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 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.

Solution:

$$U(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = \lambda\delta(\mathbf{r}_1 - \mathbf{r}_2)\delta(\mathbf{r}_1 - \mathbf{r}_3) \tag{1}$$

The potential is diagonal in spin space.
As in the lecture, we express U in terms of creation and annihilation operators:

$$\sum_{i\neq j\neq k} U(\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k) \Leftrightarrow \sum_{i,j,k,l,m,n} U_{i,j,k;l,m,n} a_i^\dagger a_j^\dagger a_k^\dagger a_l a_m a_n \tag{2}$$

where

$$U_{i,j,k;l,m,n} = \langle i,j,k|\, U\, |l,m,n\rangle \tag{3}$$

$$= \int \mathrm{d}r_1\, \mathrm{d}r_2\, \mathrm{d}r_3\, \mathrm{d}r_1'\, \mathrm{d}r_2'\, \mathrm{d}r_3' \sum_{\sigma_1,\sigma_2,\sigma_3,\sigma_1',\sigma_2',\sigma_3'} \langle i,j,k|(r_1,\sigma_1),(r_2,\sigma_2),(r_3,\sigma_3)\rangle \times \tag{4}$$

$$\times \langle (r_1,\sigma_1),(r_2,\sigma_2),(r_3,\sigma_3)|\, U\, |(r_1',\sigma_1'),(r_2',\sigma_2'),(r_3',\sigma_3')\rangle \times \tag{5}$$

$$\times \langle (r_1',\sigma_1'),(r_2',\sigma_2'),(r_3',\sigma_3')|l,m,n\rangle \tag{6}$$

$$= \sum_{\sigma_1,\sigma_2,\sigma_3} \int \mathrm{d}r_1\, \mathrm{d}r_2\, \mathrm{d}r_3 \times \tag{7}$$

$$\times\, \psi^*_{(i,\sigma_1)}(r_1)\psi^*_{(j,\sigma_2)}(r_2)\psi^*_{(k,\sigma_3)}(r_3) U(r_1,r_2,r_3) \psi_{(l,\sigma_1)}(r_1)\psi_{(m,\sigma_2)}(r_2)\psi_{(n,\sigma_3)}(r_3) \tag{8}$$

$$= \lambda \sum_{\sigma_1,\sigma_2,\sigma_3} \int \mathrm{d}r_1\, \psi^*_{(i,\sigma_1)}(r_1)\psi^*_{(j,\sigma_2)}(r_1)\psi^*_{(k,\sigma_3)}(r_1)\psi_{(l,\sigma_1)}(r_1)\psi_{(m,\sigma_2)}(r_1)\psi_{(n,\sigma_3)}(r_1) \tag{9}$$

Here and in the following we write r instead of $\mathbf{r}$ and $\mathrm{d}r$ instead of $\mathrm{d}^d r$ for brevity. Introducing field operators, we obtain:

$$U = \lambda \sum_{\sigma_1,\sigma_2,\sigma_3} \int \mathrm{d}r_1 \, \psi^\dagger_{\sigma_1}(r_1)\psi^\dagger_{\sigma_2}(r_1)\psi^\dagger_{\sigma_3}(r_1)\psi_{\sigma_1}(r_1)\psi_{\sigma_2}(r_1)\psi_{\sigma_3}(r_1) \tag{10}$$

Note that all field operators share the same position argument, as we are considering a contact interaction potential.

(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).

Solution: The diagrams contributing to the first order correction to the Green's function have one interaction vertex each.
The Green's function is defined as

$$G_{\sigma,\sigma'}(\mathbf{r},t;\mathbf{r}',t') = -\mathrm{i}\,\langle\phi_0|\,\mathcal{T}\psi_\sigma(\mathbf{r},t)\psi^\dagger_{\sigma'}(\mathbf{r}',t')\,|\phi_0\rangle \tag{11}$$

All connected diagrams with one interaction vertex:

