1 Mean-field approximation

We often use a mean-field approximation to decouple interactions. In the process, we get a self-consistent equation as a constraint. A famous example that uses mean-field theory is BCS superconductivity. Consider the Hamiltonian

$$H = \sum_{i,j} t_{ij} c_i^\dagger c_j + \frac{1}{2} \sum_{i,j,k,l} V_{ijkl} c_i^\dagger c_j^\dagger c_k c_l \tag{1}$$

We write $c_i^\dagger c_j^\dagger$ and $c_k c_l$ as fluctuations from the mean.

$$c_i^\dagger c_j^\dagger = \left(c_i^\dagger c_j^\dagger - \langle c_i^\dagger c_j^\dagger\rangle\right) + \langle c_i^\dagger c_j^\dagger\rangle \tag{2}$$

$$c_k c_l = \left(c_k c_l - \langle c_k c_l\rangle\right) + \langle c_k c_l\rangle \tag{3}$$

The Hamiltonian becomes

$$\begin{aligned} H =& \sum_{i,j} t_{ij} c_i^\dagger c_j + \frac{1}{2} \sum_{i,j,k,l} V_{ijkl} \Big(\left(c_i^\dagger c_j^\dagger - \langle c_i^\dagger c_j^\dagger\rangle\right) + \langle c_i^\dagger c_j^\dagger\rangle \Big) \Big((c_k c_l - \langle c_k c_l\rangle) + \langle c_k c_l\rangle \Big) & (4) \\ =& \sum_{i,j} t_{ij} c_i^\dagger c_j + \frac{1}{2} \sum_{i,j,k,l} V_{ijkl} \left(c_i^\dagger c_j^\dagger \langle c_k c_l\rangle + \langle c_i^\dagger c_j^\dagger\rangle c_k c_l - \langle c_i^\dagger c_j^\dagger\rangle \langle c_k c_l\rangle + \left(c_i^\dagger c_j^\dagger - \langle c_i^\dagger c_j^\dagger\rangle\right)\left(c_k c_l - \langle c_k c_l\rangle\right) \right) & (5) \end{aligned}$$

Assuming that the fluctuations are small, we can drop the term $\left(c_i^\dagger c_j^\dagger - \langle c_i^\dagger c_j^\dagger\rangle\right)\left(c_k c_l - \langle c_k c_l\rangle\right)$. Since the Hamiltonian is Hermitian, we get $t_{ij} = t_{ji}^*$ and $V_{ijkl} = V_{lkji}^*$. We define the order parameter,

$$\Delta_{ij} = \sum_{k,l} V_{ijkl} \langle c_k c_l\rangle \tag{6}$$

$$\Delta_{lk}^* = \sum_{i,j} V_{lkji}^* \langle c_i^\dagger c_j^\dagger\rangle = \sum_{i,j} V_{ijkl} \langle c_i^\dagger c_j^\dagger\rangle \tag{7}$$

The Hamiltonian becomes

$$H = \sum_{i,j} t_{ij} c_i^\dagger c_j + \frac{1}{2} \sum_{i,j} \left(\Delta_{ij} c_i^\dagger c_j^\dagger + \Delta_{ji}^* c_i c_j \right) - \frac{1}{2} \sum_{i,j,k,l} V_{ijkl} \langle c_i^\dagger c_j^\dagger\rangle \langle c_k c_l\rangle \tag{8}$$

We split the first term as

$$\begin{aligned} \sum_{i,j} t_{ij} c_i^\dagger c_j =& \frac{1}{2} \sum_{i,j} \left(t_{ij} c_i^\dagger c_j + t_{ij} c_i^\dagger c_j \right) & (9) \\ =& \frac{1}{2} \sum_{i,j} \left(t_{ij} c_i^\dagger c_j + t_{ij} \left(\delta_{ij} - c_j c_i^\dagger \right) \right) & (10) \\ =& \frac{1}{2} \sum_{i,j} \left(t_{ij} c_i^\dagger c_j - t_{ji} c_i c_j^\dagger \right) + \frac{1}{2} \mathrm{Tr}(t) & (11) \end{aligned}$$

to get

$$H = \frac{1}{2} \sum_{i,j} \left(t_{ij} c_i^\dagger c_j - t_{ji} c_i c_j^\dagger + \Delta_{ij} c_i^\dagger c_j^\dagger + \Delta_{ji}^* c_i c_j \right) + \frac{1}{2} \mathrm{Tr}(t) - \frac{1}{2} \sum_{i,j,k,l} V_{ijkl} \langle c_i^\dagger c_j^\dagger\rangle \langle c_k c_l\rangle \tag{12}$$

