TALENT course on "Many-body Methods for NP"

July 2015 - Numerical exercises on SCGF theory

We will consider hamiltonians with up to 2-body interactions in the following general form:

$$\hat{H} = \hat{H}_0 + \hat{H}_1$$

where:

$$H_0 = \sum_{\alpha\beta} u_{\alpha\beta}\, a^\dagger_\alpha a_\beta$$

$$H_1 = \frac{1}{4} \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta,\gamma\delta}\, a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma$$

and $v_{\alpha\beta,\gamma\delta}$ are antisymmetrized: $v_{\alpha\beta,\gamma\delta} = \langle\alpha\beta|H_1|\gamma\delta - \delta\gamma\rangle$

In all cases to be considered in our exercises, H_0 will be a pure 1-body potential and H_2 a pure 2-body interaction (although this is not necessarily always the case).

For both our pairing model and the nuclear-matter calculations, $\hat{H}_0$ will define <u>both</u> our single-particle basis ($\alpha, \beta, \gamma \ldots$) and the particle and hole orbits that define our <u>reference state</u> [$n, m, \ldots$ for the unoccupied (particle) orbits and $i, j, k, \ldots$ for the occupied (hole) ones].
This in not the case in general but we won't need worry about it for now.

The non interacting propagator (assuming that the basis $\{|\alpha\rangle\}$ diagonalises H_0) is given by:

$$g^{(0)}_{\alpha\beta}(\omega) = \delta_{\alpha\beta}\left\{ \frac{\delta_{n,\alpha}\,\delta_{n\notin F}}{\omega - \varepsilon^{(0)}_n + i\eta} + \frac{\delta_{i,\alpha}\,\delta_{i\in F}}{\omega - \varepsilon^{(0)}_i - i\eta} \right\}$$

where: $H_0|\alpha\rangle = \varepsilon^{(0)}_\alpha |\alpha\rangle$

and we take the $+(-)$ sign is α is unoccupied (occupied) in the reference state

The complete propagator, which we want to calculate, is:

$$g_{\alpha\beta}(\omega) = \sum_n \frac{(\mathcal{X}^n_\alpha)^* \mathcal{X}^n_\beta}{\omega - \varepsilon^+_n + i\eta} + \sum_k \frac{\mathcal{Y}^k_\alpha (\mathcal{Y}^k_\beta)^*}{\omega - \varepsilon^-_k - i\eta}$$

with the following definitions

$$\begin{cases} \mathcal{X}^n_\alpha \equiv \langle \Psi^{A+1}_n | a^\dagger_\alpha | \Psi^A_0 \rangle \\ \varepsilon^+_n \equiv E^{A+1}_n - E^A_0 \\ \hat{H}|\Psi^{A+1}_n\rangle = E^{A+1}_n |\Psi^A_0\rangle \end{cases} \qquad \begin{cases} \mathcal{Y}^k_\beta = \langle \Psi^{A-1}_k | a_\beta | \Psi^A_0 \rangle \\ \varepsilon^-_k = E^A_0 - E^{A-1}_k \\ H|\Psi^{A-1}_k\rangle = E^{A-1}_k |\Psi^A_0\rangle \end{cases}$$

In general the irreducible self-energy has the following analytical structure

$$\Sigma^{\star}_{\alpha\beta}(\omega) = \Sigma^{\infty}_{\alpha\beta} + \sum_r \frac{(m^r_\alpha)^* m^r_\beta}{\omega - E_r + i\eta} + \sum_q \frac{m^q_\alpha (m^q_\beta)^*}{\omega - E^q_r - i\eta}$$

$$= \Sigma^{\infty}_{\alpha\beta} + \tilde{\Sigma}_{\alpha\beta}(\omega)$$

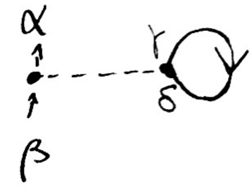
which has a energy independent part Σ^{∞} and a dinamic part $\tilde{\Sigma}(\omega)$ that represents contributions from dynamical excitations in the system.

In order to calculate the propagator, $g_{\alpha\beta}(\omega)$, we need an approximation for $\Sigma^*(\omega)$.

At first order Σ^∞ is given by the following formula (and diagram)

$$\Sigma^{\infty(1)}_{\alpha\beta} = -i\, v_{\alpha\gamma,\beta\delta}\, g^{(0)}_{\gamma\delta}(\tau \to 0^-)$$

$$= \int_{C\uparrow} \frac{d\omega}{2\pi i}\, v_{\alpha\gamma,\beta\delta}\, g^{(0)}_{\delta\gamma}(\omega)$$

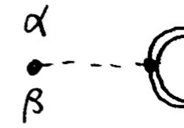


You should check that:

$$\Sigma^{\infty(1)}_{\alpha\beta} = \sum_{i=1}^{A} v_{\alpha i,\beta i}$$

The exact Σ^∞ turns out to be the same diagram contracted with the unperturbed propagator $g_{\alpha\beta}$ instead

$$\Sigma^{\infty}_{\alpha\beta} = i\, v_{\alpha\gamma,\beta\delta}\, g_{\delta\gamma}(\tau = 0^-) = \int_{C\uparrow} \frac{d\omega}{2\pi i}\, v_{\alpha\gamma,\beta\delta}\, g_{\delta\gamma}(\omega) \quad :$$



Show that

$$\Sigma^{\infty}_{\alpha\beta} = \sum_{\gamma\delta} v_{\alpha\gamma,\beta\delta}\, \rho_{\delta\gamma}$$

and re-express $\rho_{\delta\gamma}$ in terms of y^k_δ and y^k_γ.

