I EG-X Model - Trying BCS theory

I.1 BCS Theory on the EG-X Model

I.1.1 Self-consistent calculation of the superconducting gaps

This does not really work! I neglect interband pairing at some point, so i throw away 6 out of 9 gap equations I have, also the GF ansatz works with diagonal Matsubara GFs, so I dont think it works here.

Compare [**Bruus_Flensberg_2004**]. Notable here: Multiple bands, and the gaps in each band depend in a complicated manner on the parameters U_α and the orbital Green's functions.

Define normal Green's function:

$$\mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\tau) = -\left\langle T_\tau d_{n\mathbf{k}\uparrow}(\tau) d^\dagger_{n\mathbf{k}\uparrow}(0)\right\rangle \tag{I.1}$$

Anomalous Green's function:

$$\mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\tau) = -\left\langle T_\tau d_{n-\mathbf{k}\downarrow}(\tau) d^\dagger_{n\mathbf{k}\uparrow}(0)\right\rangle \tag{I.2}$$

Equations of motion (Heisenberg equation), follow [**Bruus_Flensberg_2004**]:

$$\partial_\tau \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\tau) = -\delta(\tau) + \left\langle T_\tau \left[d_{n\mathbf{k}\uparrow}, H_{BdG}\right](\tau) d^\dagger_{n\mathbf{k}\uparrow}(0)\right\rangle \tag{I.3}$$

$$\partial_\tau \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\tau) = \left\langle T_\tau \left[d_{n-\mathbf{k}\downarrow}, H_{BdG}\right](\tau) d^\dagger_{n\mathbf{k}\uparrow}(0)\right\rangle \tag{I.4}$$

To calculate the commutators, use the relation (for operators A, B, C):

$$[A, BC] = ABC - BCA = (\{A,B\} - BA)C - B(\{C,A\} - AC) \tag{I.5}$$

$$\begin{aligned}
\left[d^\dagger_{n-\mathbf{k}\downarrow}, H_0\right] &= \sum_{n'\mathbf{k}'\sigma'} \xi_{n'\mathbf{k}'} \left[d^\dagger_{n-\mathbf{k}\downarrow}, d^\dagger_{n'\mathbf{k}'\sigma'} d_{n'\mathbf{k}'\sigma'}\right] && \text{(I.6)}\\
&= \sum_{n'\mathbf{k}'\sigma'} \xi_{n'\mathbf{k}'} \left(\{d^\dagger_{n-\mathbf{k}\downarrow}, d^\dagger_{n'\mathbf{k}'\sigma'}\} - d^\dagger_{n'\mathbf{k}'\sigma'} d^\dagger_{n-\mathbf{k}\downarrow}\right) d_{n'\mathbf{k}'\sigma'} && \text{(I.7)}\\
&- d^\dagger_{n'\mathbf{k}'\sigma'} \left(\{d_{n'\mathbf{k}'\sigma'}, d^\dagger_{n-\mathbf{k}\downarrow}\} - d^\dagger_{n-\mathbf{k}\downarrow} d_{n'\mathbf{k}'\sigma'}\right) && \text{(I.8)}\\
&= \sum_{n'\mathbf{k}'\sigma'} \xi_{n'\mathbf{k}'} \left(-d^\dagger_{n'\mathbf{k}'\sigma'} d^\dagger_{n-\mathbf{k}\downarrow} d_{n'\mathbf{k}'\sigma'} - d^\dagger_{n'\mathbf{k}'\sigma'} \delta_{n'\mathbf{k}'\sigma', n-\mathbf{k}\uparrow} + d^\dagger_{n'\mathbf{k}'\sigma'} d^\dagger_{n-\mathbf{k}\downarrow} d_{n'\mathbf{k}'\sigma'}\right) && \text{(I.9)}\\
&= -\xi_{n\mathbf{k}} d^\dagger_{n\mathbf{k}\uparrow} && \text{(I.10)}
\end{aligned}$$