Let $E_0 = \frac{1}{2}\mathrm{Tr}(t) - \frac{1}{2}\sum_{i,j,k,l} V_{ijkl} \langle c_i^\dagger c_j^\dagger\rangle \langle c_k c_l\rangle$. We get the mean-field Hamiltonian

$$H = \frac{1}{2} \sum_{i,j} \begin{pmatrix} c_i^\dagger & c_i \end{pmatrix} \begin{pmatrix} t_{ij} & \Delta_{ij} \\ \Delta_{ji}^* & -t_{ji} \end{pmatrix} \begin{pmatrix} c_j \\ c_j^\dagger \end{pmatrix} + E_0 \tag{13}$$

and the self-consistent equation

$$\Delta_{ij} = \sum_{k,l} V_{ijkl} \langle c_k c_l\rangle \tag{14}$$

1.1 Self-consistent equation as a fixed point

The expectation value, $\langle c_k c_l \rangle$, depends on the order parameter, Δ_{ij}, that we input into the mean-field Hamiltonian. We construct a vector, $\boldsymbol{x}$, using the order parameter.

$$\boldsymbol{x} = \begin{pmatrix} \Delta_{11} \\ \vdots \\ \Delta_{NN} \end{pmatrix} \tag{15}$$

The self-consistent equation can be represented as

$$\boldsymbol{x} = \boldsymbol{f}(\boldsymbol{x}) \tag{16}$$

where the function $\boldsymbol{f}$ calculates the RHS of Eq. (14). Therefore, the self-consistent solution is the fixed point of the function $\boldsymbol{f}$. Alternatively, we can define the function $\boldsymbol{F}(\boldsymbol{x}) = \boldsymbol{f}(\boldsymbol{x}) - \boldsymbol{x}$.

$$0 = \boldsymbol{f}(\boldsymbol{x}) - \boldsymbol{x} = \boldsymbol{F}(\boldsymbol{x}) \tag{17}$$

The self-consistent solution is the root of the function $\boldsymbol{F}$.

2 Iterative methods for root finding

These notes are based on Modified Broyden's method for accelerating convergence in self-consistent calculations. Let $|x\rangle$ be the input vector and $|f\rangle$ be the output vector in the self-consistent equation. We define the residual vector $|F\rangle = |f\rangle - |x\rangle$. To find the self-consistent solution, we want to minimize the norm of $|F\rangle$.

2.1 Linear mixing

The simplest method is to iteratively calculate the self-consistent equation and use a linear combination of input and output vectors.

$$|x^{(m+1)}\rangle = (1-\alpha)\,|x^{(m)}\rangle + \alpha\,|f^{(m)}\rangle = |x^{(m)}\rangle + \alpha\,|F^{(m)}\rangle \tag{18}$$

where $\alpha \in (0, 1]$ is an empirically chosen parameter. We can see how this iterative procedure mixes the output vectors.

$$|x^{(1)}\rangle = (1-\alpha)\,|x^{(0)}\rangle + \alpha\,|f^{(0)}\rangle \tag{19}$$
$$|x^{(2)}\rangle = (1-\alpha)^2\,|x^{(0)}\rangle + (1-\alpha)\alpha\,|f^{(0)}\rangle + \alpha\,|f^{(1)}\rangle \tag{20}$$
$$|x^{(3)}\rangle = (1-\alpha)^3\,|x^{(0)}\rangle + (1-\alpha)^2\alpha\,|f^{(0)}\rangle + (1-\alpha)\alpha\,|f^{(1)}\rangle + \alpha\,|f^{(2)}\rangle \tag{21}$$
$$\vdots \tag{22}$$
$$|x^{(m)}\rangle = (1-\alpha)^m\,|x^{(0)}\rangle + \alpha \sum_{n=0}^{m-1} (1-\alpha)^{m-n-1}\,|f^{(n)}\rangle \tag{23}$$

If α is small, then we can approximate $(1-\alpha) \approx e^{-\alpha}$.

$$|x^{(m)}\rangle = e^{-m\alpha}\,|x^{(0)}\rangle + \alpha \sum_{n=0}^{m-1} e^{-(m-n-1)\alpha}\,|f^{(n)}\rangle \tag{24}$$

I.e., the input vector is a sum of output vectors weighted by an exponential decay.

