Instabilities to generic single particle reduced density matrix

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Assume we have a many-body system described by $\hat{H}_{\text{total}} = \hat{H}_0 + \hat{H}_{\text{int}}$. The original system has symmetry decribed by group G. Without spontaneus symmetry breaking, the single particle density matrix $\hat{\rho}_0$ will be consistant with G and unchanged under the symmetry operations in G. Under the general Hatree-Fock variational scheme deribed in the previous notes, the mean field Hamiltonian can be chosen as

$$\hat{H}_{\text{mf}}^0 = \hat{H}_0 + \sum_i \alpha_i \hat{O}_i \tag{1}$$

where, $\hat{H}_{\text{mf}}^0$ respects to the original symmetry G.

Now let's consider the possible smmetry breaking phase will symmetry breaking terms $\hat{O}_l$ appearing in the mean field Hamiltonian, which reads

$$\hat{H}_{\text{mf}} = \hat{H}_{\text{mf}}^0 + \sum_l \lambda_l \hat{O}_l \tag{2}$$

Our task is to find out if the variational ground state will lose it stability against those symmetry breaking variational parameters λ_l by checking the second order derivative of the total variational enegry E_{total} versus λ_l.

Similar to the previous notes, the variational process will be different for special and general Hartree-Fock cases. Let's consider the special Hartree-Fock case first.

1 special Hartree-Fock

In the special Hartree-Fock case the expectation value of the interaction energy under the slater determinant ground state determined by $\hat{H}_{\text{mf}}$ can be expressed as the bilinear form of the single particle operators $\hat{O}_i$, as

$$E_{\text{interact}} = \sum_{ij} U_{ij} \langle \hat{O}_i \rangle \langle \hat{O}_j \rangle \tag{3}$$

$$E_{\text{total}} = E_{\text{mf}} - \sum_i \alpha_i \langle \hat{O}_i \rangle + \sum_{ij} U_{ij} \langle \hat{O}_i \rangle \langle \hat{O}_j \rangle \tag{4}$$

then

$$\frac{\partial E_{\text{total}}}{\partial \alpha_i} = -\sum_j \alpha_j \frac{\partial \langle \hat{O}_j \rangle}{\partial \alpha_i} + \sum_{jj'} U_{jj'} \left(\frac{\partial \langle \hat{O}_j \rangle}{\partial \alpha_i} \langle \hat{O}_{j'} \rangle + \frac{\partial \langle \hat{O}_{j'} \rangle}{\partial \alpha_i} \langle \hat{O}_j \rangle \right) \tag{5}$$

which can be expressed as

$$\left[\frac{\partial E_{\text{total}}}{\partial \boldsymbol{\alpha}} \right]^T = -\boldsymbol{\alpha}^T \boldsymbol{A} + \mathbf{O}^T \mathbf{U}^T \boldsymbol{A} + \mathbf{O}^T \mathbf{U} \boldsymbol{A} = [\mathbf{O}^T (\mathbf{U}^T + \mathbf{U}) - \boldsymbol{\alpha}^T] \boldsymbol{A} \tag{6}$$

,where $\boldsymbol{A}_{ij} = \frac{\partial \langle \hat{O}_i \rangle}{\partial \alpha_j}$.

At mean field saddle point

$$\left[\frac{\partial E_{\text{total}}}{\partial \boldsymbol{\alpha}} \right]^T = 0$$

$$\Rightarrow \quad (\mathbf{U}^T + \mathbf{U}) \mathbf{O} = \boldsymbol{\alpha} \tag{7}$$

Now let's consider the second order derivative.

$$\frac{\partial^2 E_{\text{total}}}{\partial\alpha_i\partial\alpha_{i'}} = -\sum_j \alpha_j \frac{\partial^2\langle\hat{O}_j\rangle}{\partial\alpha_i\partial\alpha_{i'}} - \frac{\partial\langle\hat{O}_{i'}\rangle}{\partial\alpha_i} + \sum_{jj'} (U_{jj'} + U_{j'j}) \frac{\partial^2\langle\hat{O}_j\rangle}{\partial\alpha_i\partial\alpha_{i'}}\langle\hat{O}_{j'}\rangle$$

$$+ \sum_{jj'} (U_{jj'} + U_{j'j}) \frac{\partial\langle\hat{O}_j\rangle}{\partial\alpha_i}\frac{\partial\langle\hat{O}_{j'}\rangle}{\partial\alpha_{i'}} = [\mathbf{O}^T(\mathbf{U}^T + \mathbf{U}) - \boldsymbol{\alpha}^T]\boldsymbol{B} - \boldsymbol{A} + \boldsymbol{A}^T(\mathbf{U}^T + \mathbf{U})\boldsymbol{A} \tag{8}$$

$$= \quad -\boldsymbol{A} + \boldsymbol{A}^T(\mathbf{U}^T + \mathbf{U})\boldsymbol{A} = \boldsymbol{\Gamma}$$

Now we have proved that for special HF to obtain the second order derivative of the total energy only the first order derivative of the single particle density matrix (matrix $\boldsymbol{A}$) is needed.