$$\begin{aligned}
&\left[d_{n-\mathbf{k}\downarrow}, -\sum_{m\mathbf{k}'} \Delta^*_m d_{m-\mathbf{k}'\downarrow} d_{m\mathbf{k}'\uparrow}\right] && \text{(I.11)}\\
&= -\sum_{m\mathbf{k}'} \Delta^*_m \left(\{d_{n-\mathbf{k}\downarrow}, d_{m-\mathbf{k}'\downarrow}\} - d_{m-\mathbf{k}'\downarrow} d_{n-\mathbf{k}\downarrow}\right) d_{m\mathbf{k}'\uparrow} && \text{(I.12)}\\
&- d_{m-\mathbf{k}'\downarrow} \left(\{d_{m\mathbf{k}'\uparrow}, d_{n-\mathbf{k}\downarrow}\} - d_{n-\mathbf{k}\downarrow} d_{m\mathbf{k}'\uparrow}\right) && \text{(I.13)}\\
&= -\sum_{m\mathbf{k}'} \Delta^*_m \left(\delta_{n-\mathbf{k}\downarrow, m-\mathbf{k}'\downarrow} - d_{m-\mathbf{k}'\downarrow} d_{n-\mathbf{k}\downarrow}\right) d_{m\mathbf{k}'\uparrow} + d_{m-\mathbf{k}'\downarrow} d_{n-\mathbf{k}\downarrow} d_{m\mathbf{k}'\uparrow} && \text{(I.14)}\\
&= -\Delta^*_n d_{n\mathbf{k}\uparrow} && \text{(I.15)}
\end{aligned}$$

$$\begin{aligned}
\partial_\tau \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k}, \tau) &= -\xi_{n\mathbf{k}} \langle T_\tau(d^\dagger_{n-\mathbf{k}\downarrow}(\tau) d^\dagger_{n\mathbf{k}\uparrow}(0))\rangle - \Delta^*_n \langle T_\tau(d_{n\mathbf{k}\uparrow}(\tau) d^\dagger_{n\mathbf{k}\uparrow}(0))\rangle && \text{(I.16)}\\
&= \xi_{n\mathbf{k}} \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k}, \tau) + \Delta^*_n \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k}, \tau) && \text{(I.17)}
\end{aligned}$$

Similarly:

$$\begin{aligned}
[d_{n-\mathbf{k}\uparrow}, H_0] &= \sum_{n'\mathbf{k}'\sigma'} \xi_{n'\mathbf{k}'} \left[d^\dagger_{n-\mathbf{k}\downarrow}, d^\dagger_{n'\mathbf{k}'\sigma'} d_{n'\mathbf{k}'\sigma'}\right] && \text{(I.18)}\\
&= \xi_n d^\dagger_{n\mathbf{k}\uparrow} && \text{(I.19)}
\end{aligned}$$

$$\left[d_{n-\mathbf{k}\uparrow}, -\sum_{m\mathbf{k}'} \Delta_m d^\dagger_{m-\mathbf{k}'\uparrow} d^\dagger_{m-\mathbf{k}'\downarrow}\right] \tag{I.20}$$

$$= -\Delta_n d^\dagger_{n-\mathbf{k}\downarrow} \tag{I.21}$$

$$\partial_\tau \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\tau) = -\delta(\tau) + \xi_{n\mathbf{k}} \langle T_\tau d_{n\mathbf{k}\uparrow}(\tau) d^\dagger_{n\mathbf{k}\uparrow}\rangle - \Delta_n \langle T_\tau d_{n-\mathbf{k}\downarrow}(\tau) d^\dagger_{n\mathbf{k}\uparrow}(0)\rangle \tag{I.22}$$

$$= -\delta(\tau) - \xi_{n\mathbf{k}} \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\tau) + \Delta_n \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\tau) \tag{I.23}$$

$$\tag{I.24}$$

All in all:

$$\partial_\tau \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\tau) = -\delta(\tau) - \xi_{n\mathbf{k}} \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\tau) + \Delta_n \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\tau) \tag{I.25}$$

$$\partial_\tau \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\tau) = \xi_{n\mathbf{k}} \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\tau) + \Delta_n^* \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\tau) \tag{I.26}$$

