbf{k})$.

b) By linear response theory, in the correlation function description the induced magnetization can be written in the form

$$\langle \mathbf{M}(\mathbf{r}, t) \rangle = -i \int_\infty^t dt' \langle [\mathbf{M}(\mathbf{r}, t), \delta H(t')] \rangle_{\text{eq}}, \tag{9}$$

where the perturbation term in the Hamiltonian is

$$\delta H(t) = -\int d\mathbf{r} \mathbf{M}(\mathbf{r}, t) \mathbf{H}(\mathbf{r}, t) \tag{10}$$

and the expectation value $\langle\ \rangle_{\text{eq}}$ is taken in the equilibrium ensemble. We note that because of the translational invariance of the equilibrium system one has

$$\langle [\mathbf{M}(\mathbf{r}, t), \mathbf{M}(\mathbf{r}', t')] \rangle_{\text{eq}} = \int \frac{d\omega}{\pi} \int \frac{d\mathbf{k}}{(2\pi)^3} \chi''(\mathbf{k}, \omega) e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}') - i\omega(t-t')}. \tag{11}$$

Here $\chi(\mathbf{k}, \omega) = \chi'(\mathbf{k}, \omega) + i\chi''(\mathbf{k}, \omega)$ is the Fourier transformed dynamic susceptibility. Its real and imaginary parts are denoted by one and two primes, respectively.

Show that

$$\mathbf{M}(\mathbf{k}, z) = \int \frac{d\omega'}{\pi i} \frac{\chi''(k, \omega')}{\omega'(\omega' - z)} \mathbf{H}(\mathbf{k}). \tag{12}$$

Hint: The system is rotational invariant. *(2.5 points)*

c) *Show that*

$$\chi''(k, \omega) = \frac{\chi D k^2 \omega}{\omega^2 + (Dk^2)^2}. \tag{13}$$

(1.5 points)

Hint: Use the identity

$$\lim_{\epsilon \to 0} \frac{1}{\omega' - \omega - i\epsilon} = P \frac{1}{\omega' - \omega} + \pi i \delta(\omega - \omega') \tag{14}$$

where P denotes the principal value of the integral.

Problem 3 *Linear response function*

The Onsager's regression law (seen in class) reads

$$\overline{\delta \mathcal{A}_i}(t) = \beta \sum_j f_j \left\langle \delta \mathcal{A}_i(t) \delta \mathcal{A}_j(0) \right\rangle , \tag{15}$$

where $\delta \mathcal{A}_i$ is the deviation from the equilibrium average of the dynamical variable $\mathcal{A}_i$ and f_j the external forces. Let us consider the case of a single dynamical variable under an periodic external force $f(t) = f_\omega \cos \omega t$.

a) Writing $\chi(\omega)$ as the Fourier transform of the dynamical susceptibility, show that $\overline{\delta \mathcal{A}_i}(t)$ has a reactive part, in phase with the force and controlled by the real part of $\chi(\omega)$ and a dissipative part, out of phase by $\pi/2$ with the force, and controlled by the imaginary part of $\chi(\omega)$. *(2 point)*

b) *EXTRA:* One important property of the susceptibility $\chi(t)$ is causality: $\chi(t) = 0$ if $t < 0$. This allows us to define the Laplace transform

$$\chi(z) = \int_0^\infty dt e^{izt} \chi(t), \tag{16}$$

for any complex value z such that $Im(z) > 0$. Express $\chi(z)$ in terms of the Laplace transform of the Kubo function and show that the Laplace transform of $\overline{\delta \mathcal{A}_i}(t)$ can be given independently of f_A. *(1 point)*

Problem 4 *Brownian particle*

a) In classical mechanics a Brownian particle is a heavy particle of mass M in a heat bath of light particles of mass m, with $m/M \ll 1$. If the heavy particle is moving with velocity $\vec{v}$, the fluid viscosity leads to a net force $\vec{\mathcal{F}} = -\alpha \vec{v}$, where α is the friction coefficient. Consider a one-dimensional Brownian particle and show that the velocity autocorrelation function is an exponentially decreasing function in the Markovian approximation. *(1 point)*

b) Let us study the limit $m/M \to 0$, that is, the Brownian particle is infinitely heavy. The classical Hamiltonian for the system composed of the fluid and the Brownian particle is

$$H = \sum_\alpha \frac{p_\alpha^2}{2m} + \frac{1}{2} \sum_{\alpha \neq \beta} V(\vec{r}_{\alpha\beta}) + \frac{P^2}{2M} + \sum_\alpha U(\vec{R} - \vec{r}_\alpha), \tag{17}$$

where p_α are the momenta of the fluid particles, V their potential energy, P and $\vec{R}$ the momentum and position of the Brownian particle and U its potential energy in the fluid.

Write down the Liouvillian corresponding to H and identify the Liouvillians for the fluid, $\mathcal{L}_f$, the free-Brownian particle, $\mathcal{L}_B$, the term representing the action of the fluid particles on the heavy particle, $\mathcal{L}_{f\to B}$ and the action of the heavy particle on the fluid, $\mathcal{L}_{B\to f}$. *(1 point)*

c) Following the ideas that lead to Langevin-Mori equation, show that the memory matrix is given by $\gamma_{ij} = \delta_{ij}\gamma(t)$, where

$$\gamma(t) = \frac{1}{MkT}\left\langle \dot{P}_i; e^{i\mathcal{QLQ}t}\dot{P}_i \right\rangle, \tag{18}$$

where the projector $\mathcal{Q}$ is given by

$$\mathcal{Q} = \mathbb{1} - \vec{P}\frac{1}{MkT}\vec{P}. \tag{19}$$

(2 point)

d) Use the limit $m/M \to 0$ to find an approximate form for the Liouvillian $\mathcal{L} \to \mathcal{L}_0$, such that $\mathcal{L}_0\vec{P} = 0$. In this limit, obtain an expression for $\gamma(t)$ in terms of the instantaneous force that the fluid particles exert on the Brownian particle. *(2 point)*