2 Eigenstates of interaction vertex matrix U

From equation (7), at the stationary point, $\boldsymbol{\alpha} = \mathbf{U}\mathbf{O}$. Both $\boldsymbol{\alpha}$ and $\mathbf{O}$ can be expanded by the eigenvectors of the interaction vertex matrix $\mathbf{U}$, as

$$\boldsymbol{\alpha} = \sum_{l=0}^{M} a_l \boldsymbol{u}_l \qquad \text{and} \qquad \mathbf{O} = \sum_{l=0}^{M} b_l \boldsymbol{u}_l$$

$$\text{with} \qquad \mathbf{O}\boldsymbol{u}_l = \lambda_l \boldsymbol{u}_l \tag{9}$$

$$\text{so} \qquad a_l = \lambda_l b_l$$

Thus the coupled multi-variable self consistant problem becomes many independent single variable self consistant problem in different "eigen channels".

3 How to obtain the first order derivative?

This is very straight forward. The key understanding is that the second order perturbation theory is NOT applied to single particle basis $|n>$ but on many particle ground state $|G_0>$, from which we have

$$H_{\text{mf}} = H_{\text{mf0}} + \delta H_{\text{mf}}$$

$$\text{with} \qquad \delta H_{\text{mf}} = \sum_i \delta\lambda_i O_i = \sum_i \delta\lambda_i O_{i,\text{mn}} c_m^\dagger c_n \tag{10}$$

$$\text{and} \qquad |G> = |G_0> + \sum_{m\notin\text{occ}}\sum_{n\in\text{occ}}\sum_i \frac{\delta\lambda_i O_{i,\text{mn}}}{E_{G0} - (E_m - E_n)}|\text{mn}>$$

$$\Rightarrow \; <G|O_i|G> = <G_0|O_i|G_0> + \sum_j \delta\lambda_j \sum_{m\notin\text{occ}}\sum_{n\in\text{occ}} \left[\frac{O_{i,\text{nm}}O_{j,\text{mn}}}{-(E_m - E_n)} + \frac{O_{j,\text{nm}}O_{i,\text{mn}}}{-(E_m - E_n)}\right]$$

$$\Rightarrow \qquad \frac{\partial <O_i>}{\partial\lambda_j} = \sum_{m\notin\text{occ}}\sum_{n\in\text{occ}}\left[\frac{O_{i,\text{nm}}O_{j,\text{mn}} + O_{j,\text{nm}}O_{i,\text{mn}}}{(E_n - E_m)}\right]$$

$$= -\mathbb{O}_i^\dagger\mathbb{O}_j - \mathbb{O}_j^\dagger\mathbb{O}_i$$

$$\text{where} \qquad \mathbb{O}_{i,(mn)} = \frac{1}{\sqrt{E_m - E_n}} O_{i,(mn)}$$

In above equation, the (mn) denotes that two indices m and n will be combined to one and the two dimentional matrix will become one dimentional vector.

4 Generalization to lattice models

For lattice models in condensd matter physics, the total crystal momentum k will be conserved and the many-body Hamiltonian reads,

$$
\begin{aligned}
H_0 &= \sum_k \hat{h}_{\alpha\beta}(\boldsymbol{k}) c_\alpha^\dagger(\boldsymbol{k}) c_\beta(\boldsymbol{k}) \\
H_{\text{int}} &= \sum_{kk'q} \hat{V}_{\beta\beta'\alpha'\alpha}(\boldsymbol{k}, \boldsymbol{k}', \boldsymbol{q}) c_\beta^\dagger(\boldsymbol{k}+\boldsymbol{q}) c_{\beta'}^\dagger(\boldsymbol{k}'-\boldsymbol{q}) c_{\alpha'}(\boldsymbol{k}') c_\alpha(\boldsymbol{k})
\end{aligned} \tag{11}
$$

Suppose we are looking for orders at particular momentum $\boldsymbol{Q}$, all the possible orders can be expressed as

$$
\hat{O}_i(\boldsymbol{Q}) = \sum_k f_{\alpha\beta}^{(i)}(\boldsymbol{k}) c_\alpha^\dagger(\boldsymbol{k}+\boldsymbol{Q}) c_\beta(\boldsymbol{k}) \tag{12}
$$

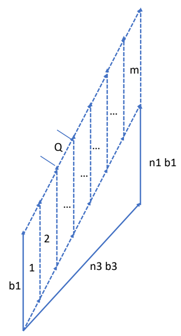
And the corresponding mean field Hamiltonian reads

$$
H_{\text{mf}} = H_0 + \sum_i \lambda_i \hat{O}_i(\boldsymbol{Q}) + \sum_i \lambda_i^* \hat{O}_i(-\boldsymbol{Q}) \tag{13}
$$

