Analytical Tools for Quantum Many-Body Physics (WS 22/23)
Exercise Sheet 1

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The goal of this exercise sheet is to give some examples of free fermionic states for which Wick's theorem can be retrieved from an explicit algebraic calculation, and to reveal the role of Green's functions in linear response theory.

1. **Explicit calculation of correlation functions for free fermions**
   To get a feeling of how Wick's theorem follows from an explicit algebraic calculation, consider a Slater determinant $|\psi\rangle = \prod_{\alpha=1}^{N_p} \hat{f}_\alpha^\dagger |0\rangle = \hat{f}_{N_p}^\dagger ... \hat{f}_1^\dagger |0\rangle$ consisting of N_p fermionic orthonormal states created by the operators $\hat{f}_\alpha^\dagger = \sum_{j=1}^N \psi_\alpha(j) \hat{c}_j^\dagger$, with $\hat{c}_j^\dagger$ being the creation operators for fermions in e.g. one of N sites of the system.

   - As a warm-up, consider another Slater determinant $|\phi\rangle = \prod_{\beta=1}^{N_p} \hat{d}_\beta^\dagger |0\rangle$ with $\hat{d}_\beta^\dagger = \sum_{j=1}^N \phi_\beta(j) \hat{c}_j^\dagger$, and show that the overlap $\langle\phi|\psi\rangle$ can be calculated as:
   $$\langle\phi|\psi\rangle = \det \mathbb{O} \ , \quad \text{with } \ \mathbb{O} = \Big(\langle\phi_\beta|\psi_\alpha\rangle\Big)_{\alpha,\beta=1,\dots,N_p} = \begin{pmatrix} \langle\phi_1|\psi_1\rangle & \cdots & \langle\phi_1|\psi_{N_p}\rangle \\ \vdots & \ddots & \vdots \\ \langle\phi_{N_p}|\psi_1\rangle & \cdots & \langle\phi_{N_p}|\psi_{N_p}\rangle \end{pmatrix} . \tag{1}$$

   - Adopting the same strategy, calculate now the correlation function $\langle\psi|\hat{n}_i\hat{n}_j|\psi\rangle$, with $\hat{n}_j = \hat{c}_j^\dagger \hat{c}_j$, and show that the result can be brought to the form predicted by Wick's theorem:
   $$\langle\psi|\hat{n}_i\hat{n}_j|\psi\rangle = \delta_{i,j} G_0(i,i) + G_0(i,i)G_0(j,j) - G_0(i,j)G_0(j,i) \tag{2}$$
   with $G_0(i,j) = \langle\psi|\hat{c}_i^\dagger \hat{c}_j|\psi\rangle = \sum_{\alpha=1}^{N_p} \psi_\alpha^*(i)\psi_\alpha(j)$ being the two-point function.

   Now consider a thermal state $\hat{\rho} = Z^{-1} \mathrm{e}^{-\beta \hat{H}}$ with $\hat{H}$ being a Hamiltonian of non-interacting fermions, and $Z = \mathrm{tr}\big(\mathrm{e}^{-\beta\hat{H}}\big)$. Show that also in this case the density-density correlation $\langle\hat{n}_i\hat{n}_j\rangle_\beta = \mathrm{tr}\big(\hat{\rho}\,\hat{n}_i\hat{n}_j\big)$ can be calculated using Wick's theorem through the formula:
   $$\langle\hat{n}_i\hat{n}_j\rangle_\beta = \delta_{i,j}\langle\hat{n}_i\rangle_\beta - \langle\hat{c}_i^\dagger\hat{c}_j\rangle_\beta \langle\hat{c}_j^\dagger\hat{c}_i\rangle_\beta + \langle\hat{n}_i\rangle_\beta\langle\hat{n}_j\rangle_\beta \ . \tag{3}$$

