Time-dependent Hartree-Fock Approximation for Magnetoroton Spectrum above Composite-Fermion Ground State

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In this note, we will give a quick review on the general setup of Hartree-Fock methods, particularly the iterative *Roothaan equation*. We will work in a second-quantized language.

CONTENTS

I. HARTREE-FOCK

The general setup of Hartre-Fock mean-field approximation is that, given N *nearly non-interacting* fermions, the many-body effect of the N-particle wave function will be dominated by the single-particle fermionic exchange effect. Thus Slater determinant of N *orthonormal* Hartree-Fock single-particle wave functions turns out to be a good approximation for the many-particle wave functions

$$\Psi(\boldsymbol{r}_1,\cdots,\boldsymbol{r}_N)=\frac{1}{\sqrt{N!}}\begin{vmatrix}\psi_1(\boldsymbol{r}_1) & \cdots & \psi_N(\boldsymbol{r}_1)\\ \vdots & \ddots & \vdots\\ \psi_1(\boldsymbol{r}_N) & \cdots & \psi_N(\boldsymbol{r}_N)\end{vmatrix},\quad \text{or } |\Psi_{HF}\rangle\equiv\prod_{\alpha=1}^{N}C_\alpha^\dagger|0\rangle$$

with α runs over *both* momentum, spin and internal discrete indices like band/valley/orbital etc.

Here HF single-particles are truely occupied, as is constructed in the second quantized form. In terms of the *single-particle density operator* $\hat{\rho}=\sum_\alpha|\psi_\alpha\rangle\langle\psi_\alpha|$, we have the single-particle density matrix $P_{\alpha\beta}\equiv\langle\psi_\alpha|\hat{\rho}|\psi_\beta\rangle=\delta_{\alpha\beta}$ in these HF single-particle states. In fact, clearly such density matrix is nothing but the two-point correlator

$$P_{\alpha\beta}\equiv\langle\Psi_{HF}|C_\beta^\dagger C_\alpha|\Psi_{HF}\rangle.$$

The order of subsctipt is important here! Inserting the identity operator resolution within the Fock space $\mathbb{1}=\sum_{\alpha_1}|\alpha_1\rangle\langle\alpha_1|+\sum_{\alpha_1\alpha_2}|\alpha_1\alpha_2\rangle\langle\alpha_1\alpha_2|+\cdots$ to the middle of f-bilinear and noting that only $(N-1)$-particle states contribute, we get

$$\begin{aligned}P_{\alpha\beta}&=\sum_{\alpha_1,\cdots,\alpha_{N-1}}\langle\Psi_{HF}|C_\beta^\dagger|\alpha_1,\cdots,\alpha_{N-1}\rangle\langle\alpha_1,\cdots,\alpha_{N-1}|C_\alpha|\Psi_{HF}\rangle\\&=\sum_{\alpha_1,\cdots,\alpha_{N-1}}\langle\alpha,\alpha_1,\cdots,\alpha_{N-1}|\Psi_{HF}\rangle\langle\Psi_{HF}|\beta,\alpha_1,\cdots,\alpha_{N-1}\rangle\equiv\langle\alpha|\mathrm{tr}_{N-1}\{\hat{\rho}^N\}|\beta\rangle\end{aligned}$$

which is exactly the definition of single-particle density matrix — by tracing out the $(N-1)$-particle states for the many-body (but *pure state*) density matrix $\hat{\rho}^N\equiv|\Psi_{HF}\rangle\langle\Psi_{HF}|$.

The left question is, *what are these N Hartree-Fock single-particle states look like?*

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A. Roothaan Equation

Suppose we have a set of M *known* states $\{\phi_i\}$ in hand ($M \geq N$ and hereafter we suppose they are orthonormal), we can always try to expand the above N HF single-particle states with these basis — as long as $\{\phi_i\}$ is complete. However, usually completeness means *countable infinite* number of basis. Due to computation limitation, in practice we will always truncate such expansion with *finite* M basis

$$|\psi_\alpha\rangle = \sum_{i=1}^{M} d_{i\alpha}|\phi_i\rangle, \quad \text{or } C_\alpha^\dagger = \sum_i d_{i\alpha} f_i^\dagger.$$