Fourier transform:

$$(-\mathrm{i}\omega_n + \xi_{n\mathbf{k}}) \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\mathrm{i}\omega_n) = -1 + \Delta_n \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\mathrm{i}\omega_n) \tag{I.27}$$

$$(-\mathrm{i}\omega_n - \xi_{n\mathbf{k}}) \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\mathrm{i}\omega_n) = \Delta_n^* \mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k},\mathrm{i}\omega_n) \tag{I.28}$$

This algebraic expression can be easily solved:

$$(-\mathrm{i}\omega_n - \xi_{n\mathbf{k}}) \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\mathrm{i}\omega_n) = \frac{\Delta_n^*}{-\mathrm{i}\omega_n + \xi_{n\mathbf{k}}}(-1 + \Delta_n \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\mathrm{i}\omega_n)) \tag{I.29}$$

$$(-\mathrm{i}\omega_n - \xi_{n\mathbf{k}} - \frac{|\Delta_n|^2}{-\mathrm{i}\omega_n + \xi_{n\mathbf{k}}}) \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\mathrm{i}\omega_n) = \frac{-\Delta_n^*}{-\mathrm{i}\omega_n + \xi_{n\mathbf{k}}} \tag{I.30}$$

$$(\frac{(-\mathrm{i}\omega_n - \xi_{n\mathbf{k}})(-\mathrm{i}\omega_n + \xi_{n\mathbf{k}}) - |\Delta_n|^2}{-\mathrm{i}\omega_n + \xi_{n\mathbf{k}}}) \mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\mathrm{i}\omega_n) = \frac{-\Delta_n^*}{-\mathrm{i}\omega_n + \xi_{n\mathbf{k}}} \tag{I.31}$$

$$\mathcal{F}_{n\downarrow n\uparrow}(\mathbf{k},\mathrm{i}\omega_n) = \frac{-\Delta_n^*}{(-\mathrm{i}\omega_n - \xi_{n\mathbf{k}})(-\mathrm{i}\omega_n + \xi_{n\mathbf{k}}) - |\Delta_n|^2} \tag{I.32}$$

$$= \frac{-\Delta_n^*}{(\mathrm{i}\omega_n)^2 - \xi_{n\mathbf{k}}^2 - |\Delta_n|^2} \tag{I.33}$$

$$= \frac{-\Delta_n^*}{(\mathrm{i}\omega_n)^2 - E_{n\mathbf{k}}} \tag{I.34}$$

$$(-\mathrm{i}\omega_n + \xi_{n\mathbf{k}})\mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k}, \mathrm{i}\omega_n) = -1 + \frac{-|\Delta_n|^2}{(\mathrm{i}\omega_n)^2 - \xi_{n\mathbf{k}}^2 - |\Delta_n|^2} \tag{I.35}$$

$$= \frac{-(\mathrm{i}\omega_n)^2 + \xi_{n\mathbf{k}}^2 + |\Delta_n|^2 - |\Delta_n|^2}{(\mathrm{i}\omega_n)^2 - \xi_{n\mathbf{k}}^2 - |\Delta_n|^2} \tag{I.36}$$

$$= \frac{-(\mathrm{i}\omega_n)^2 + \xi_{n\mathbf{k}}^2}{(\mathrm{i}\omega_n)^2 - \xi_{n\mathbf{k}}^2 - |\Delta_n|^2} \tag{I.37}$$

$$= \frac{(\mathrm{i}\omega_n + \xi_{n\mathbf{k}})(-\mathrm{i}\omega_n + \xi_{n\mathbf{k}})}{(\mathrm{i}\omega_n)^2 - \xi_{n\mathbf{k}}^2 - |\Delta_n|^2} \tag{I.38}$$

$$\mathcal{G}_{n\uparrow n\uparrow}(\mathbf{k}, \mathrm{i}\omega_n) = \frac{\mathrm{i}\omega + \xi_{n\mathbf{k}}}{(\mathrm{i}\omega_n)^2 - \xi_{n\mathbf{k}}^2 - |\Delta_n|^2} \tag{I.39}$$

$$= \frac{\mathrm{i}\omega + \xi_{n\mathbf{k}}}{(\mathrm{i}\omega_n)^2 - E_{n\mathbf{k}}} \tag{I.40}$$

with the energies $E_{n\mathbf{k}} = \pm\sqrt{\xi_{n\mathbf{k}}^2 + |\Delta_n|^2}$.

