Solution of Hartree-Fock equations

1. Take the initial single-particle hamiltonian $h_{\mu\nu}$
2. Find eigenvectors of h:

$$\sum_{\nu} h_{\mu\nu} x_{\nu}^{(\lambda)} = \epsilon_{\lambda} x_{\mu}^{(\lambda)}$$

3. Take the A lowest-energy eigenvectors

$$x_{\mu}^{(h)}, \quad h = 1, \ldots, A$$

4. The largest s.p. energy is the Fermi level
5. Find the density matrix

$$\rho_{\mu\nu} = \sum_{h=1}^{A} x_{\mu}^{(h)} x_{\nu}^{(h)*}$$

Note that the HF equation $[h,\rho]=0$ is met by construction

6. Calculate $\Gamma(\rho)$
7. Go back to 2.

Hartree Fock stability condition

HF minimum should correspond to the positive second derivative of the energy.

$$\rho = \rho^{(0)} + \rho^{(1)} + \rho^{(2)} + \ldots \quad \left(\rho^{(0)} >> \rho^{(1)} >> \rho^{(2)} >> \ldots\right)$$

$$\rho^2 = \rho \quad \Longrightarrow \quad \boxed{\begin{aligned} \rho^{(1)} &= \left[\left[\rho^{(1)}, \rho^{(0)}\right], \rho^{(0)}\right] \\ \rho^{(2)} &= \left[\left[\rho^{(2)}, \rho^{(0)}\right], \rho^{(0)}\right] + \frac{1}{2}\left[\left[\rho^{(1)}, \rho^{(0)}\right], \rho^{(1)}\right] \end{aligned}}$$

This implies that independent variations are only in the ph channel (pp and hh matrix elements of $\rho^{(1)}$ and $\rho^{(2)}$ vanish)

$$E = E^{(0)} + E^{(1)} + E^{(2)} + \ldots$$

$$E^{(0)} = \mathrm{Tr}\left(T\rho^{(0)}\right) + \frac{1}{2}\mathrm{Tr}\left(\Gamma^{(0)}\rho^{(0)}\right)$$

$$E^{(1)} = \mathrm{Tr}\left(\left[h^{(0)}, \rho^{(0)}\right]\left[\rho^{(0)}, \rho^{(1)}\right]\right)$$

$$E^{(2)} = \mathrm{Tr}\left(\left[h^{(0)}, \rho^{(0)}\right]\left[\rho^{(0)}, \rho^{(21)}\right]\right)$$

$$+ \frac{1}{2}\mathrm{Tr}\left(\rho^{(1)}\left[\left[h^{(0)}, \rho^{(1)}\right] + \left[\Gamma^{(1)}, \rho^{(0)}\right], \rho^{(0)}\right]\right)$$

$$E^{(1)} = 0$$

$$E^{(2)} = \frac{1}{2}\left(\rho^{(1)}\middle|M^{(0)}\middle|\rho^{(1)}\right) > 0$$

$$M^{(0)}\rho^{(1)} = \left[\left[h^{(0)}, \rho^{(1)}\right] + \left[\Gamma^{(1)}, \rho^{(0)}\right], \rho^{(0)}\right]$$

The HF stability matrix (must be positively defined)

Constrained Hartree-Fock

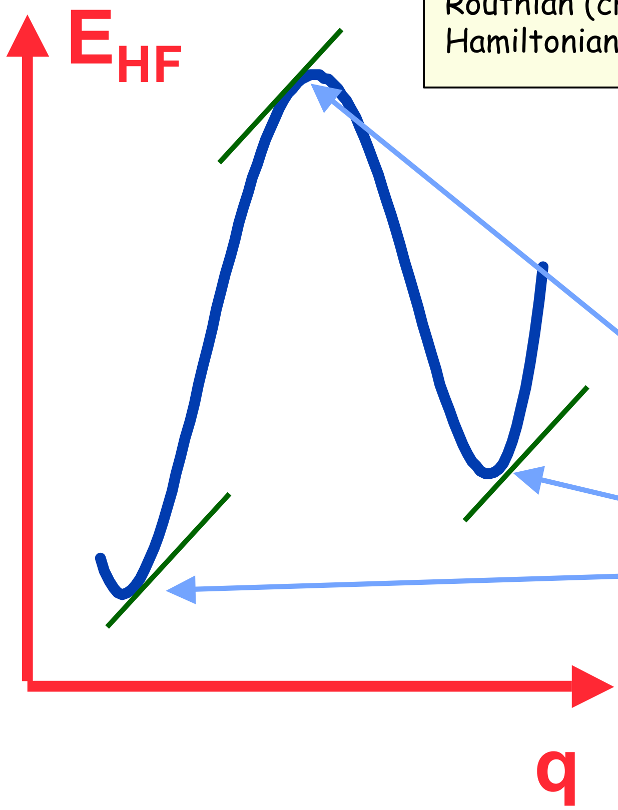
Often, we are interested not only in the local HF minima but also in the whole potential energy surface (PES)

$$\delta\left\langle \Psi \middle| \hat{H} \middle| \Psi \right\rangle = 0 \quad \text{at a fixed value of } q = \left\langle \Psi \middle| \hat{Q} \middle| \Psi \right\rangle$$

Routhian (cranked Hamiltonian)

$$\hat{H}' = \hat{H} - \lambda \hat{Q}$$

$$\delta\left\langle \Psi \middle| \hat{H}' \middle| \Psi \right\rangle = 0$$



$$\lambda = \frac{dE}{dq}$$

Collective coordinate

- Several ways of solving the CHF equations (linear constraint, quadratic constraint, gradient method)
- Usually: many-dimensional surfaces
- Static picture - fluctuations are not included!

Self-consistent HF symmetries

$$\left[\hat{H}, S\right] = 0 \Rightarrow S\Gamma\left[\hat{\rho}\right]S^{+} = \Gamma\left[S\hat{\rho}S^{+}\right]$$

$$\Rightarrow Sh\left[\hat{\rho}\right]S^{+} = h\left[S\hat{\rho}S^{+}\right]$$

If $\hat{\rho}_{(i)}$ has a certain symmetry then $\hat{\rho}_{(i+1)}$ has the same symmetry.

- If a certain symmetry for the solution is expected, one can start with an initial density which has this symmetry
- If one starts with a certain symmetry, one will always stay within this symmetry (if the deepest minimum is deformed, one will never get to it starting with a spherically symmetric density matrix)
- The above discussion can be generalized to density dependent interactions satisfying the condition:

$$SV\left[\hat{\rho}\right]S^{-1} = V\left[S\hat{\rho}S^{-1}\right]$$

If we have a solution with a (spontaneously) broken symmetry *S*...

$$S\hat{\rho}S^{+} = \hat{\rho}_1 \neq \hat{\rho}$$

$$\Downarrow$$

$$h(\hat{\rho}_1) = Sh(\hat{\rho})S^{+}$$

$$\Downarrow$$

$$\left[h(\hat{\rho}_1), \hat{\rho}_1\right] = S\left[h(\hat{\rho}), \hat{\rho}\right]S^{+} = 0$$

...then every transformed (rotated) state is also a solution of the HF equations!

Goldstone Theorem

$$\hat{\rho}_1 = S\hat{\rho}S^{+} \quad \Rightarrow \quad M^{(0)}\hat{\rho}_1 = 0$$

If a symmetry is broken, there appears a zero-energy mode (Goldstone boson!)