Here we transpoes the expansion matrix by default for further convenience. The density matrix in the new basis can be immediately obtained

$$P_{ij} \equiv \langle\phi_i|\hat{\rho}|\phi_j\rangle = \sum_{\alpha\beta}\langle\phi_i|\psi_\alpha\rangle\langle\psi_\alpha|\hat{\rho}|\psi_\beta\rangle\langle\psi_\beta|\phi_j\rangle = \sum_{\alpha,\text{filled}} d_{j\alpha}^* d_{i\alpha}.$$

This can also be directly obtained from in the second-quantized language

$$P_{ij} \equiv \langle\Psi_{HF}|f_j^\dagger f_i|\Psi_{HF}\rangle = \cdots.$$

The left task is to find the optimal choice of the expansion coefficients $d_{i\alpha}$ in terms of the *variation principle*.

1. *Mean-field Hamiltonian and Energy*

For most physical model, translation symmetry is present and momentum is a good quantum number. From now on we will explicit separate out the momentum-dependence so that the full quadratic Hamiltonian in terms of the creation/annihilation operators in hand reads

$$\hat{H} = \sum_{\boldsymbol{k},ij} f_{\boldsymbol{k},\alpha}^\dagger [\kappa(\boldsymbol{k})]_{ij} f_{\boldsymbol{k},j} + \sum_{\boldsymbol{q}} \hat{\rho}_e(\boldsymbol{q}) V_q \hat{\rho}_e(-\boldsymbol{q}), \quad \text{with charge density } \hat{\rho}_e(\boldsymbol{q}) \equiv \sum_{\boldsymbol{k},ij} f_{\boldsymbol{k},i}^\dagger [\varrho_{\boldsymbol{q}}(\boldsymbol{k})]_{ij} f_{\boldsymbol{k}+\boldsymbol{q},j}. \tag{1}$$

Hermicity of the Coulomb interaction gives an extra constraint on the matrix coefficient of the charge density operator

$$[\varrho_{\boldsymbol{q}}(\boldsymbol{k})]^\dagger \equiv [\varrho_{-\boldsymbol{q}}([\boldsymbol{k}+\boldsymbol{q}])], \tag{2}$$

where $[\cdots]$ in the argument means modulo with the composite-fermion BZ.

As a result, we get the mean-field Hamiltonian

$$\hat{H}_{HF} = \sum_{\boldsymbol{k},ij} f_{\boldsymbol{k},i}^\dagger \Big\{ \kappa(\boldsymbol{k}) + \mathcal{HF}\{P\}(\boldsymbol{k}) \Big\}_{ij} f_{\boldsymbol{k},j}, \tag{3}$$

with the *generalized Hartree-Fock functional* acting on a matrix-valued function carrying momentum-$\boldsymbol{q}$ defined in my `neat_TDHF.ipynb` notes that

$$\begin{aligned} \mathcal{HF}\{M_{\boldsymbol{q}}\}(\boldsymbol{k}) &:= (\mathcal{H}+\mathcal{F})\{M_q\}(\boldsymbol{k}) \\ &= \sum_{\boldsymbol{G}} V_{q+G} \varrho_{\boldsymbol{q}+\boldsymbol{G}}(\boldsymbol{k}) \sum_{\boldsymbol{k}'} \text{tr}\Big\{ \varrho_{\boldsymbol{q}+\boldsymbol{G}}^\dagger \cdot M_{\boldsymbol{q}} \Big\}(\boldsymbol{k}') - \sum_{\boldsymbol{q}'} V_{q'} \varrho_{\boldsymbol{q}'}(\boldsymbol{k}) M_{\boldsymbol{q}}(\boldsymbol{k}+\boldsymbol{q}) \varrho_{\boldsymbol{q}'}(\boldsymbol{k}+\boldsymbol{q})^\dagger. \end{aligned} \tag{4}$$

And the mean-field energy reads

$$E_{MF} = \sum_{\boldsymbol{k},ij} \Big\{ P_{ji} \big(\kappa + \mathcal{HF}\{P\}\big)_{ij} \Big\}(\boldsymbol{k}) = \sum_{\boldsymbol{k}} \sum_{ij} \Big\{ \sum_\alpha d_{i\alpha}^* d_{j\alpha} \big(\kappa + \mathcal{HF}\{P\}\big) \Big\}(\boldsymbol{k}) \tag{5}$$

