Interlude: how to express $\langle \hat H \rangle$ in terms of spectral function

Consider real-time equation of motion for $\hat\psi(1) \equiv \psi(x_1, t_1)$

$$i\partial_{t_1} \hat\psi(1) \overset{(GF11.2)}{=} [\hat\psi(1), \hat H] = h_0(1)\,\hat\psi(1) + \int dx_2\, \psi^\dagger(1)\, V(1,2)\, \psi(2)\, \psi(1) \tag{1}$$

$\int dx_1\, \frac{1}{2}\psi^\dagger(1) \times$ Eq.(1):

$$\int dx_1 \frac{1}{2} \psi^\dagger(1)\, i\partial_{t_1} \psi(1) = \frac{1}{2}\hat H_0 + \hat H' \tag{2}$$

$$\Rightarrow \langle \hat H \rangle = \langle \underbrace{\tfrac{1}{2}\hat H_0}_{(8.2)} + \underbrace{\tfrac{1}{2}\hat H_0 + \hat H'}_{(2)} \rangle \tag{3}$$

$$= \frac{1}{2}\int dx_1 \langle \hat\psi^\dagger(1) \left(h_0(1) + i\partial_{t_1}\right) \hat\psi(1) \rangle \tag{4}$$

$$\overset{(GF30.2)}{=} \frac{1}{2}\int dx_1 \left(h_0(1) + i\partial_{t_1}\right) \underbrace{\langle \hat\psi^\dagger(2)\, \hat\psi(1) \rangle}_{(GF30.2)} \Big|_{\substack{t_1 = t_2 \\ x_1 = x_2}} \tag{5}$$

$$i\xi\, \mathcal{G}^<(x_1, t_1; x_2, t_2) = \int \frac{d\omega}{2\pi} e^{-i\omega(t_1 - t_2)} \underbrace{i\xi\, \mathcal{G}^<(x_1, x_2, \omega)}_{\substack{(GF60.2) \\ 2\pi\, n_\xi(\omega)\, A_{\psi(x_1)\psi^\dagger(x_2)}(\omega)}} \tag{6}$$

$$\Longrightarrow \langle \hat H \rangle = \int dx_1 \int d\omega\, \frac{1}{2}\left(h_0(1) + \omega\right) n_\xi(\omega)\, \underbrace{A(x_1, x_2; \omega)\Big|_{x_1 = x_2}}_{} \tag{1}$$

If system is translationally invariant:

$$= \int \frac{d^3 p}{(2\pi)^3} e^{i\vec p\cdot(\vec x_1 - \vec x_2)} A_{\vec p}(\omega) \tag{2}$$

$$\langle \hat H \rangle = Vd \int \frac{d^3 p}{(2\pi)^3} \frac{1}{2}\left(\frac{\vec p^{\,2}}{2m} + \omega\right) n_\xi(\omega)\, A_\sigma(\omega, \vec p) \tag{3}$$

occupation probability of excitations with energy ω

density of excitations with energy ω and momentum $\vec p$.

In absence of interactions: $A_\sigma(\omega, \vec p) = \delta\!\left(\omega - \frac{p^2}{2m}\right)$, and (4)

energy density:

$$\frac{\langle \hat H \rangle}{Vd} = \sum_\sigma \int \frac{d\vec p}{2\pi} \frac{p^2}{2m}\, n_\xi\!\left(p^2/2m\right) \tag{5}$$

↑ thermal occupancy of single-particle excitations. ✓

With interactions, $A_{\vec p}(\omega)$ will be broadened, i.e. spectral weight is shifted away from $p^2/2m$; (3) specifies how thermal weighting has to be done in this case.

Perturbation theory in the interaction

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Adopt interaction representation w.r.t. $\hat{H}'$ (GF12, GF16)

$$\hat{U}(\tau) = e^{-\tau \hat{H}} \equiv e^{-\tau \hat{H}_0} \hat{U}_I(\tau) \qquad (1)$$

$$\hat{U}_I(\tau) = T_\tau \, e^{-\int_0^\tau d\tau' \hat{H}_I'(\tau')} \qquad \text{(in analogy to GF13.6)} \qquad (2)$$

$$\hat{U}_I^{-1}(\tau) = \bar{T}_\tau \, e^{\int_0^\tau d\tau' \hat{H}_I'(\tau')}$$

T_τ: time-ordering: larger times to left

$\bar{T}_\tau$: anti-timeordering " " " right

$$\hat{A}_I(\tau) \equiv e^{\tau \hat{H}_0} \hat{A} e^{-\tau \hat{H}_0} \qquad (3)$$

does not depend only on $\tau_1 - \tau_2$!

