Quantum theory of condensed matter I

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Tue	10:00 - 12:00	H33
Thu	10:00 - 12:00	H33
Tue	12:00 - 14:00	9.2.01

Sheet 10

1. Diffusion, velocity autocorrelation function, classical propagator, and classical Kubo formula

Your aim is to show that the results obtained in the 1st lecture of Week 9 and in Sheet 8 can be reproduced using the velocity auto-correlation function $\mathrm{w}_{\alpha\beta}(t) = \langle v_\alpha(t) v_\beta(0)\rangle$: i.e. the classical analogue of the Kubo formula for a 2D electron gas at zero temperature reads $\hat{\sigma}(\omega) = e^2\nu\hat{D}(\omega)$, where ν is the density of states at the Fermi level, the diffusion tensor $D_{\alpha\beta}(\omega) = \int_0^\infty \mathrm{d}t \exp(i\omega t)\langle v_\alpha(t) v_\beta(0)\rangle$, indices α, β denote x or y directions and angular brackets denote the average over ensemble, i.e. over disorder realizations and angles, as specified below.

1. Consider a 2D electron gas at zero temperature and perpendicular magnetic field. Find the classical propagator $G(\phi, t; \phi_0, t_0)$, – the conditional probability to find particle at the Fermi surface with velocity $\mathbf{v} = v_F \mathbf{n}_\phi$, where the unit vector $\mathbf{n}_\phi = (\cos\phi, \sin\phi)^T$, provided at $t = t_0$ it has velocity $\mathbf{v}_0 = v_F \mathbf{n}_{\phi_0}$. The Boltzmann equation for the propagator reads
$$(\partial_t + \omega_c\partial_\phi + \widehat{\mathrm{St}})G(\phi, t; \phi_0, t_0) = 2\pi\delta(\phi - \phi_0)\delta(t - t_0).$$
Hints: Recall that the collision operator is diagonal in the eigen basis of ∂_ϕ, i.e. $\widehat{\mathrm{St}}\{e^{in\phi}\} = -\tau_n^{-1} e^{in\phi}$, while $2\pi\delta(\phi) = \sum_{n=-\infty}^{\infty} \exp(in\phi)$. Seek for the solution in the form $G = \sum_{n=-\infty}^{\infty} g_n(t - t_0)\theta(t - t_0)\exp[in(\phi - \phi_0)]$, where $\theta(t)$ is the step function. **3 Points)**

2. The propagator G fully describes the stochastic classical dynamics in the ensemble-averaged disordered system. In particular, the velocity autocorrelation function is given by
$$D_{\alpha\beta}(t) = v_F^2 \langle\langle n_\alpha(\phi) G(\phi, t; \phi_0, t_0) n_\beta(\phi_0)\rangle\rangle_{\phi,\phi_0},$$
where angular brackets denote angular averages. Find the diffusion tensor $D(t)$ as well as the correspondent dynamic conductivity in magnetic field given by $\hat{\sigma}(\omega) = e^2\nu\hat{D}(\omega) = e^2\nu\int_{-\infty}^{\infty} \mathrm{d}t\hat{D}(t)\exp(i\omega t)$. Hints: You will find it easier to deal with $v_\pm(t) = \langle v_x(t) \pm iv_y(t)\rangle_\phi = v_F\langle G(\phi, t; \phi_0, t_0)\exp(\pm i\phi)\rangle_\phi$, which will give directly $D_{xx} \pm iD_{yx}$ etc. **(2 Points)**

2. Wick's theorem

1. Show that, for a system of non-interacting fermions described by the Hamiltonian in the energy basis
$$\hat{H} = \sum_\alpha \epsilon_\alpha \hat{c}_\alpha^\dagger \hat{c}_\alpha \left(= \sum_{i=1}^{N} \hat{h}_i \right),$$
the following relation for the many-body grandcanonical expectation value holds:
$$\langle \hat{c}_{\alpha_1}^\dagger \hat{c}_{\alpha_2}^\dagger \hat{c}_{\alpha_3} \hat{c}_{\alpha_4}\rangle = \langle \hat{c}_{\alpha_1}^\dagger \hat{c}_{\alpha_4}\rangle\langle \hat{c}_{\alpha_2}^\dagger \hat{c}_{\alpha_3}\rangle \delta_{\alpha_1\alpha_4}\,\delta_{\alpha_2\alpha_3} - \langle \hat{c}_{\alpha_1}^\dagger \hat{c}_{\alpha_3}\rangle\langle \hat{c}_{\alpha_2}^\dagger \hat{c}_{\alpha_4}\rangle \delta_{\alpha_1\alpha_3}\,\delta_{\alpha_2\alpha_4},$$

where

$$\langle \hat{c}^\dagger_{\alpha_1}\hat{c}^\dagger_{\alpha_2}\hat{c}_{\alpha_3}\hat{c}_{\alpha_4}\rangle \equiv \frac{1}{Z}\,\mathrm{Tr}\,\left\{\hat{c}^\dagger_{\alpha_1}\hat{c}^\dagger_{\alpha_2}\hat{c}_{\alpha_3}\hat{c}_{\alpha_4}\;\exp\left[-\beta(H-\mu N)\right]\right\}$$

and Z is the grandcanonical partition function. The trace is taken over the full Fock space. Hint: Consider the use of the eigenbasis of $\hat{h}$. **(2 Points)**

