Direct calculation of a self-consistent one-body Green's function

The one body Green's functions is used to understand and predict photoemission and inverse photoemission spectra. The Green's functions can be obtained by solving the Dyson equation which contains an effective potential, the self-energy. The self-energy is usually written as a functional of the self-consistent Green's functions. This leads to a complicated non-linear problem, that in practice is solved either perturbatively or self-consistently. However on the one hand, the perturbative solution, obtained with standard approximations to the self-energy, cannot describe the multiple plasmon satellites in the photoemission spectrum. And on the other hand, the self-consistent calculations are very expensive in computing time, do not always converge, and can converge to wrong values [1]. In this work we investigate the possibility to solve the Dyson equation directly. To this end, we studied GW approximation of the self energy, in a model where all the quantities are diagonal in the same basis. We thus obtained an explicit expression for the Green's function. The good news is that solution correctly describes the position of the multiple plasmon satellites. The bad news is that part of the spectrum has negative values. Thus, the next step of this work will be to explain this artefacts, and to try to go beyond the diagonal approximation.