Note:
$$U_I(\tau_1, \tau_2) \overset{(3a)}{\equiv} U(\tau_1) U^{-1}(\tau_2) \overset{(3b)}{=} T_\tau \, e^{-\int_{\tau_2}^{\tau_1} d\tau' \hat{H}_I'(\tau')} \qquad (4)$$

Proof:
$$\left.\begin{aligned} -\partial_{\tau_1} U_I(\tau_1,\tau_2) &\overset{(3a)}{=} H_I'(\tau_1) \hat{U}_I(\tau_1,\tau_2) \\ -\partial_{\tau_2} U_I(\tau_1,\tau_2) &\overset{(3a)}{=} \hat{U}_I(\tau_1,\tau_2) H_I'(\tau_2) \end{aligned}\right\} \text{these equations are solved by (3b)} \qquad (5)$$

GF in interaction representation:

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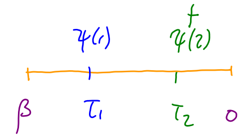
$\beta \geq \tau_1 \geq \tau_2 \geq 0$:
$$\mathcal{G}(1,2) = -\frac{1}{Z} \mathrm{Tr}\left\{ e^{-\beta \hat{H}} \left(e^{\tau_1 \hat{H}} \overset{\equiv \hat{\psi}(x_1)}{\hat{\psi}_1} e^{-\tau_1 \hat{H}} \right) \left(e^{\tau_2 \hat{H}} \hat{\psi}_2^\dagger e^{-\tau_2 \hat{H}} \right) \right\} \qquad (1)$$

$$= -\frac{1}{\mathrm{Tr}\{e^{-\beta \hat{H}}\}} \mathrm{Tr}\Big\{ e^{-\beta \hat{H}_0} \hat{U}_I(\beta) \; \hat{U}_I^{-1}(\tau_1) \overbrace{e^{\tau_1 \hat{H}_0} \hat{\psi}_1 e^{-\tau_1 \hat{H}_0}}^{= \hat{\psi}(x_1,\tau_1) \equiv \hat{\psi}(1)} \hat{U}_I(\tau_1) \qquad (2)$$
$$\times \hat{U}_I^{-1}(\tau_2) e^{\tau_2 \hat{H}_0} \hat{\psi}_2^\dagger e^{-\tau_2 \hat{H}_0} \hat{U}_I(\tau_2) \Big\}$$

$$= -\frac{\mathrm{Tr}\left\{ e^{-\beta \hat{H}_0} \hat{U}_I(\beta,\tau_1) \hat{\psi}_I(1) \; \hat{U}_I(\tau_1,\tau_2) \hat{\psi}_I^\dagger(\tau) \; U_I(\tau_2) \right\}}{\mathrm{Tr}\{ e^{-\beta \hat{H}_0} \hat{U}_I(\beta) \}} \qquad (3)$$

$$\mathcal{G}(1,2) = -\frac{\langle T_\tau \, \hat{U}_I(\beta) \hat{\psi}_I(1) \hat{\psi}_I^\dagger(2) \rangle_0}{\langle T_\tau \hat{U}_I(\beta) \rangle_0} \qquad (4)$$

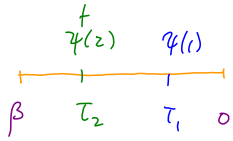


where $\langle \ldots \rangle_0 = \mathrm{Tr}\, e^{-\beta \hat{H}_0}$ (5)

Similarly, for $\underline{0 \geq \tau_2 \geq \tau_1 \geq 0}$: $\boxed{\text{PT13}}$

$$\mathcal{G}(1,2) = -\zeta \, \frac{1}{Z} \mathrm{Tr}\left\{ e^{-\beta \hat{H}} \left(e^{\tau_2 \hat{H}} \hat{\psi}_2^{+} e^{-\tau_2 \hat{H}} \right) \left(e^{\tau_1 \hat{H}} \hat{\psi}_1 e^{-\tau_1 \hat{H}} \right) \right\} \tag{1}$$

$$= -\zeta \, \frac{\mathrm{Tr}\left\{ e^{-\beta \hat{H}_0} \hat{\mathcal{U}}_I(\beta, \tau_2) \hat{\psi}^{+}(\tau_2) \hat{u}_I(\tau_2, \tau_1) \hat{\psi}_I(1) \hat{u}_I(\tau_1) \right\}}{\mathrm{Tr}\left\{ e^{-\beta \hat{H}_0} \hat{\mathcal{U}}_I(\beta) \right\}} \tag{2}$$



$$= -\frac{\langle T_\tau \, \hat{\mathcal{U}}_I(\beta) \, \hat{\psi}_I(1) \, \hat{\psi}_I^{+}(2) \rangle_0}{\langle T_\tau \hat{\mathcal{U}}_I(\beta) \rangle_0} \tag{3}$$

So, (3) holds for both $\tau_1 > \tau_2$ and $\tau_1 < \tau_2$.

