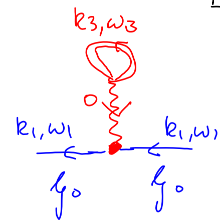
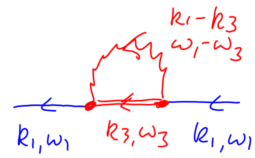
Comments:

PT 58

For translationally invariant systems, we have



$$\bar{\Sigma}_H(i\omega_1, k_1) \overset{(45.2)}{=} (-\xi)\, 2\,\tilde{v}(0) \int d(k_3)\, \frac{1}{\beta}\sum_{\omega_3} \bar{\mathcal{G}}(i\omega_3, k_3)\, e^{i\omega_3 0^+} \quad (1)$$



$$\bar{\Sigma}_F(i\omega_1, k_1) \overset{(45.6)}{=} -\int d(k_3)\, \frac{1}{\beta}\sum_{\omega_3'} \bar{\mathcal{G}}(i\omega_3, k_3)\, \tilde{v}(k_1-k_3) \quad (2)$$

$\bar{\Sigma}_{H+F}(i\omega_1, k_1)$ is <u>independent</u> of $i\omega_1$, and <u>real</u>, hence $\Gamma_k^{H+F} \overset{(53.7)}{=} 0$ (3)

(check this, using spectral representation for $\mathcal{G}(i\omega_n)$!)

$\Rightarrow$ they do <u>not</u> contribute to quasi-particle decay! The reason for this is the single-particle nature of the HF approximation: it does not allow for the creation of particle-hole pairs (such as )

Relation between HF equations and single-particle wave functions

PT 59

Consider single-particle Hamiltonian $h_0(1)$ with eigenfunctions $\varphi^0_\lambda(x_1)$:

$$\left(h_0(1) - E^0_\lambda\right)\varphi^0_\lambda(x_1) = 0 \quad (1)$$

Free GF satisfies
$$\left(-\partial_{\tau_1} - h_0(1)\right)\mathcal{G}_0(1,2) \overset{(57.2)}{=} \delta(1,2) = \delta(\tau_1-\tau_2)\,\delta(x_1-x_2) \quad (2)$$

Matsubara transform:
$$\mathcal{G}_0(1,2) = \frac{1}{\beta}\sum_n \bar{\mathcal{G}}(i\omega_n; x_1, x_2)\, e^{-i(\tau_1-\tau_2)\omega_n} \quad (3)$$

(3) into (2):
$$\left[i\omega_n - h_0(1)\right]\bar{\mathcal{G}}_0(i\omega_n; x_1, x_2) = \delta(x_1 - x_2) \quad (4)$$

Solution of (4):
$$\bar{\mathcal{G}}_0(i\omega_n; x_1, x_2) = \sum_\lambda \frac{\varphi^0_\lambda(x_1)\,\varphi^{0*}_\lambda(x_2)}{i\omega_n - E^0_\lambda} \quad (5)$$

Check:
$$\left[i\omega_n - h_0(1)\right](5) = \sum_\lambda \frac{\cancel{(i\omega_n - E^0_\lambda)}\,\varphi^0_\lambda(x_1)\,\varphi^{0*}_\lambda(x_2)}{\cancel{i\omega_n - E^0_\lambda}} \underset{\text{(completeness)}}{=} \delta(x_1 - x_2) \checkmark \quad (6)$$