   Hint: Use the spectral representation of $\hat{H} = \sum_\ell \epsilon_\ell \hat{f}_\ell^\dagger \hat{f}_\ell$, with the operators $\hat{f}_\ell^\dagger = \sum_j V_{j,\ell}\,\hat{c}_j^\dagger$ creating the single-particle eigenstates of $\hat{H}$. The following identities may also be useful:
   $$\mathrm{e}^{-\beta\,\epsilon_\ell \hat{f}_\ell^\dagger \hat{f}_\ell}\,\hat{f}_\ell^\dagger = \mathrm{e}^{-\beta\,\epsilon_\ell}\,\hat{f}_\ell^\dagger\,\mathrm{e}^{-\beta\,\epsilon_\ell \hat{f}_\ell^\dagger \hat{f}_\ell} \ , \ \ \mathrm{e}^{-\beta\,\epsilon_\ell \hat{f}_\ell^\dagger \hat{f}_\ell}\,\hat{f}_\ell = \mathrm{e}^{\beta\,\epsilon_\ell}\,\hat{f}_\ell\,\mathrm{e}^{-\beta\,\epsilon_\ell \hat{f}_\ell^\dagger \hat{f}_\ell} \ .$$

2. **Green's functions and linear response theory**
   Consider a system described by an unperturbed time-independent Hamiltonian $\hat{H}_0$. Show that the operator $\hat{G}_0^{\mathrm{ret}}(t,t') = -i\,\Theta(t-t')\,\mathrm{e}^{-i\hat{H}_0(t-t')}$, with $\Theta(t-t')$ being the Heaviside step function, is a Green's function for the unperturbed Schrödinger equation, in the sense that it satisfies:
   $$\big(i\partial_t - \hat{H}_0\big)\hat{G}_0^{\mathrm{ret}}(t,t') = \delta(t-t')\,\hat{I} \ , \tag{4}$$
   where $\hat{I}$ denotes the identity operator. Now consider adding a small perturbation $\hat{V}(t)$ to the Hamiltonian, switched on adiabatically at time $t \to -\infty$. Show that the solution to $\big(i\partial_t - \hat{H}_0 + \hat{V}(t)\big)|\psi(t)\rangle = 0$ can be approximated to first order in $\hat{V}$ as follows:
   $$|\psi(t)\rangle \simeq |\psi_0(t)\rangle + \int_{-\infty}^{+\infty} dt'\,\hat{G}_0^{\mathrm{ret}}(t,t')\hat{V}(t')|\psi_0(t')\rangle \ , \tag{5}$$

where $|\psi_0(t)\rangle$ corresponds to the unperturbed solution $|\psi_0(t)\rangle = \mathrm{e}^{-i\hat{H}_0(t-t')}|\psi_0(t')\rangle$, and $|\psi(t)\rangle$ satsfies the initial condition $|\psi(t \to -\infty)\rangle = |\psi_0(t \to -\infty)\rangle = |\psi_0\rangle$. Assume now the perturbation consists of an amplitude, or external field, $F(t)$ coupled to an observable $\hat{B}$, i.e. $V(t) = F(t)\hat{B}$ and that we are interested in calculating the change $\delta\langle\hat{A}\rangle(t)$ of the expectation value of an observable $\hat{A}$ in presence of the perturbation $\hat{V}$, defined as $\delta\langle\hat{A}\rangle(t) = \langle\psi(t)|\hat{A}|\psi(t)\rangle - \langle\psi_0(t)|\hat{A}|\psi_0(t)\rangle$. Show that $\delta\langle\hat{A}\rangle(t)$ has the form:

$$\delta\langle\hat{A}\rangle(t) = \int_{-\infty}^{+\infty} dt'\, F(t')\, G^{\mathrm{ret}}_{AB}(t,t') \tag{6}$$

where $G^{\mathrm{ret}}_{AB}(t,t') = \langle\psi_0(t)|\hat{A}\,\hat{G}^{\mathrm{ret}}_0(t,t')\hat{B}|\psi_0(t')\rangle + \mathrm{c.c.} = -i\,\Theta(t-t')\langle\psi_0|\big[\hat{A}_I(t), \hat{B}_I(t')\big]|\psi_0\rangle$ is the two-time AB retarded Green's function, and $\hat{A}_I(t) = \mathrm{e}^{i\hat{H}_0(t-t_0)}\,\hat{A}\,\mathrm{e}^{-i\hat{H}_0(t-t_0)}\big|_{t_0\to-\infty}$ (similarly for $\hat{B}_I(t)$).