2.2 Anderson's mixing

We extend linear mixing by adding another layer of mixing. Assuming that a linear interpolation of the input results in a linear interpolation of the output, we get

$$
\begin{aligned}
|\bar{x}^{(m)}\rangle =& (1-\beta)\,|x^{(m)}\rangle + \beta\,|x^{(m-1)}\rangle && (25)\\
|\bar{f}^{(m)}\rangle =& (1-\beta)\,|f^{(m)}\rangle + \beta\,|f^{(m-1)}\rangle && (26)\\
|\bar{F}^{(m)}\rangle =& |\bar{f}^{(m)}\rangle - |\bar{x}^{(m)}\rangle && (27)\\
=& (1-\beta)\,|F^{(m)}\rangle + \beta\,|F^{(m-1)}\rangle && (28)\\
& && (29)
\end{aligned}
$$

Let $|\Delta F^{(m)}\rangle = |F^{(m)}\rangle - |F^{(m-1)}\rangle$. We get

$$
|\bar{F}^{(m)}\rangle = |F^{(m)}\rangle - \beta\,|\Delta F^{(m)}\rangle \tag{30}
$$

We can find an optimal β by solving $\partial_\beta \langle \bar{F}^{(m)}|\bar{F}^{(m)}\rangle = 0$.

$$
\begin{aligned}
\partial_\beta \langle \bar{F}^{(m)}|\bar{F}^{(m)}\rangle =& \partial_\beta \left(\langle F^{(m)}| - \beta\,\langle \Delta F^{(m)}|\right)\left(|F^{(m)}\rangle - \beta\,|\Delta F^{(m)}\rangle\right) && (31)\\
=& 2\beta\,\langle \Delta F^{(m)}|\Delta F^{(m)}\rangle - \langle \Delta F^{(m)}|F^{(m)}\rangle - \langle F^{(m)}|\Delta F^{(m)}\rangle && (32)
\end{aligned}
$$

$$
\begin{aligned}
\beta =& \frac{\langle \Delta F^{(m)}|F^{(m)}\rangle + \langle F^{(m)}|\Delta F^{(m)}\rangle}{2\,\langle \Delta F^{(m)}|\Delta F^{(m)}\rangle} && (33)\\
=& \frac{\mathrm{Re}(\langle F^{(m)}|\Delta F^{(m)}\rangle)}{\langle \Delta F^{(m)}|\Delta F^{(m)}\rangle} && (34)
\end{aligned}
$$

The second derivative is strictly positive, so this β minimizes the norm. We then mix the mixed input and output vectors.

$$
|x^{(m+1)}\rangle = (1-\alpha)\,|\bar{x}^{(m)}\rangle + \alpha\,|\bar{f}^{(m)}\rangle = |\bar{x}^{(m)}\rangle + \alpha\,|\bar{F}^{(m)}\rangle \tag{35}
$$

Again, $\alpha \in (0,1]$ is an empirically chosen parameter.

2.3 Broyden's method

Broyden's method is the multidimensional extension of Newton's method. For the scalar case, we can expand F using a taylor expansion.

$$
0 = F(x) \approx F(x_0) + F'(x_0)(x - x_0) \tag{36}
$$

$$
x \approx x_0 - \frac{F(x_0)}{F'(x_0)} \tag{37}
$$

Approximating the derivative using finite-diferences, we get

$$
\begin{aligned}
F'(x_n) \approx& \frac{F(x_n) - F(x_{n-1})}{x_n - x_{n-1}} && (38)\\
x_{n+1} =& x_n - \frac{F(x_n)}{F'(x_n)} && (39)
\end{aligned}
$$

For the multidimensional case, we use the Jacobian to expand $|F\rangle$.

$$
\begin{aligned}
0 = |F\rangle =& |F^{(m)}\rangle + J^{(m)}\left(|x\rangle - |x^{(m)}\rangle\right) && (40)\\
|x\rangle =& |x^{(m)}\rangle - \left(J^{(m)}\right)^{-1} |F^{(m)}\rangle && (41)
\end{aligned}
$$

Let

$$|\Delta x^{(m)}\rangle = |x^{(m)}\rangle - |x^{(m-1)}\rangle \tag{42}$$
$$|\Delta F^{(m)}\rangle = |F^{(m)}\rangle - |F^{(m-1)}\rangle \tag{43}$$

Using finite differences, the Jacobian is approximated as

$$J^{(m)}|\Delta x^{(m)}\rangle = |\Delta F^{(m)}\rangle \tag{44}$$

We can update the estimate of the Jacobian using

$$J^{(m)} = J^{(m-1)} + \frac{|\Delta F^{(m)}\rangle - J^{(m-1)}|\Delta x^{(m)}\rangle}{\langle \Delta x^{(m)}|\Delta x^{(m)}\rangle}\langle \Delta x^{(m)}| \tag{45}$$