Would an Ansatz analogous to (59.5) work as solution to HF eq. (57.1)? $\boxed{\text{PT60}}$

$$\left(-\partial_{\tau_1} - h_0(1)\right)\mathcal{G}(1,2) = \delta(1,2) - \xi \overset{\tau_1=\tau_1'}{\int} dx_1'\, v(x_1,x_1')\left[\mathcal{G}(1,2)\mathcal{G}(1',1'_+) + \xi\,\mathcal{G}(1,1'_+)\mathcal{G}(1',2)\right] \qquad (1)$$

$$= \delta(1,2) + v_H(x_1)\,\mathcal{G}(1,2) - \int dx_1'\, v_F(x_1,x_1')\,\mathcal{G}(1',2) \qquad (2)$$

where
$$v_H(x_1) \equiv -\xi \int dx_1'\, v(x_1,x_1')\underbrace{\mathcal{G}(1',1'_+)}_{i n(1')} \qquad (3)$$
$$v_F(x_1,x_1') \equiv v(x_1,x_1')\underbrace{\mathcal{G}(1,1'_+)}_{G^<(1,1')} \qquad (4)$$

equal time correlators:
$$\mathcal{G}(1,1'_+) = -i\langle T_\tau\, \psi(1)\,\psi^\dagger(1'_+)\rangle = \begin{cases} i\, n(1) & \text{if } x_1 = x_1' \\ G^<(1,1') & \text{if } x_1 \neq x_1' \end{cases} \quad \text{(GF 36.4)}$$

Matsubara-transform (2):

$$\left(i\omega_1 - h_0(1) - v_H(x_1)\right)\bar{\mathcal{G}}(i\omega_1; x_1, x_2) = \delta(x_1 - x_2) - \int dx_1'\, v_F(x_1,x_1')\,\bar{\mathcal{G}}(i\omega_1; x_1', x_2) \qquad (5)$$

$\boxed{\text{PT61}}$

Ansatz for solution (analogous to 59.5):
$$\bar{\mathcal{G}}(i\omega_n; x_1, x_2) = \sum_\lambda \frac{\psi_\lambda(x_1)\,\psi^*_\lambda(x_2)}{i\omega_n - E_\lambda} \qquad (1)$$

Insert into (60.5):

$$\sum_\lambda \Big[\Big(i\omega_1 - \underbrace{h_0(1) - v_H(x_1)\Big)\,\psi_\lambda(x_1) + \int dx_1'\, v_F(x_1,x_1')\,\psi_\lambda(x_1')}_{\equiv\, E_\lambda \psi^*_\lambda(x_1)}\Big]\frac{\psi^*_\lambda(x_2)}{i\omega_n - E_\lambda} = \delta(x_1 - x_2) \qquad (2)$$

This is satisfied provided that the single-particle wave functions obey

$$\left(h_0(1) + v_H(x_1)\right)\psi_\lambda(x_1) - \int dx_1'\, v_F(x_1,x_1')\,\psi_\lambda(x_1') = E_\lambda\,\psi_\lambda(x_1) \qquad (3)$$

"HF-eq. for single-particle wavefunctions"

and completeness:
$$\sum_\lambda \psi_\lambda(x_1)\,\psi^*_\lambda(x_2) = \delta(x_1 - x_2) \qquad (4)$$

with
$$\overset{\tau_1=\tau_1'}{\mathcal{G}(1,1'_+)} = \frac{1}{\beta}\sum_{\omega_1}\bar{\mathcal{G}}(i\omega_1; x_1, x_1')\, e^{i0^+\omega_1} \overset{(1)}{=} \sum_\lambda \psi_\lambda(x_1)\,\psi^*_\lambda(x_1')\overbrace{\sum_{\omega_1}\frac{e^{i0^+\omega_1}}{i\omega_1 - E_\lambda}}^{(65.4)\;\; n_\xi(E_\lambda)} \qquad (5)$$

needed in (60.3), (60.4)

(3) to (5), with (60.3), (60.4), have to be solved <u>self-consistently</u>.

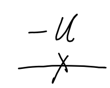
Comments: (from Rickayzen, p. 89)

Since the Hartree-Fock approximation sums a larger class of diagrams than the Hartree approximation, it might seem that it is a better approximation. However, this is not always the case, especially when long-range forces are involved. In such situation corrections to the exchange diagrams are very important and reduce their effect. In fact, the Hartree approximation, being based on a classical, self-consistent picture, works well when classical considerations can give a good answer. Typically, this occurs when macroscopic effects are paramount, for example in discussions of the long-waevelength collective modes such as plasma oscillations and sound waves, and of the effects of slowly varying external forces.

