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Advanced Theoretical Condensed Matter Physics — SS11

Exercise 2

(Please return your solutions before Tu. 3.5.2011)

2.1. In-Class Exercise: Wick's Theorem in the Matsubara Formalism

Recall from the lecture that in order to perform the perturbation expansion in terms of Feynman diagrams, a technical fact relating an arbitrary order Green's function to products of single particle Green's functions, *Wick's theorem*, is required. A proof of Wick's theorem in the zero-temperature formalism is relatively straightforward, due to the fact that at zero temperature, the expectation values of *normal*-ordered product of creation / annihilation operators vanishes, and therefore the *time*-ordered product of those operators are the same as the the sum. But in the case of finite-temperature, since groud-state expectation values do no vanish, Wick's theorem needs to be proven in a slightly different way. This exercise will guide you through the steps required to prove Wick's theorem in the Matsubara formalism.

We start with the usual definition of the n-particle Green's function in the Matsubara formalism:

$$\begin{aligned}\mathcal{G}_0^{(n)}(\nu_1\tau_1,\ldots,\nu_n\tau_n;\nu_1'\tau_1',\ldots,\nu_n'\tau_n')\\ = (-1)^n \left\langle T_\tau \left[\hat{c}_{\nu_1}(\tau_1)\cdots\hat{c}_{\nu_n}(\tau_n)\hat{c}^\dagger_{\nu_n'}(\tau_1')\cdots\hat{c}^\dagger_{\nu_1'}(\tau_1')\right]\right\rangle_0 \quad (1)\end{aligned}$$

Here the indices ν_i denote arbitrary quantum numbers ($\vec{r}$, σ etc) assigned to particle i, τ_i are the imaginary time variables, and the "0" subscript denotes average with respect to a non-interacting Hamiltonian H_0. Time evolution of the creation and annihilation operators are also defined with respect to H_0, i.e.,

$$\hat{c}(\tau) = e^{\tau H_0} c e^{-\tau H_0} \quad (2)$$

We first simplify our expression in (1) by introducing the operator symbol

$$d_i(\sigma_i) = \begin{cases} \hat{c}_{\nu_i}(\tau_i), & i \in [1,n] \\ \hat{c}^\dagger_{\nu'_{2n+1-i}}(\tau'_{2n+1-i}), & i \in [n+1, 2n] \end{cases}$$

and furthermore we define the permutations of the $2n$ operators as

$$P(d_1(\sigma_1)\cdots d_{2n}(\sigma_{2n})) = d_{P_1}(\sigma_{P_1})\cdots d_{P_{2n}}(\sigma_{P_{2n}})$$

a) Using the definition of the Green's function given in (1), argue that it can be rewritten in the form

$$\begin{aligned}\mathcal{G}_0^{(n)}(i_1,\ldots,i_{2n}) = (-1)^n \sum_{P\in S_{2n}} (\pm 1)^P \theta(\sigma_{P_1}-\sigma_{P_2})\cdots\theta(\sigma_{P_{n-1}}-\sigma_{P_n})\times\\ \times \langle d_{P_1}(\sigma_{P_1})\cdots d_{P_{2n}}(\sigma_{P_{2n}})\rangle_0 \quad (3)\end{aligned}$$

The easiest way to show Wick's theorem for finite temperatures is through the equation of motion of the n-particle Green's function. Since in (3) we have a product of θ-functions and H_0-averaged product of the $d_{P_i}(\sigma_i)$ operators, we expect that a derivative with respect to a time variable, τ_1 for example, will produce 2 kinds of contributions: one coming from the derivative of the θ-function, and another coming from the derivative of the expectation value itself.

b) Differentiate (1) with respect to τ_1. What do you obtain for the equation of motion? Show that differentiation with respect to an arbitrary index i yields the following expression

$$\mathcal{G}_{0i}^{-1}\mathcal{G}_0^{(n)} = -\partial_{\tau_i}^{\theta}\mathcal{G}_0^{(n)} \tag{4}$$

where the quantities $\mathcal{G}_{0i}^{-1}$ and h_0 are defined in the following way

$$\mathcal{G}_{0i}^{-1} = -\partial_\tau - h_0, \qquad H_0 = \sum_{\nu\nu'} h_{0,\nu\nu'}c_\nu^\dagger c_{\nu'} \tag{5}$$

$$-\partial_\tau \mathcal{G}_0(\nu\tau,\nu'\tau') - \sum_{\nu''} h_{0,\nu\nu''}\mathcal{G}_0(\nu''\tau,\nu'\tau') = \delta(\tau-\tau')\delta_{\nu\nu'} \tag{6}$$

and $\partial_{\tau_i}^{\theta}$ only operates on the θ-functions.