We can see that this improves the estimate by plugging in Eq. (45) to Eq. (44).

$$J^{(m)}|\Delta x^{(m)}\rangle = J^{(m-1)}|\Delta x^{(m)}\rangle + \frac{|\Delta F^{(m)}\rangle - J^{(m-1)}|\Delta x^{(m)}\rangle}{\langle \Delta x^{(m)}|\Delta x^{(m)}\rangle}\langle \Delta x^{(m)}|\Delta x^{(m)}\rangle \tag{46}$$
$$= J^{(m-1)}|\Delta x^{(m)}\rangle + |\Delta F^{(m)}\rangle - J^{(m-1)}|\Delta x^{(m)}\rangle \tag{47}$$
$$= |\Delta F^{(m)}\rangle \tag{48}$$

Using the Sherman-Morrison formula, we can directly update the inverse Jacobian.

$$\left(J + |u\rangle\langle v|\right)^{-1} = J^{-1} - \frac{J^{-1}|u\rangle\langle v|J^{-1}}{1 + \langle v|J^{-1}|u\rangle} \tag{49}$$

Let $G^{(m)} = -\left(J^{(m)}\right)^{-1}$.

$$G^{(m+1)} = G^{(m)} - \frac{|\Delta x^{(m)}\rangle + G^{(m)}|\Delta F^{(m)}\rangle}{\langle \Delta x^{(m)}|G^{(m)}|\Delta F^{(m)}\rangle}\langle \Delta x^{(m)}|G^{(m)} \tag{50}$$

We get the update equations

$$|x^{(m+1)}\rangle = |x^{(m)}\rangle + G^{(m)}|F^{(m)}\rangle \tag{51}$$
$$G^{(m)} = G^{(m-1)} - \frac{|\Delta x^{(m)}\rangle + G^{(m-1)}|\Delta F^{(m)}\rangle}{\langle \Delta x^{(m)}|G^{(m-1)}|\Delta F^{(m)}\rangle}\langle \Delta x^{(m)}|G^{(m-1)} \tag{52}$$

This is called Broyden's "good" method and minimizes the Frobenius norm $||J^{(m)} - J^{(m-1)}||$.

2.3.1 Broyden's "bad" method

Previously, we approximated the Jacobian using finite differences as $J^{(m)}|\Delta x^{(m)}\rangle = |\Delta F^{(m)}\rangle$. Alternatively, we can approximate the inverse Jacobian as $|\Delta x^{(m)}\rangle = -G^{(m)}|\Delta F^{(m)}\rangle$. The update equation becomes

$$G^{(m)} = G^{(m-1)} - \frac{|\Delta x^{(m)}\rangle + G^{(m-1)}|\Delta F^{(m)}\rangle}{\langle \Delta F^{(m)}|\Delta F^{(m)}\rangle}\langle \Delta F^{(m)}| \tag{53}$$

This method minimizes the Frobenius norm $||G^{(m)} - G^{(m-1)}||$. Usually, storing the full inverse Jacobian is prohibitive. Let

$$|Z^{(m)}\rangle = \frac{|\Delta x^{(m)}\rangle + G^{(m-1)}|\Delta F^{(m)}\rangle}{\langle \Delta F^{(m)}|\Delta F^{(m)}\rangle} \tag{54}$$

Then $G^{(m)} = G^{(m-1)} - |Z^{(m)}\rangle \langle \Delta F^{(m)}|$. After iterating, we get

$$G^{(1)} = G^{(0)} - |Z^{(1)}\rangle \langle \Delta F^{(1)}| \tag{55}$$

$$G^{(2)} = G^{(0)} - |Z^{(1)}\rangle \langle \Delta F^{(1)}| - |Z^{(2)}\rangle \langle \Delta F^{(2)}| \tag{56}$$

$$G^{(3)} = G^{(0)} - |Z^{(1)}\rangle \langle \Delta F^{(1)}| - |Z^{(2)}\rangle \langle \Delta F^{(2)}| - |Z^{(3)}\rangle \langle \Delta F^{(3)}| \tag{57}$$

$$\vdots \tag{58}$$

$$G^{(m)} = G^{(0)} - \sum_{n=1}^{m} |Z^{(n)}\rangle \langle \Delta F^{(n)}| \tag{59}$$

