Karlsruher Institut für Technologie Institute for Condensed Matter Theory
Institute for Quantum Materials and Technologies

Condensed Matter Theory II: Many-Body Theory (TKM II) SoSe 2023

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Homework assignment 4
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1. Three-particle interaction: (10 + 10 + 10 + 5 points)

In the lectures, we formulated the Feynman diagrammatic rules for fermions and analyzed the perturbative expansion of the Green's function in the case of a pairwise interaction between particles.

Consider a model system of fermions with spin S that interact through the three-body contact interaction potential: $U_3(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \lambda\, \delta(\mathbf{r}_1 - \mathbf{r}_2)\delta(\mathbf{r}_1 - \mathbf{r}_3)$. The corresponding operator $\widehat{U}_3$ now contains six field operators.

(a) In analogy to the discussion of pairwise interaction in the lecture, write the interaction potential in terms of creation and annihilation operators and field operators.

(b) Draw all diagrams needed for the calculation of the Green's function to first order in λ. You can assume, that disconnected diagrams cancel as is the case for a pairwise interaction (this can be shown).

(c) Using these diagrams, find the total 1st-order correction to the free Green's function in momentum space. Assume, that the non-interacting system is translational invariant and diagonal in spin-space, $G_{0\sigma,\sigma'}(\varepsilon, \mathbf{r}, \mathbf{r}') \to G_0(\varepsilon, \mathbf{r} - \mathbf{r}')\delta_{\sigma,\sigma'}$. The correction should be written in terms of λ, S, $G_0(\varepsilon, \mathbf{k})$, n_0 where n_0 is the particle density.

(d) Calculate the interaction-induced change in the ground state energy $E - E_0$ to first order. Start by drawing the contributing diagrams.

2. Exchange correlation energy (10 + 5 points)

Consider the Hartree and Fock interaction energies in real space and the effect of Pauli repulsion.

(a) Consider a noninteracting ground state $|g\rangle$ with Fermi momentum p_F and a generic repulsive interaction

$$\hat{V} = \frac{1}{2}\sum_{\sigma\sigma} \int \mathrm{d}^3\mathbf{x} \int \mathrm{d}^3\mathbf{x}' U(|\mathbf{x} - \mathbf{x}'|)\psi^\dagger_\sigma(\mathbf{x})\psi^\dagger_{\sigma'}(\mathbf{x}')\psi_{\sigma'}(\mathbf{x}')\psi_\sigma(\mathbf{x}), \tag{1}$$

with $U(r) > 0$.
Express $\langle g|\hat{V}|g\rangle$ in terms of the equal-time correlation function

$$C_{\sigma\sigma'}(\mathbf{x} - \mathbf{x}') = \langle g|\psi^\dagger_\sigma(\mathbf{x})\psi^\dagger_{\sigma'}(\mathbf{x}')\psi_{\sigma'}(\mathbf{x}')\psi_\sigma(\mathbf{x})|g\rangle. \tag{2}$$

Write the correlation function as a time-ordered product, use Wick's theorem and identify the Hartree and Fock contributions. Calculate the spatial dependence of $C_{\sigma\sigma'}(\mathbf{x} - \mathbf{x}')$ for different spin combinations.

(b) Now assume a short-range interaction

$$U(\mathbf{x}-\mathbf{x}') = U_0\delta(\mathbf{x}-\mathbf{x}') \tag{3}$$

and a spin-polarized ground state $|P\rangle$ with $N_\downarrow = \left(\frac{1-P}{2}\right) N_0$ spin-down electrons and $N_\uparrow = \left(\frac{1+P}{2}\right) N_0$ spin-up electrons, where N_0 is the total electron number. How does the interaction energy depend on the polarization? Interpret the result.