Übungen zur Theorie der Kondensierten Materie II SS 18

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1. Free fermions and off-diagonal long-range order (10 + 15 + 25 Points)

Here we show that a system of noninteracting fermions does not exhibit off-diagonal long-range order (ODLRO).

(a) To this end, Fourier transform the two-particle density matrix

$$\rho^{(2)}_{\alpha,\beta;\alpha',\beta'}(\boldsymbol{R},\boldsymbol{r};\boldsymbol{R}',\boldsymbol{r}') = \left\langle c^\dagger_\alpha\!\left(\boldsymbol{R}+\frac{\boldsymbol{r}}{2}\right) c^\dagger_\beta\!\left(\boldsymbol{R}-\frac{\boldsymbol{r}}{2}\right) c_{\beta'}\!\left(\boldsymbol{R}'-\frac{\boldsymbol{r}'}{2}\right) c_{\alpha'}\!\left(\boldsymbol{R}'+\frac{\boldsymbol{r}'}{2}\right)\right\rangle$$

with respect to the center of masses $\boldsymbol{R}$, $\boldsymbol{R}'$ (conjugate momenta $\boldsymbol{K}$, $\boldsymbol{K}'$) and relative coordinates $\boldsymbol{r}$, $\boldsymbol{r}'$ (conjugate momenta $\boldsymbol{k}$, $\boldsymbol{k}'$). Here c ($c^\dagger$) are fermionic annihilation (creation) operators and α refers to the electron's spin. Now perform the Wick contractions assuming that there are no interactions between the particles. For simplicity, we take the electron gas to be unpolarized with respect to its spin.

(b) Use the completeness $\sum_{S=0,1}\sum_{m=-S}^{S} |S,m\rangle\langle S,m| = \mathbb{1}$ of the singlet ($S=0$, $m=0$) and triplet ($S=1$, $m=-1,0,1$) wavefunctions within the Hilbert space of two spin-1/2 degrees of freedom to decompose the Kronecker deltas in spin space into singlet and triplet contributions.

(c) Show that the result can be brought into the form

$$\rho^{(2)}_{\alpha,\beta;\alpha',\beta'}(\boldsymbol{R},\boldsymbol{r};\boldsymbol{R}',\boldsymbol{r}') = \sum_{\boldsymbol{K},\boldsymbol{k},S,m} \lambda_{\boldsymbol{K},\boldsymbol{k},S,m}\, \phi_{\boldsymbol{K},\boldsymbol{k},S,m}(\boldsymbol{R},\boldsymbol{r},\alpha,\beta)\phi^*_{\boldsymbol{K},\boldsymbol{k},S,m}(\boldsymbol{R}',\boldsymbol{r}',\alpha',\beta'). \tag{1}$$

Normalize the wavefunctions to a constant that does not scale with the system size and find $\lambda_{\boldsymbol{K},\boldsymbol{k},S,m}$. Use this result to conclude that the system has no ODLRO.

2. ODLRO in the BCS state (25 + 10 + 10 + 5 Points)

Let us next proof that the BCS ground state $|\mathrm{BCS}\rangle$ is characterized by ODLRO.

(a) As a warm-up, express all finite expectation values

$$\langle \mathrm{BCS}| c^\dagger_{\boldsymbol{k}_1\alpha} c^\dagger_{\boldsymbol{k}_2\beta} c_{\boldsymbol{k}'_2\beta'} c_{\boldsymbol{k}'_1\alpha'} |\mathrm{BCS}\rangle \tag{2}$$

in terms of $u_{\boldsymbol{k}}$ and $v_{\boldsymbol{k}}$ which determine the relation between the electron operators $c_{\boldsymbol{k}\alpha}$ and the Bogoliubov operators

$$\alpha_{\boldsymbol{k}\uparrow} = u^*_{\boldsymbol{k}} c_{\boldsymbol{k}\uparrow} - v_{\boldsymbol{k}} c^\dagger_{-\boldsymbol{k}\downarrow}, \qquad \alpha^\dagger_{-\boldsymbol{k}\downarrow} = u_{\boldsymbol{k}} c^\dagger_{-\boldsymbol{k}\downarrow} + v^*_{\boldsymbol{k}} c_{\boldsymbol{k}\uparrow} \tag{3}$$

diagonalizing the BCS mean-field Hamiltonian.

(b) With the help of these expressions, show that the eigenvalues λ and eigenvectors $\phi_\lambda(\boldsymbol{k}_1, \alpha, \boldsymbol{k}_2, \beta)$ of the two-particle density matrix of the system (at zero temperature) have to satisfy

$$2v_{\boldsymbol{k}_1}^2 v_{\boldsymbol{k}_2}^2 \phi_\lambda(\boldsymbol{k}_1, \alpha, \boldsymbol{k}_2, \alpha) = \lambda \phi_\lambda(\boldsymbol{k}_1, \alpha, \boldsymbol{k}_2, \alpha), \tag{4}$$

$$2v_{\boldsymbol{k}_1}^2 v_{\boldsymbol{k}_2}^2 \phi_\lambda(\boldsymbol{k}_1, \uparrow, -\boldsymbol{k}_2, \downarrow) = \lambda \phi_\lambda(\boldsymbol{k}_1, \uparrow, -\boldsymbol{k}_2, \downarrow), \tag{5}$$

$$2u_{\boldsymbol{k}} v_{\boldsymbol{k}} \sum_{\boldsymbol{k}' \neq \boldsymbol{k}} u_{\boldsymbol{k}'} v_{\boldsymbol{k}'} \phi_\lambda(\boldsymbol{k}', \uparrow, -\boldsymbol{k}', \downarrow) = (\lambda - 2v_{\boldsymbol{k}}^2) \phi_\lambda(\boldsymbol{k}, \uparrow, -\boldsymbol{k}, \downarrow), \tag{6}$$

with $\boldsymbol{k}_1 \neq \boldsymbol{k}_2$.

(c) Convince yourself that the first two equations only yield eigenvalues of order unity. Show that Eq. (6) leads to

$$1 = 2 \sum_{\boldsymbol{k}} \frac{u_{\boldsymbol{k}}^2 v_{\boldsymbol{k}}^2}{\lambda - 2v_{\boldsymbol{k}}^4} \tag{7}$$

in the superconducting phase.

(d) Use Eq. (7) to proof that the BCS wavefunction exhibits ODRLO.