To calculate the band gap in band n:

$$\Delta_n(\mathbf{k}) = -\sum_{\alpha} [G_{k\uparrow}]^*_{\alpha n} \Delta_\alpha [G_{-k\downarrow}]^*_{\alpha n} \tag{I.41}$$

$$= \sum_{\alpha\mathbf{k}'} U_\alpha [G_{k\uparrow}]^*_{\alpha n} \langle c_{-k'\alpha\downarrow} c_{k'\alpha\uparrow}\rangle [G_{-k\downarrow}]^*_{\alpha n} \tag{I.42}$$

$$= \sum_{\alpha\mathbf{k}'} U_\alpha [G_{k\uparrow}]^*_{\alpha n} [G_{-k\downarrow}]^*_{\alpha n} \sum_m [G_{-k'\downarrow}]_{\alpha m} [G_{k'\uparrow}]_{\alpha m} \langle d_{-k'm\downarrow} d_{k'm\uparrow}\rangle \tag{I.43}$$

Can now use $\mathcal{F}$ and fourier-transform:

$$\langle d_{-k'm\downarrow} d_{k'm\uparrow}\rangle = \mathcal{F}^*_{m\downarrow m\uparrow}(\mathbf{k}', \tau = 0^+) \tag{I.44}$$

$$= \frac{1}{\beta} \sum_{\mathrm{i}\omega_n} e^{-\mathrm{i}\omega_n 0^+} \mathcal{F}^*_{m\downarrow m\uparrow}(\mathbf{k}', \mathrm{i}\omega_n) \tag{I.45}$$

The summation over the Matsubara frequencies can be solved via the Residue theorem (the poles z_0 of $\mathcal{F}$ are the energies $\pm E_{m\mathbf{k}}$):

$$\frac{1}{\beta}\sum_{\mathrm{i}\omega_n} e^{-\mathrm{i}\omega_n 0^+}\mathcal{F}^*_{m\downarrow m\uparrow}(\mathbf{k}', \mathrm{i}\omega_n) \tag{I.46}$$

$$= \sum_{z_0 \mathrm{poles of} \mathcal{F}} e^{-z_0 0^+} n_F(z_0) Res_{z_0}\mathcal{F}^*_{m\downarrow m\uparrow}(\mathbf{k}', z_0) \tag{I.47}$$

$$= e^{-E_{m\mathbf{k}}0^+} n_F(E_{m\mathbf{k}}) Res_{E_{m\mathbf{k}}} \frac{-\Delta_m}{(\mathrm{i}\omega_n)^2 - E_{m\mathbf{k}}} + e^{E_{m\mathbf{k}}0^+} n_F(-E_{m\mathbf{k}}) Res_{-E_{m\mathbf{k}}} \frac{-\Delta_m}{(\mathrm{i}\omega_n)^2 - E_{m\mathbf{k}}} \tag{I.48}$$

with residue:

$$Res_{E_{m\mathbf{k}}} \frac{1}{(\mathrm{i}\omega_n)^2 - z_0^2} = \frac{1}{\partial_z|_{z_0=E_{m\mathbf{k}}}((\mathrm{i}\omega)^2 - z_0^2)} = \frac{1}{2E_{m\mathbf{k}}} \tag{I.49}$$

So we have

$$\langle d_{-k'm\downarrow} d_{k'm\uparrow}\rangle = -\Delta_m \left(\frac{n_F(E_{m\mathbf{k}})}{2E_{m\mathbf{k}}} - \frac{n_F(-E_{m\mathbf{k}})}{2E_{m\mathbf{k}}}\right) \tag{I.50}$$