To obtain a perturbation expansion in $\hat{H}'$, use (compare 13.5):

$$\hat{\mathcal{U}}_I(\tau, \tau') \overset{(11.2)}{=} \sum_{n=0}^{\infty} \left(-1/\hbar\right)^n \frac{1}{n!} \int_{\tau'}^{\tau} d\tau_1 \int_{\tau'}^{\tau} d\tau_2 \ldots \int_{\tau'}^{\tau} d\tau_n \; T\left[\hat{H}_I'(\tau_1) \hat{H}_I'(\tau_2) \ldots \hat{H}_I'(\tau_n) \right] \tag{4}$$

To calculate $\langle H' \, H' \ldots \psi(1) \, \psi^{+}(2) \rangle$, we need to know how to calculate correlators of higher order GF's, using "Wick's theorem".

Higher order GF: $\boxed{\text{PT14}}$

always even # of operators (n creation, n annihilation)

Define:
$$\mathcal{G}^{(n)}(\tau_1, \ldots, \tau_{2n}) \equiv (-)^n \langle T_\tau \left[\hat{A}_1(\tau_1) \hat{A}_2(\tau_2) \ldots \hat{A}_{2n}(\tau_{2n}) \right] \rangle \tag{1}$$

Boundary condition:
$$\mathcal{G}^{(n)}(\tau_1, \ldots, \tau_i = 0, \ldots \tau_{2n}) = \zeta \, \mathcal{G}^{(n)}(\tau_1, \ldots, \tau_i = \beta, \ldots, \tau_{2n}) \tag{2}$$

Proof:

$$(\text{LHS})_2 = \zeta^{2n-i} \, \mathrm{Tr}\left\{ e^{-\beta \hat{H}} T_\tau \left[\hat{A}_1(\tau_1) \ldots \hat{A}_{i-1}(\tau_{i-1}) \overbrace{\hat{A}_{i+1}(\tau_{i+1}) \ldots \hat{A}_{2n}(\tau_{2n})}^{2n-i \text{ swaps}} \right] \hat{A}_i(0) \right\} \tag{3}$$

$$= \zeta^{2n-i} \, \mathrm{Tr}\left\{ e^{-\beta \hat{H}} \underbrace{e^{\beta \hat{H}} \hat{A}_i(0) e^{-\beta \hat{H}}}_{\hat{A}_i(\beta)} T_\tau \left[\hat{A}_1(\tau_1) \ldots \hat{A}_{i-1}(\tau_{i-1}) \, \hat{A}_{i+1}(\tau_{i+1}) \ldots \hat{A}_{2n}(\tau_{2n}) \right] \right\} \tag{4}$$

$$= \underbrace{\zeta^{2n-i+i-1}}_{= \zeta} \mathrm{Tr}\left\{ e^{-\beta H} T_\tau \left[\overbrace{\hat{A}_1(\tau_1) \ldots \hat{A}_{i-1}(\tau_{i-1})}^{i-1 \text{ swaps}} \hat{A}_i(\beta) \, \hat{A}_{i+1}(\tau_{i+1}) \ldots \hat{A}_{2n}(\tau_{2n}) \right] \right\} = (\text{RHS})_2 \tag{5}$$

For future reference: (14.2) implies that Matsubara transform has the form:

$$\mathcal{G}(\tau_1, \cdots, \tau_{2n}) = \frac{1}{\beta^{2n-1}} \sum_{\omega_{\ell_1}} \sum_{\omega_{\ell_2}} \cdots \sum_{\omega_{\ell_{2n}}} \bar{\mathcal{G}}(\omega_{\ell_1}, \cdots, \omega_{\ell_{2n}}) \, e^{-i \sum_{j=1}^{2n} \omega_{\ell_j} \tau_j} \qquad (1)$$

with $\omega_\ell = \left\{ \begin{matrix} 2\pi n T \\ 2\pi(n+1/2)T \end{matrix} \right\}$ for bosonic/fermionic operators, as in (23.2).

Since we always have $H \neq H(\tau)$ for problems treatable with Matsubara formalism, GF must satisfy translational invariance:

$$\mathcal{G}(\tau_1 + \tau', \tau_2 + \tau', \ldots \tau_{2n} + \tau') = \mathcal{G}(\tau_1, \cdots, \tau_{2n}) \qquad \forall \; \tau' \in [0, \beta] \qquad (2)$$

which is possible only if $$\sum_{j=1}^{2n} \omega_{\ell_j} = 0 \qquad (3)$$

Thus, there $\bar{\mathcal{G}}(\omega_{\ell_1}, \cdots, \omega_{\ell_n})$ is understood to be nonzero only if (3) holds.