2. Derive from 2.1 that, for noninteracting fermions, in every other single particle basis $\{|n\rangle\}$ the following relation holds:

$$\langle \hat{c}^\dagger_{n_1}\hat{c}^\dagger_{n_2}\hat{c}_{n_3}\hat{c}_{n_4}\rangle = \langle \hat{c}^\dagger_{n_1}\hat{c}_{n_4}\rangle\langle \hat{c}^\dagger_{n_2}\hat{c}_{n_3}\rangle - \langle \hat{c}^\dagger_{n_1}\hat{c}_{n_3}\rangle\langle \hat{c}^\dagger_{n_2}\hat{c}_{n_4}\rangle.$$

Note that this is valid even if in this basis the Hamiltonian

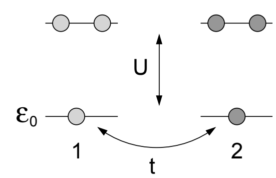
$$\hat{H} = \sum_{n,m} h_{nm}\hat{c}^\dagger_n\hat{c}_m$$

contains non-diagonal terms, h_{nm} for $n \neq m$. Hint: Diagonalize H first, using a unitary transformation $\hat{c}_n = \sum_\alpha u_{n\alpha}\hat{c}_\alpha$. Apply the equation proven in 2.1. Use, e.g., the fact that $\partial\langle\hat{n}_\alpha\rangle/\partial\epsilon_\beta = 0$ for $\alpha \neq \beta$, together with $\langle\hat{n}_\alpha\rangle = -\beta^{-1}\partial\ln Z/\partial\epsilon_\alpha$. Perform the canonical transformation in the reverse direction. **(3 Points)**

3. Double site Hubbard model (oral)

The Hubbard Hamiltonian for a two site system reads explicitly:

$$\begin{aligned}\hat{H} &= \epsilon_0\left(\hat{c}^\dagger_{1\uparrow}\hat{c}_{1\uparrow} + \hat{c}^\dagger_{1\downarrow}\hat{c}_{1\downarrow} + \hat{c}^\dagger_{2\uparrow}\hat{c}_{2\uparrow} + \hat{c}^\dagger_{2\downarrow}\hat{c}_{2\downarrow}\right) + t\left(\hat{c}^\dagger_{1\uparrow}\hat{c}_{2\uparrow} + \hat{c}^\dagger_{2\downarrow}\hat{c}_{1\downarrow} + \hat{c}^\dagger_{2\uparrow}\hat{c}_{1\uparrow} + \hat{c}^\dagger_{1\downarrow}\hat{c}_{2\downarrow}\right)\\ &+ U\left(\hat{c}^\dagger_{1\uparrow}\hat{c}_{1\uparrow}\hat{c}^\dagger_{1\downarrow}\hat{c}_{1\downarrow} + \hat{c}^\dagger_{2\uparrow}\hat{c}_{2\uparrow}\hat{c}^\dagger_{2\downarrow}\hat{c}_{2\downarrow}\right).\end{aligned}$$



1. Calculate the two particle eigenenergies analytically. Treat the case of parallel and antiparallel spin separately. Assume a fixed $t < 0$ and plot the results as a function of U/t.
Hint: For the antiparallel case consider the basis of the corresponding Hilbert space:

$$\hat{c}^\dagger_{1\uparrow}\hat{c}^\dagger_{1\downarrow}|0\rangle, \quad \hat{c}^\dagger_{2\uparrow}\hat{c}^\dagger_{2\downarrow}|0\rangle, \quad \hat{c}^\dagger_{1\uparrow}\hat{c}^\dagger_{2\downarrow}|0\rangle, \quad \hat{c}^\dagger_{2\uparrow}\hat{c}^\dagger_{1\downarrow}|0\rangle.$$

Calculate the matrix elements of $\hat{H}$ in this basis and diagonalize the resulting 4×4 matrix.

2. Calculate the ground state in the Hartree-Fock approximation and compare it with the exact result from 3.1.

Frohes Schaffen!