The n_F term can be written as:

$$n_F(E_{m\mathbf{k}'}) - n_F(-E_{m\mathbf{k}'}) = \frac{1}{e^{\beta E_{m\mathbf{k}'}} + 1} - \frac{1}{e^{-\beta E_{m\mathbf{k}'}} + 1} \tag{I.51}$$

$$= \frac{e^{-\frac{1}{2}\beta E_{m\mathbf{k}'}}}{e^{-\frac{1}{2}\beta E_{m\mathbf{k}'}}} \frac{1}{e^{\beta E_{m\mathbf{k}'}} + 1} - \frac{e^{\frac{1}{2}\beta E_{m\mathbf{k}'}}}{e^{\frac{1}{2}\beta E_{m\mathbf{k}'}}} \frac{1}{e^{-\beta E_{m\mathbf{k}'}} + 1} \tag{I.52}$$

$$= \frac{e^{-\frac{1}{2}\beta E_{m\mathbf{k}'}} - e^{\frac{1}{2}\beta E_{m\mathbf{k}'}}}{e^{\frac{1}{2}\beta E_{m\mathbf{k}'}} + e^{-\frac{1}{2}\beta E_{m\mathbf{k}'}}} \tag{I.53}$$

$$= -\tanh\left(\frac{\beta E_{m\mathbf{k}'}}{2}\right) \tag{I.54}$$

This results in the self-concistency equation for the gap:

$$\Delta_n(\mathbf{k}) = \sum_{\alpha m \mathbf{k}'} U_\alpha [G_{k\uparrow}]^*_{\alpha n} [G_{-k\downarrow}]^*_{\alpha n} [G_{-k'\downarrow}]_{\alpha m} [G_{k'\uparrow}]_{\alpha m} \Delta_m(\mathbf{k}') \frac{\tanh\left(\frac{\beta E_{m\mathbf{k}'}}{2}\right)}{2E_{m\mathbf{k}'}} \tag{I.55}$$

Using time-reversal symmetry $[G_{-\mathbf{k}\downarrow}]^*_{\alpha m} = [G_{\mathbf{k}\uparrow}]_{\alpha m}$ this expression gets a bit simpler:

$$\Delta_n(\mathbf{k}) = \sum_{\alpha m \mathbf{k}'} U_\alpha |[G_{k\uparrow}]_{\alpha n}|^2 |[G_{k'\uparrow}]_{\alpha m}|^2 \Delta_m(\mathbf{k}') \frac{\tanh\left(\frac{\beta E_{m\mathbf{k}'}}{2}\right)}{2E_{m\mathbf{k}'}} \tag{I.56}$$

I.1.2 Computational Implementation

Use scipys `fixed_point` solver to solve the gap equation self-consistently.

Flatten $\Delta_n(\mathbf{k})$ the following way, to put it into the solver ($\mathbf{k}$ discretized in some way):

$$x = \begin{pmatrix} \Re(\Delta_1(\mathbf{k}_1)) \\ \Re(\Delta_1(\mathbf{k}_2)) \\ \vdots \\ \Re(\Delta_2(\mathbf{k}_1)) \\ \vdots \\ \Re(\Delta_3(\mathbf{k}_1)) \\ \vdots \\ \Im(\Delta_1(\mathbf{k}_1)) \\ \vdots \\ \Im(\Delta_2(\mathbf{k}_1)) \\ \vdots \\ \Im(\Delta_3(\mathbf{k}_1)) \\ \vdots \end{pmatrix} \tag{I.57}$$

so that accessing a certain element takes the form:

$$\Re\Delta_n(\mathbf{k}) = x\left[\mathrm{index}(\mathbf{k}) + \frac{\mathrm{len}(x)\cdot n}{6}\right] \tag{I.58}$$

$$\Im\Delta_n(\mathbf{k}) = x\left[\mathrm{index}(\mathbf{k}) + \frac{\mathrm{len}(x)\cdot n}{6} + \frac{1}{2}\mathrm{len}(x)\right] \tag{I.59}$$