Take now the case where τ_i and τ_j' are next to each other. There are 2 such terms in (1), corresponding to τ_i being either smaller or larger than τ_j'. This corresponds to different arguments of the θ-functions.

c) Calculate the right-hand side of (4) for the times τ_i and τ_j' as described above.

d) With the help of the equal-time (anti-)commutation relations

$$\left[\hat{c}_{\nu_i}(\tau_i), \hat{c}_{\nu_j'}^\dagger(\tau_i)\right]_{B,F} = \delta_{\nu_i,\nu_j'}$$
$$\left[\hat{c}_{\nu_i}(\tau_i), \hat{c}_{\nu_j}(\tau_i)\right]_{B,F} = 0$$

show that (4) can be rewritten as

$$\mathcal{G}_{0i}^{-1}\mathcal{G}_0^{(n)} = \sum_{j=1}^{n} \delta_{\nu_i,\nu_j'}\delta(\tau_i-\tau_j')(-1)^x \mathcal{G}_0^{n-1}(\underbrace{\nu_1\tau_1,\ldots,\nu_n\tau_n}_{\text{without}i};\underbrace{\nu_1'\tau_1',\ldots,\nu_n'\tau_n'}_{\text{without}j}) \tag{7}$$

e) Determine x by looking at the various definitions of Green's functions and minus signs picked up when commutating fermions. Integrating (7) according to (5) and obtain Wick's theorem:

$$\begin{aligned}&\mathcal{G}_0^{(n)}(\nu_1\tau_1,\ldots,\nu_n\tau_n;\nu_1'\tau_1',\ldots,\nu_n'\tau_n')\\ &\quad= \sum_{j=1}^{n}(\pm 1)^{i+j}\mathcal{G}_0(\nu_i\tau_i,\ldots,\nu_j'\tau_j')\mathcal{G}_0^{n-1}(\underbrace{\nu_1\tau_1,\ldots,\nu_n\tau_n}_{\text{without}i};\underbrace{\nu_1'\tau_1',\ldots,\nu_n'\tau_n'}_{\text{without}j})\end{aligned} \tag{8}$$

2.2 Homework Exercise: Feynman Diagrams in 1^{st} Order Perturbation Theory

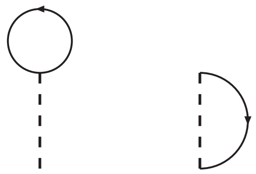
Generally, Green's function cannot be calculated exactly, but one has to use appropriate approximations. In this exercise, we want to use perturbation theory and to practice the calculation of Feynman diagrams. For that purpose, consider the Hamiltonian $\mathcal{H}$ of interacting electrons,

$$\mathcal{H} \;\equiv\; \mathcal{H}_0 + V \;=\; \sum_{\mathbf{k},\sigma} (\epsilon(\mathbf{k}) - \mu)\, c^\dagger_{\mathbf{k}\sigma}\, c_{\mathbf{k}\sigma} \;+\; \sum_{\substack{\mathbf{k},\mathbf{k}',\mathbf{q}\\ \sigma,\sigma'}} V^{\sigma,\sigma'}_{\mathbf{q}}\; c^\dagger_{\mathbf{k}+\mathbf{q},\sigma}\, c^\dagger_{\mathbf{k}'-\mathbf{q},\sigma'}\, c_{\mathbf{k}'\sigma'}\, c_{\mathbf{k}\sigma}.$$