2. Variation with Lagrangian Multiplier

For *each* HF single-particle states, we have an orthogonality condition $1 = \langle\psi_\alpha|\psi_\alpha\rangle = \sum_i d^*_{i\alpha} d_{i\alpha}$. So there are N-independent variation constraint and we can handle them with Lagrangian multipliers as ε_α. To sum up, we can define the functional

$$\mathcal{L}[d, d^*] := \sum_{ij} \left\{ \sum_\alpha d^*_{i\alpha} d_{j\alpha} \big(\kappa + \mathcal{HF}\{P\}\big) \right\} - \sum_\alpha \varepsilon_\alpha \left(\sum_i d^*_{i\alpha} d_{i\alpha} - 1 \right).$$

Saddle-point condition $\delta\mathcal{L}/\delta d^*_{i\alpha} = 0$ then gives i equations

$$\sum_j \big(\kappa + \mathcal{HF}\{P\}\big)_{ij} d_{j\alpha} = d_{i\alpha}\varepsilon_\alpha \tag{6}$$

or in short matrix form, the iterative *Roothaan equation*

$$\boldsymbol{F[d]d = d\varepsilon}, \quad \text{with the } M \times M \text{ Fock operator } \boldsymbol{F} \equiv \kappa + \mathcal{HF}\{P\}. \tag{7}$$

Equation (7) is nonlinear because the Fock operator $\boldsymbol{F}$ itself also depends on the expansion coefficient $d_{i\alpha}$. In practice it has to be solved iteratively: starting with a guess expansion $d^{(0)}_{i,\alpha}$, calculating the Fock operator $\boldsymbol{F[d]}$, then obtain a new expansion $d^{(1)}_{i,\alpha}$ from the eigenvector and so on.

B. Stability: Thouless Representation

II. TDHF AND COLLECTIVE EXCITATION OF MAGNETOROTON

A. Collective Spectrum

The general definition of a particle, in both high-energy and condensed-matter community is the **pole of Green functions**. Particularly, the particle-hole excitation spectrum can be obtained from the dynamics of the Green function constructed from the given PH bilinear

$$\hat{O}_{\boldsymbol{q}} \equiv \sum_{\alpha\beta} \hat{O}_{\boldsymbol{q};\alpha\beta} = \sum_{\boldsymbol{k},\alpha\beta} C^\dagger_{\boldsymbol{k},\alpha} [\phi_{\boldsymbol{q}}(\boldsymbol{k})]_{\alpha\beta} C_{\boldsymbol{k}+\boldsymbol{q},\beta}. \tag{8}$$

For each species of PH bilinear $\hat{O}_{q;\alpha\beta}$, we can evaluate the dynamics of the Green function

$$-i\frac{\partial}{\partial t}\hat{G}_{\alpha\beta;\mu\nu}(\boldsymbol{q}, t) \equiv -i\frac{\partial}{\partial t}\langle \mathcal{T}\hat{O}_{\alpha\beta}(\boldsymbol{q}, t)\hat{O}_{\mu\nu}(-\boldsymbol{q}; 0)\rangle = -i\langle \mathcal{T}[\hat{H}, \hat{O}_{\boldsymbol{q};\alpha\beta}]\hat{O}_{-\boldsymbol{q};\mu\nu}\rangle - \delta(t)\langle[\hat{O}_{\boldsymbol{q};\alpha\beta}, \hat{O}_{-\boldsymbol{q};\mu\nu}]\rangle,$$

with the last unimportant *source term*. **What TDHF does is to approximate (with Wick's contraction) the commutator $[\hat{H}, \hat{O}_{\boldsymbol{q};\alpha\beta}]$ with *original bilinears*, so that the RHS is still linear combination of Green functions**

$$\langle[\hat{H}, \hat{O}_{\boldsymbol{q};\alpha\beta}]\rangle_{\text{TDHF}} = \sum_{\mu\nu} \mathcal{H}_{\boldsymbol{q};\alpha\beta,\mu\nu} \hat{O}_{\boldsymbol{q};\mu\nu}$$

so that the pole of the Green function could be immediately obtained from diagonalization of the matrix $\mathcal{H}$ of dimension $\dim(\alpha)^4$ for each $\boldsymbol{q}$.