The Hartree approximation is also useful for starting an iterative solution of a problem. To iniate the Hartree approximation, on needs to make a guess at the one-point function v(1), the self-consistent potential. This is used to generate the Green's functions, which can in turn be used to calculate an improved potential. The process can then be continued, at least in principle.

Application: Density-response to an external potential (Rickayzen, §3.8)

External potential: $H'(t_1) = \int dx_1 \, \hat{\rho}(x_1) \, \mathcal{U}(t_1, \vec{r}_1)$ (1)



(includes sum on spin, $\sum_{\sigma_1}$)

density $\hat{\rho}(x_1) \equiv \hat{\psi}^{\dagger}(x_1)\,\hat{\psi}(x_1) - \bar{\rho}(x_1)$ (2)

defined w.r.t. background: $\bar{\rho}(x_1) = \langle \hat{\psi}^{\dagger}(x_1)\,\hat{\psi}(x_1) \rangle = \rho_{\text{ions}}$ (3)

so that $\langle \hat{\rho}(x_1) \rangle = 0$ (4)

[The subtraction of $\bar{\rho}$ in (2) is equivalent to a "normal ordering prescription".]

Response of the density to external perturbation is given by Kubo formula:

$$\delta\rho(1) = \int_{-\infty}^{\infty} d2 \; \mathcal{G}^{R}_{\rho\rho}(1,2)\, \mathcal{U}(2) \qquad (5)$$

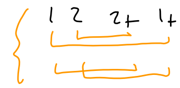
Thermal Density-density correlator:

$\boxed{PT64}$

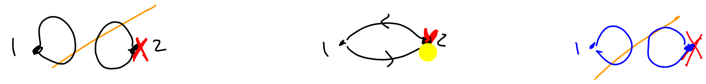
$$\mathcal{G}_{\rho\rho}(1,2) = -\langle T_\tau\, \hat\rho(1)\,\hat\rho(2)\rangle = -\langle T_\tau \big(\hat\psi^\dagger(1_+)\hat\psi(1) - \bar\rho(1)\big)\big(\hat\psi^\dagger(2_+)\hat\psi(2) - \bar\rho(2)\big)\rangle \tag{1}$$

$$= -\langle T_\tau\, \hat\psi^\dagger(1_+)\,\hat\psi(1)\,\hat\psi^\dagger(2_+)\,\hat\psi(2)\rangle + \bar\rho(1)\bar\rho(2) = -\mathcal{G}(1,2;1_+,2_+) + \bar\rho(1)\bar\rho(2) \tag{2}$$

In absence of interactions, this would factorize as (3)



$$\mathcal{G}^0_{\rho\rho}(1,2)\,U(2) = \Big[-\cancel{\mathcal{G}^0(1,1^+)\,\mathcal{G}^0(2,2^+)} - \zeta\,\mathcal{G}^0(1,2_+)\,\mathcal{G}^0(2,1^+) + \cancel{\bar\rho(1)\,\bar\rho(2)}\Big]\,U(2) \tag{4}$$



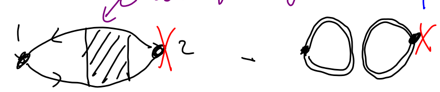
$$= -\zeta\,\mathcal{G}^0(1,2_+)\,\mathcal{G}^0(2,1^+)\,U(2) \tag{5}$$

subtract disconnected terms

With interactions, we'll have:

lots of diagrams!

$$\mathcal{G}_{\rho\rho}(1,2)\,U(2) = \tag{6}$$



A popular approximation scheme for such diagrams is RPA ("random phase approximation"), which describes physics of screening.