The second order approximation to the self-energy is given by

$$\tilde{\Sigma}^{(2)}_{\alpha\beta}(\omega) = (-)\int \frac{d\omega_1}{2\pi i}\int \frac{d\omega_2}{2\pi i}\, v_{\alpha\lambda,\mu\nu}\, g^{(0)}_{\mu\xi}(\omega_1)$$

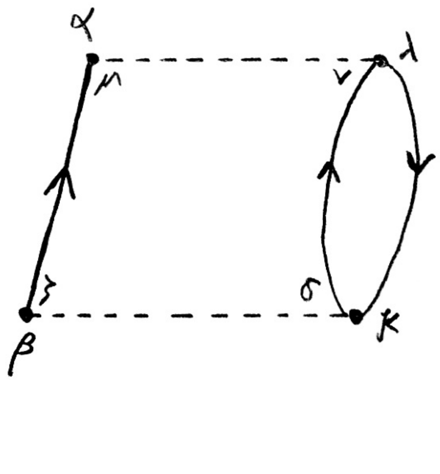
$$\times\, g^{(0)}_{\nu\sigma}(\omega-\omega_1+\omega_2)\, g^{(0)}_{\kappa\lambda}(\omega_2)\, v_{\xi\sigma,\beta\kappa} .$$

(repeated indices are implicitely summed)

$$= \frac{1}{2}\sum_{\substack{n_1,n_2>F\\ k\leq F}} \frac{v_{\alpha k, n_1 n_2}\; v_{n_1 n_2,\beta k}}{\omega - \left(\varepsilon^{(0)}_{n_1} + \varepsilon^{(0)}_{n_2} - \varepsilon^{(0)}_{k}\right) + i\eta} +$$

$$+ \frac{1}{2}\sum_{\substack{n>F\\ k_1,k_2\leq F}} \frac{v_{\alpha n, k_1 k_2}\; v_{k_1 k_2,\beta n}}{\omega - \left(\varepsilon^{(0)}_{k_1} + \varepsilon^{(0)}_{k_2} - \varepsilon^{(0)}_{n}\right) + i\eta}$$

that correspond to the following Feynman diagram:



[NOTE that rearranging the sums to be over $n_1 < n_2$ and $k_1 < k_2$ gets rid of the factor $\frac{1}{2}$ an reduces the dimensions of matrices to diagonalize later!

We will solve the Dyson eq. to find $g_{\alpha\beta}(\omega)$

$$g_{\alpha\beta}(\omega) = g^{(0)}_{\alpha\beta}(\omega) + g^{(0)}_{\alpha\gamma}(\omega) \Sigma^{*}_{\gamma\delta}(\omega)\, g_{\delta\beta}(\omega)$$

To see how to solve this it is convenient to re-express things as follows:

$(\chi^{n}_{\alpha})^{*}, \ \psi^{k}_{\beta} \quad \rightarrow \quad \underline{Z}^{i}$ vector in indices α with $i = n$ or k

$m^{r}_{\alpha}, \ m^{q}_{\alpha} \quad \rightarrow \quad \underline{\underline{M}}$ matrix in the indices α and r/q

Since $\pm i\eta$ at the denominators always go to zero ($\eta \to 0$) we can discard it an write:

$$g^{(0)}(\omega) = \frac{1}{\omega - \mathrm{diag}\{\varepsilon^{(0)}\}}$$

$$g(\omega) = \sum_{i} \underline{Z}^{i} \frac{1}{\omega - \varepsilon^{+/-}_{i}} (\underline{Z}^{i})^{\dagger}$$

$$\Sigma^{*}(\omega) = \underline{\underline{\Sigma}}^{\infty} + \underline{\underline{M}}^{\dagger} \frac{1}{\omega - \mathrm{diag}(E^{r})} \underline{\underline{M}}$$

We can then readjust the Dyson eq. be extracting the poles of each solution $\varepsilon_i^{+/-}$ we are looking for:

$$\lim_{\omega \to \varepsilon_i} (\omega - \varepsilon_i) \left\{ g(\omega) = g^{(0)}(\omega) + g^{(0)}(\omega) \underline{\underline{\Sigma}}^{\star}(\omega) g(\omega) \right\}$$

$$\underline{Z}^i (\underline{Z}^i)^\dagger = \frac{1}{\omega - \mathrm{diag}(\varepsilon^{(0)})} \underline{\underline{\Sigma}}^{\star}(\omega) \, \underline{Z}^i \, (\underline{Z}^i)^\dagger \Big|_{\omega = \varepsilon_i}$$

$$\boxed{\underline{Z}^i = \frac{1}{\omega - \mathrm{diag}(\varepsilon^{(0)})} \left[\underline{\underline{\Sigma}}^{\infty} + M^\dagger \frac{1}{\omega - \mathrm{diag}(E)} M \right] \underline{Z}^i \Big|_{\omega = \varepsilon_i}}$$

defining

$$\underline{W}^i = \frac{1}{\omega - \mathrm{diag}(E^{r/q})} M \underline{Z}^i \Big|_{\omega = \varepsilon_i}$$

(vector in the r and q indices

one finds the eigenvalue problem:

$$\varepsilon_i^{+/-} \begin{pmatrix} \underline{Z} \\ \\ \underline{W} \end{pmatrix}^i = \left(\begin{array}{c|c|c} \mathrm{diag}\{\varepsilon^{(0)}\} + \Sigma^{\infty} & M^{(r)} & M^{(q)} \\ \hline M^{(r)\dagger} & \mathrm{diag}\{E^{(r)}\} & \\ \hline M^{(q)\dagger} & & \mathrm{diag}\{E^{(q)}\} \end{array} \right) \begin{pmatrix} \underline{Z}^i \\ \\ \underline{W}^i \end{pmatrix}$$