HFB densities

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Abstract

Basic relations used for computation of various densities.

1 General case

HFB problem in general case is given by:

$$\begin{pmatrix} h_{\uparrow\uparrow} & h_{\uparrow\downarrow} & 0 & \Delta \\ h_{\downarrow\uparrow} & h_{\downarrow\downarrow} & -\Delta & 0 \\ 0 & -\Delta^* & -h^*_{\uparrow\uparrow} & -h^*_{\uparrow\downarrow} \\ \Delta^* & 0 & -h^*_{\downarrow\uparrow} & -h^*_{\downarrow\downarrow} \end{pmatrix} \begin{pmatrix} u_{n\uparrow} \\ u_{n\downarrow} \\ v_{n\uparrow} \\ v_{n\downarrow} \end{pmatrix} = E_n \begin{pmatrix} u_{n\uparrow} \\ u_{n\downarrow} \\ v_{n\uparrow} \\ v_{n\downarrow} \end{pmatrix} \tag{1}$$

and corresponding densities are constructed as follow:

$$n_\sigma(\boldsymbol{r}) = \sum_{|E_n|<E_c} |v_{n,\sigma}(\boldsymbol{r})|^2 f_\beta(-E_n), \tag{2}$$

$$\tau_\sigma(\boldsymbol{r}) = \sum_{|E_n|<E_c} |\nabla v_{n,\sigma}(\boldsymbol{r})|^2 f_\beta(-E_n), \tag{3}$$

$$\nu(\boldsymbol{r}) = \frac{1}{2} \sum_{|E_n|<E_c} (u_{n,\uparrow}(\boldsymbol{r}) v^*_{n,\downarrow}(\boldsymbol{r}) - u_{n,\downarrow}(\boldsymbol{r}) v^*_{n,\uparrow}(\boldsymbol{r})) f_\beta(-E_n), \tag{4}$$

$$\boldsymbol{j}_\sigma(\boldsymbol{r}) = \sum_{|E_n|<E_c} \mathrm{Im}[v_{n,\sigma}(\boldsymbol{r}) \nabla v^*_{n,\sigma}(\boldsymbol{r})] f_\beta(-E_n), \tag{5}$$

where subscripts $\sigma = \{\uparrow, \downarrow\}$ indicate spin, E_n denotes quasi-particle energy and E_c is energy cut-off scale. Fermi distribution function $f_\beta(E) = 1/(\exp(\beta E) + 1)$ is introduced to model temperature $k_B T = 1/\beta$ effects. In zero temperature limit $T = 0$ Fermi distribution function reduces to $f_\beta(E) = \theta(-E)$, where $\theta(x)$ is Heaviside step function. Note also that $f_\beta(E) = 1 - f_\beta(-E)$.

Relation 1: If vector $\varphi_+ = (u_{n\uparrow}, u_{n\downarrow}, v_{n\uparrow}, v_{n\downarrow})^T$ is solution of Eq. (1) with eigenvalue E_n, then also vector $\varphi_- = (v^*_{n\uparrow}, v^*_{n\downarrow}, u^*_{n\uparrow}, u^*_{n\downarrow})^T$ is solution with eigenvalue $-E_n$.

Conclusion 1: It is sufficient to extract only solutions for positive eigenvalues E_n.

2 Case where $h_{\uparrow\downarrow} = h_{\downarrow\uparrow} = 0$

If $h_{\uparrow\downarrow} = h_{\downarrow\uparrow} = 0$ (typically it corresponds to no spin-orbit case) then Eq. (1) decouples into two sets of equations:

$$\begin{pmatrix} h_{\uparrow\uparrow} & \Delta \\ \Delta^* & -h^*_{\downarrow\downarrow} \end{pmatrix} \begin{pmatrix} u_{n\uparrow} \\ v_{n\downarrow} \end{pmatrix} = E_n \begin{pmatrix} u_{n\uparrow} \\ v_{n\downarrow} \end{pmatrix}, \tag{6}$$

$$\begin{pmatrix} h_{\downarrow\downarrow} & -\Delta \\ -\Delta^* & -h^*_{\uparrow\uparrow} \end{pmatrix} \begin{pmatrix} u_{n\downarrow} \\ v_{n\uparrow} \end{pmatrix} = E_n \begin{pmatrix} u_{n\downarrow} \\ v_{n\uparrow} \end{pmatrix}. \tag{7}$$

Relation 2: If vector $\varphi_+ = (u_{n\uparrow}, v_{n\downarrow})^T$ is solution of Eq. (6) with eigenvalue E_n, then vector $\varphi_- = (v^*_{n\uparrow}, u^*_{n\downarrow})^T$ is solution of Eq. (7) with eigenvalue $-E_n$.