In this note, we consider only the commensurate case, where $\boldsymbol{Q}$ satisfies,

$$
m\boldsymbol{Q} = n_1 \boldsymbol{b}_1 + n_2 \boldsymbol{b}_2 + n_3 \boldsymbol{b}_3 \tag{14}
$$

Now we need to find out a convenient numerical protocol to determine the reduced BZ, which I described below. First, pick two basis vectors which satisfy $\boldsymbol{b}_i \times \boldsymbol{Q} \neq 0$. If there is one choice then we are done (suppose these two basis vectors are $\boldsymbol{b}_1$ and $\boldsymbol{b}_2$) and the reduced BZ is determined by the reduced reciprocal lattic spanned by the three basis vectors as $\boldsymbol{b}_{1,}\boldsymbol{b}_2$ and $\boldsymbol{Q}$. With the equation (14), the orders with wave vector $\pm\boldsymbol{Q}$, with couple m different reduced BZs covering n_3 original BZs. The schemetic plot is showing in the following figure.



Next, we will rewrite the Hamiltonian on the n_3 copies of the original BZ, which are the No. 1 to m reduced BZ ploted schemetically above.

$$
H_{\text{mf}} = \frac{1}{n_3} \sum_{l=1}^{m} \sum_{k \in \text{mthBZ}}' \hat{h}_{\alpha\beta}(\boldsymbol{k}) c_\alpha^\dagger(\boldsymbol{k}) c_\beta(\boldsymbol{k}) + \sum_i \lambda_i \hat{O}_i(\boldsymbol{Q}) + \sum_i \lambda_i^* \hat{O}_i(-\boldsymbol{Q}) \tag{15}
$$

Next, we evaluate the trial ground state energy using the many-body ground state of the above mean field Hamiltonian. We get

$$
E_{\text{total}} = E_0 + E_{\text{int}} \tag{16}
$$

and

$$
\begin{aligned}
E_0 &= E_{\text{mf}} - \sum_i \lambda_i \langle \hat{O}_i(\boldsymbol{Q}) \rangle - \sum_i \lambda_i^* \langle \hat{O}_i(-\boldsymbol{Q}) \rangle \\
E_{\text{int}} &= \sum_{ij} U_{ij}(\boldsymbol{Q}) \langle \hat{O}_i(\boldsymbol{Q}) \rangle \langle \hat{O}_j(-\boldsymbol{Q}) \rangle
\end{aligned} \tag{17}
$$

Following the procedge described in the above sections, we obtain

$$\frac{\partial E_{\text{total}}}{\partial \lambda_i} = -\sum_j \lambda_j \frac{\partial \langle \hat{O}_j(\boldsymbol{Q}) \rangle}{\partial \lambda_i} +$$

$$\sum_{jj'} U_{j'j}(\boldsymbol{Q}) \left[\frac{\partial \langle \hat{O}_{j'}(\boldsymbol{Q}) \rangle}{\partial \lambda_i} \langle \hat{O}_j(-\boldsymbol{Q}) \rangle + \langle \hat{O}_{j'}(\boldsymbol{Q}) \rangle \frac{\partial \langle \hat{O}_j(-\boldsymbol{Q}) \rangle}{\partial \lambda_i} \right] = 0 \tag{18}$$

$$\left[\frac{\partial E_{\text{total}}}{\partial \boldsymbol{\lambda}} \right]^T = -\boldsymbol{\lambda}^T \boldsymbol{A}(\boldsymbol{Q}) + \mathbf{O}^T(-\boldsymbol{Q}) \mathbf{U}^T \boldsymbol{A}(\boldsymbol{Q}) + \mathbf{O}^T(\boldsymbol{Q}) \mathbf{U} \boldsymbol{A}(-\boldsymbol{Q}) = 0$$

For the same reason,

$$\frac{\partial E_{\text{total}}}{\partial \lambda_i^*} = -\sum_j \lambda_j^* \frac{\partial \langle \hat{O}_j(-\boldsymbol{Q}) \rangle}{\partial \lambda_i^*} +$$

$$\sum_{jj'} U_{j'j}^*(\boldsymbol{Q}) \left[\frac{\partial \langle \hat{O}_{j'}(-\boldsymbol{Q}) \rangle}{\partial \lambda_i^*} \langle \hat{O}_j(-\boldsymbol{Q}) \rangle + \langle \hat{O}_{j'}(-\boldsymbol{Q}) \rangle \frac{\partial \langle \hat{O}_j(\boldsymbol{Q}) \rangle}{\partial \lambda_i^*} \right] = 0 \tag{19}$$

Last, we evaluate the second order derivative

$$\boldsymbol{\Gamma}_{ij} = \frac{\partial^2 E_{\text{total}}}{\partial \lambda_i \partial \lambda_j} \tag{20}$$

$$= \quad \alpha\beta$$