Exercise-sheet 3 (May 23, 2017)

1 Homework - due Date: May 30, 2017 (30 points).

1.1 Particle number fluctuations in the BCS wavefunction (10 points)

Consider the variational wavefunction

$$|\tilde{\varphi}\rangle = \prod_{\boldsymbol{k}} (u_{\boldsymbol{k}} + v_{\boldsymbol{k}}\, \hat{c}^{\dagger}_{\boldsymbol{k}\uparrow} \hat{c}^{\dagger}_{-\boldsymbol{k}\downarrow})|0\rangle, \tag{1}$$

where $|0\rangle$ is the electronic vacuum and the variational coefficients satisfy the normalization condition.

$$u_{\boldsymbol{k}}^2 + v_{\boldsymbol{k}}^2 = 1. \tag{2}$$

Equation (1) can be thought of as a superposition over states with different number of zero-momentum electron pairs, i.e. the number of pairs in our variational state is allowed to fluctuate. One is therefore interested in the distribution of particles associated to $|\tilde{\varphi}\rangle$.

In the tutorial we have already shown the average particle number

$$N^* \equiv \langle\tilde{\varphi}|\hat{N}|\tilde{\varphi}\rangle = 2\sum_{\boldsymbol{k}} |v_{\boldsymbol{k}}|^2, \tag{3}$$

where $\hat{N} = \sum_{\boldsymbol{k},\sigma} \hat{c}^{\dagger}_{\boldsymbol{k}\sigma}\hat{c}_{\boldsymbol{k}\sigma}$ is the number operator.
Show that

$$\langle\tilde{\varphi}|\hat{N}^2|\tilde{\varphi}\rangle = 4\sum_{\boldsymbol{k}} |v_{\boldsymbol{k}}|^2 + 4\sum_{\boldsymbol{k},\boldsymbol{p}\neq\boldsymbol{k}} |v_{\boldsymbol{k}}|^2|v_{\boldsymbol{p}}|^2, \tag{4}$$

and hence that the absolute fluctuations of the particle number are proportional to $\sqrt{N^*}$.

For a macroscopic system $\sqrt{N^*}$ is large and, consequently, so is the uncertainty of the number of particles in the state defined in Eq. (1). This is due to the fact that $|\tilde{\varphi}\rangle$ has a fixed phase, i.e. it breaks gauge invariance.

1.2 Variational calculation of the energy (20 points)

Consider the Hamiltonian

$$\hat{H} = \sum_{\boldsymbol{k}\sigma} \xi_{\boldsymbol{k}} \hat{c}^{\dagger}_{\boldsymbol{k}\sigma} \hat{c}_{\boldsymbol{k}\sigma} + \sum_{\boldsymbol{kl}} V_{\boldsymbol{kl}} \hat{c}^{\dagger}_{\boldsymbol{k}\uparrow} \hat{c}^{\dagger}_{-\boldsymbol{k}\downarrow} \hat{c}_{-\boldsymbol{l}\downarrow} \hat{c}_{\boldsymbol{l}\uparrow}, \tag{5}$$

where $\xi_{\boldsymbol{k}} = \varepsilon_{\boldsymbol{k}} - \mu$ is the single particle energy relative to the Fermi energy.

(a) Show

$$\langle \tilde{\varphi} | \hat{H} | \tilde{\varphi} \rangle = 2 \sum_{\boldsymbol{k}} \xi_{\boldsymbol{k}} v_{\boldsymbol{k}}^2 + \sum_{\boldsymbol{kl}} V_{\boldsymbol{kl}} u_{\boldsymbol{k}} v_{\boldsymbol{k}} u_{\boldsymbol{l}} v_{\boldsymbol{k}}. \tag{6}$$

(b) Consider the change of variable $(u_{\boldsymbol{k}}, v_{\boldsymbol{k}}) = (\sin\theta_{\boldsymbol{k}}, \cos\theta_{\boldsymbol{k}})$ and minimize the functional energy in Eq. (6) with respect to $\theta_{\boldsymbol{k}}$, to show that (as explicitly done in the tutorial)

$$\Delta_{\boldsymbol{k}} = -\sum_{\boldsymbol{l}} V_{\boldsymbol{kl}} \frac{\Delta_{\boldsymbol{l}}}{2\sqrt{\xi_{\boldsymbol{l}}^2 + \Delta_{\boldsymbol{l}}^2}}, \tag{7}$$

where the definition $\Delta_{\boldsymbol{k}} = -\sum_{\boldsymbol{k}} V_{\boldsymbol{kl}} u_{\boldsymbol{l}} v_{\boldsymbol{l}}$ was used.

(NOTE: here you are supposed to simply repeat the steps done in the tutorial.)

(c) Show that if

$$V_{\boldsymbol{kl}} = \begin{cases} -V, & |\xi_{\boldsymbol{k}}|, |\xi_{\boldsymbol{l}}| \leq \hbar\omega_D \\ 0, & \text{otherwise} \end{cases} \tag{8}$$

where ω_D is the Debye frequency, one can solve Eq. (7) for Δ with

$$\Delta \approx 2\hbar\omega_D e^{-1/N(0)V}, \tag{9}$$

in the weak coupling limit (that is, $VN(0) \ll 1$ with $N(0)$ the density of states at the Fermi energy).

(d) Show that the energy associated to the BCS state (i.e. for finite Δ) is more stable than that of the free electron gas.