Conclusion 2: Having solutions of Eq. (6) one can construct solutions of Eq. (7) by using transformation: $u_{n,\uparrow} \to v^*_{n,\uparrow}$, $v_{n,\downarrow} \to u^*_{n,\downarrow}$ and $E_n \to -E_n$.
In practice we solve only Eq. (6) and we express all densities via $\{u_{n\uparrow}, v_{n\downarrow}\}$:

$$\begin{aligned}
n_\uparrow(\boldsymbol{r}) &= \sum_{|E_n|<E_c} |u_{n,\uparrow}(\boldsymbol{r})|^2 f_\beta(E_n), && (8)\\
n_\downarrow(\boldsymbol{r}) &= \sum_{|E_n|<E_c} |v_{n,\downarrow}(\boldsymbol{r})|^2 f_\beta(-E_n) && (9)\\
\tau_\uparrow(\boldsymbol{r}) &= \sum_{|E_n|<E_c} |\nabla u_{n,\uparrow}(\boldsymbol{r})|^2 f_\beta(E_n), && (10)\\
\tau_\downarrow(\boldsymbol{r}) &= \sum_{|E_n|<E_c} |\nabla v_{n,\downarrow}(\boldsymbol{r})|^2 f_\beta(-E_n), && (11)\\
\nu(\boldsymbol{r}) &= \frac{1}{2} \sum_{|E_n|<E_c} u_{n,\uparrow}(\boldsymbol{r}) v^*_{n,\downarrow}(\boldsymbol{r}) \left(f_\beta(-E_n) - f_\beta(E_n)\right), && (12)\\
\boldsymbol{j}_\uparrow(\boldsymbol{r}) &= -\sum_{|E_n|<E_c} \mathrm{Im}[u_{n,\uparrow}(\boldsymbol{r}) \nabla u^*_{n,\uparrow}(\boldsymbol{r})] f_\beta(E_n), && (13)\\
\boldsymbol{j}_\downarrow(\boldsymbol{r}) &= \sum_{|E_n|<E_c} \mathrm{Im}[v_{n,\downarrow}(\boldsymbol{r}) \nabla v^*_{n,\downarrow}(\boldsymbol{r})] f_\beta(-E_n), && (14)\\
S &= -k_B \sum_{|E_n|<E_c} \left(f_\beta(E_n) \ln\, f_\beta(E_n) + f_\beta(-E_n) \ln f_\beta(-E_n)\right). && (15)
\end{aligned}$$

3 Case where $h_{\uparrow\uparrow} = h_{\downarrow\downarrow} = h$

If $h_{\uparrow\uparrow} = h_{\downarrow\downarrow} = h$ (typically it corresponds to the spin-balanced case) then Eq. (6) takes form, as typically cited in papers (spin indices are dropped):

$$\begin{pmatrix} h & \Delta \\ \Delta^* & -h^* \end{pmatrix} \begin{pmatrix} u_n \\ v_n \end{pmatrix} = E_n \begin{pmatrix} u_n \\ v_n \end{pmatrix}. \tag{16}$$

Relation 3: If vector $\varphi_+ = (u, v)^T$ is solution of Eq. (16) with eigenvalue E_n, then vector $\varphi_- = (v^*_n, -u^*_n)^T$ is also solution with eigenvalue $-E_n$.

Conclusion 3: Having solutions of Eq. (16) for positive energies E_n one can construct all solutions of this equation.

In practice for spin-balanced case we solve Eq. (16) for positive E_n and we express all densities via these states:

$$
\begin{aligned}
n_\uparrow(\boldsymbol{r}) = n_\downarrow(\boldsymbol{r}) &= \sum_{0<E_n<E_c} \big(|v_n(\boldsymbol{r})|^2 f_\beta(-E_n) + |u_n(\boldsymbol{r})|^2 f_\beta(E_n)\big) && (17)\\
\tau_\uparrow(\boldsymbol{r}) = \tau_\downarrow(\boldsymbol{r}) &= \sum_{0<E_n<E_c} \big(|\nabla v_n(\boldsymbol{r})|^2 f_\beta(-E_n) + |\nabla u_n(\boldsymbol{r})|^2 f_\beta(E_n)\big), && (18)\\
\nu(\boldsymbol{r}) &= \sum_{0<E_n<E_c} u_n(\boldsymbol{r}) v_n^*(\boldsymbol{r}) \left(f_\beta(-E_n) - f_\beta(E_n)\right), && (19)\\
\boldsymbol{j}_\uparrow(\boldsymbol{r}) = \boldsymbol{j}_\downarrow(\boldsymbol{r}) &= \sum_{0<E_n<E_c} (\mathrm{Im}[v_n(\boldsymbol{r})\nabla v_n^*(\boldsymbol{r})] f_\beta(-E_n) \\
&\qquad - \mathrm{Im}[u_n(\boldsymbol{r})\nabla u_n^*(\boldsymbol{r})] f_\beta(E_n)), && (20)\\
S &= -2k_B \sum_{0<E_n<E_c} (f_\beta(E_n) \ln\, f_\beta(E_n) \\
&\qquad + f_\beta(-E_n) \ln f_\beta(-E_n)). && (21)
\end{aligned}
$$