We want to calculate the single-particle Matsubara Green's function $G_{\mathbf{k}\sigma}(\mathrm{i}\omega)$ by treating the potential V as a perturbation. According to Dyson's equation,

$$G_{\mathbf{k}\sigma}(\mathrm{i}\omega) = G^0_{\mathbf{k}\sigma}(\mathrm{i}\omega) + G^0_{\mathbf{k}\sigma}(\mathrm{i}\omega)\Sigma_{\mathbf{k}\sigma}(\mathrm{i}\omega)G_{\mathbf{k}\sigma}(\mathrm{i}\omega),$$

we have to calculate the self energy $\Sigma_{\mathbf{k}\sigma}(\mathrm{i}\omega)$. Restricting to 1^{st} order in V this corresponds to the evaluation of the two Feynman diagrams

.

a) General case:
   Use the Feynman rules to show that the first diagram  (Hartree term) yields

$$\Sigma^{(\mathrm{H})}_{k\sigma}(\mathrm{i}\omega) \;=\; \left(V^{\sigma,\sigma}_{\mathbf{q}=0} + V^{\sigma,-\sigma}_{\mathbf{q}=0}\right) \sum_{\mathbf{k}'} f(\epsilon(\mathbf{k}') - \mu)$$

   and the second one  (Fock term) yields

$$\Sigma^{(\mathrm{F})}_{k\sigma}(\mathrm{i}\omega) \;=\; -\sum_{\mathbf{q}} V^{\sigma,\sigma}_{\mathbf{q}} f(\epsilon(\mathbf{k}-\mathbf{q}) - \mu).$$

   Hint: Recall that for a holomorphic function $F(z)$

$$\frac{1}{\beta}\sum_{\omega} F(\mathrm{i}\omega) \;=\; -\oint_{C_1} \frac{dz}{2\pi\mathrm{i}}\, f(z)\, F(z) \;=\; \oint_{C_2} \frac{dz}{2\pi\mathrm{i}}\, f(z)\, F(z),$$

   where C_1 encloses only the poles of $f(z)$ and C_2 only those of $F(z)$.

b) Coulomb interaction:
   Consider the concrete example of a Coulomb interaction of a gas of free electrons in three dimensions. The Fourier transform of the Coulomb potential is

$$V^{\sigma,\sigma'}_{\mathbf{q}} \;=\; \begin{cases} 0 & , \quad \mathbf{q} = 0 \\ \frac{1}{V}\frac{4\pi e_0^2}{q^2} & , \quad \mathbf{q} \neq 0 \end{cases} \qquad (e_0\text{: elementary electric charge}).$$

Use the result from a) to obtain

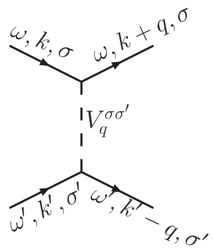
$$\Sigma_{k\sigma}(\mathrm{i}\omega) \;=\; -\sum_{\mathbf{q}} V^{\sigma\sigma}_{\mathbf{k}-\mathbf{q}}\, f(\epsilon(\mathbf{q})-\mu) \overset{T\to 0}{=} \frac{e_0^2}{2\pi} k_{\mathrm{F}} \left(2 + \frac{k_{\mathrm{F}}^2 - k^2}{k k_{\mathrm{F}}} \ln\left|\frac{k_{\mathrm{F}}+k}{k_{\mathrm{F}}-k}\right|\right).$$

Hint:

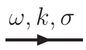
$$\int_0^x dy\, y \,\ln\left|\frac{y-1}{y+1}\right| \;=\; -x - \frac{1}{2}\left(1-x^2\right)\ln\left|\frac{x-1}{x+1}\right|$$

Feynman rules: (Matsubara representation)

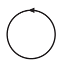
1) Draw all connected, topologically distinct diagrams of order n.

2) Each vertex corresponds to 

$= -\frac{1}{\beta} V^{\sigma,\sigma'}_{\mathbf{q}}$.

3) Each line 

corresponds to $-G^0_{\mathbf{k}\sigma}(\mathrm{i}\omega) = \dfrac{-1}{\mathrm{i}\omega - \epsilon(\mathbf{k}) + \mu}$.

4) Each non-propagating line,  and , gets a factor $e^{\mathrm{i}\omega 0^+}$.

5) Each closed fermion loop gets an additional factor (-1).

6) All internal indices (momenta, spins, energies, ...) have to be summed over.

7) For the Coulomb interaction, we have energy conservation at the vertex, i.e., $\delta_{\omega'+\omega''} = \delta_{\omega'''+\omega''''}$