In this representation, we only have to store $2m$ vectors and $G^{(0)}$ to get $G^{(m)}$. Plugging this back into the definition of $|Z^{(m)}\rangle$,

$$|Z^{(m)}\rangle = \frac{|\Delta x^{(m)}\rangle + G^{(0)} |\Delta F^{(m)}\rangle}{\langle \Delta F^{(m)} | \Delta F^{(m)}\rangle} - \sum_{n=1}^{m-1} |Z^{(n)}\rangle \frac{\langle \Delta F^{(n)} | \Delta F^{(m)}\rangle}{\langle \Delta F^{(m)} | \Delta F^{(m)}\rangle} \tag{60}$$

The update equation become

$$|x^{(m+1)}\rangle = |x^{(m)}\rangle + G^{(m)} |F^{(m)}\rangle \tag{61}$$

$$= |x^{(m)}\rangle + G^{(0)} |F^{(m)}\rangle - \sum_{n=1}^{m} |Z^{(n)}\rangle \langle \Delta F^{(n)} | F^{(m)}\rangle \tag{62}$$

A good initial guess for the inverse Jacobian is

$$G^{(0)} = \alpha I \tag{63}$$

$$\alpha = \frac{1}{2} \frac{\max(\sqrt{\langle x^{(0)} | x^{(0)}\rangle}, 1)}{\sqrt{\langle F^{(0)} | F^{(0)}\rangle}} \tag{64}$$

2.4 Modified Broyden's method

This method is similar to Broyden's "bad" method but adds a weight to each iteration. The update equation is

$$|x^{(m+1)}\rangle = |x^{(m)}\rangle + G^{(0)} |F^{(m)}\rangle - \sum_{n=1}^{m} w_n \gamma_n^{(m)} |u^{(m)}\rangle \tag{65}$$

where

$$|\Delta \bar{x}^{(m)}\rangle = \frac{|x^{(m)}\rangle - |x^{(m-1)}\rangle}{|\,|F^{(m)}\rangle - |F^{(m-1)}\rangle\,|} \tag{66}$$

$$|\Delta \bar{F}^{(m)}\rangle = \frac{|F^{(m)}\rangle - |F^{(m-1)}\rangle}{|\,|F^{(m)}\rangle - |F^{(m-1)}\rangle\,|} \tag{67}$$

$$|u^{(m)}\rangle = |\Delta \bar{x}^{(m)}\rangle + G^{(0)} |\Delta \bar{F}^{(m)}\rangle \tag{68}$$

The coefficients $\gamma_n^{(m)}$ are calculated by solving the system of equations

$$A\boldsymbol{\gamma}^{(m)} = \boldsymbol{b}^{(m)} \tag{69}$$

where

$$A_{ij} = w_0^2 \delta_{ij} + w_i w_j \langle \Delta \bar{F}^{(i)} | \Delta \bar{F}^{(j)}\rangle \qquad b_n^{(m)} = w_n \langle \Delta \bar{F}^{(n)} | F^{(m)}\rangle \tag{70}$$

A good choice for the weights is

$$w_0 = 0.01 \qquad w_n = \langle F^{(n)} | F^{(n)}\rangle^{-1/2} \tag{71}$$

This gives a higher weight to iterations that are closer to convergence.

2.4.1 Sherman-Morrison formula

$$X = J + |u\rangle \langle v| \tag{72}$$

$$Y = J^{-1} - \frac{J^{-1} |u\rangle \langle v| J^{-1}}{1 + \langle v|J^{-1}|u\rangle} \tag{73}$$

$$XY = (J + |u\rangle \langle v|) \left(J^{-1} - \frac{J^{-1} |u\rangle \langle v| J^{-1}}{1 + \langle v|J^{-1}|u\rangle} \right) \tag{74}$$

$$= 1 + |u\rangle \langle v| J^{-1} - \frac{|u\rangle \langle v| J^{-1} + |u\rangle \langle v| J^{-1} |u\rangle \langle v| J^{-1}}{1 + \langle v|J^{-1}|u\rangle} \tag{75}$$

$$= 1 + |u\rangle \langle v| J^{-1} - |u\rangle \frac{1 + \langle v| J^{-1} |u\rangle}{1 + \langle v|J^{-1}|u\rangle} \langle v| J^{-1} \tag{76}$$

$$= 1 + |u\rangle \langle v| J^{-1} - |u\rangle \langle v| J^{-1} \tag{77}$$

$$= 1 \tag{78}$$

Similarly, $YX = 1$. Therefore, $(X)^{-1} = Y$, or

$$(J + |u\rangle \langle v|)^{-1} = J^{-1} - \frac{J^{-1} |u\rangle \langle v| J^{-1}}{1 + \langle v|J^{-1}|u\rangle} \tag{79}$$