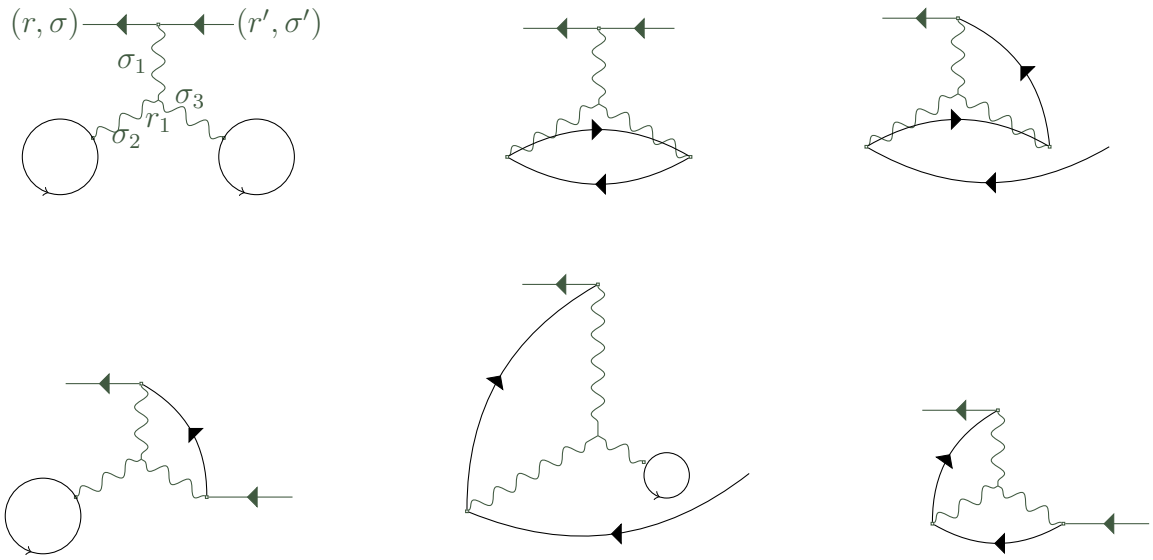

Figure 1: Diagrams J_1, J_2, J_3, J_4, J_5, J_6

As in the lecture a line with an arrow denotes a free fermionic Green's function. The arrow points from creation to annihilation. The interaction potential corresponds to three creation- and three annihilation operators (instead of two as for pairwise interaction). Therefore, we draw the interaction potential as a wavy "triangle" with three endpoints, instead of a wavy line with two endpoints. Every endpoint has one in- and one outgoing fermionic line.
All diagrams have a prefactor 3, as the operator into which $\psi_\sigma(r)$ is contracted can be chosen arbitrarily.

(c) Using these diagrams, find the total 1st-order correction to the free Green's function in energy-momentum space. Assume, that the non-interacting system is translationally 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.

Solution: The diagrams are derived from the expression

$$\mathrm{i}G^{(1)}_{\sigma,\sigma'}(\varepsilon,r,r') = -\mathrm{i}\lambda \int \mathrm{d}t \exp(\mathrm{i}\varepsilon t) \int \mathrm{d}t' \int \mathrm{d}x' \sum_{\sigma_1,\sigma_2,\sigma_3} \times \tag{12}$$

$$\times \langle 0| \mathcal{T} \left[\psi^\dagger_{0,\sigma_1}(x',t'+0)\psi^\dagger_{0,\sigma_2}(x',t'+0)\psi^\dagger_{0,\sigma_3}(x',t'+0) \right. \tag{13}$$

$$\left. \psi_{0,\sigma_1}(x',t')\psi_{0,\sigma_2}(x',t')\psi_{0,\sigma_3}(x',t')\psi_{0,\sigma}(r,t)\psi^\dagger_{0,\sigma'}(r',0) \right] |0\rangle \tag{14}$$

Second diagram:

$$J_{2,\sigma,\sigma'}(\varepsilon,k) = -\lambda \int \mathrm{d}t \exp(\mathrm{i}\varepsilon t) \int \mathrm{d}t' \int \mathrm{d}x' \sum_{\sigma_1,\sigma_2,\sigma_3} \int \mathrm{d}(r-r') \exp(\mathrm{i}k(r-r'))\times \tag{15}$$

$$\times G_{\sigma,\sigma_1}(t-t',r-x')G_{\sigma_1,\sigma'}(t',x'-r')G_{\sigma_2,\sigma_3}(0,0)G_{\sigma_3,\sigma_2}(0,0) \tag{16}$$

$$= -\lambda \sum_{\sigma_1,\sigma_2,\sigma_3} G_{\sigma_3,\sigma_2}(0,0)G_{\sigma_2,\sigma_3}(0,0) \int \mathrm{d}x' \times \tag{17}$$

$$\times \int \mathrm{d}(r-r') \exp(\mathrm{i}k(r-r'))G_{\sigma,\sigma_1}(\varepsilon,x')G_{\sigma_1,\sigma'}(\varepsilon,r-r'-x') \tag{18}$$

$$= -\lambda \sum_{\sigma_1,\sigma_2,\sigma_3} G_{\sigma_3,\sigma_2}(0,0)G_{\sigma_2,\sigma_3}(0,0)G_{\sigma,\sigma_1}(\varepsilon,k)G_{\sigma_1,\sigma'}(\varepsilon,k) \tag{19}$$

$$= -\lambda n_0^2 G^2(\varepsilon,k) \sum_{\sigma_1,\sigma_2,\sigma_3} \delta_{\sigma_2,\sigma_3}\delta_{\sigma,\sigma_1},\delta_{\sigma_1,\sigma'} \tag{20}$$

$$= -G^2(\varepsilon,k)\lambda n_0^2 \delta_{\sigma,\sigma'}(2S+1) \tag{21}$$

Here we denoted the free Green's function by G and used $G_{\sigma,\sigma'}(r=0,t=-0) = \mathrm{i}n_0\delta_{\sigma,\sigma'}$ (lecture Eq. (3.182) and free system diagonal in spin space) where n_0 is the free density.
Similarly:

$$J_{1,\sigma,\sigma'}(\varepsilon,k) = \lambda n_0^2 G^2(\varepsilon,k) \sum_{\sigma_1,\sigma_2,\sigma_3} \delta_{\sigma,\sigma'}\delta_{\sigma_2,\sigma_2}\delta_{\sigma_3,\sigma_3} \tag{22}$$

$$= \lambda n_0^2 G^2(\varepsilon,k)(2S+1)^2 \tag{23}$$

$$J_{3,\sigma,\sigma'}(\varepsilon,k) = \lambda n_0^2 G^2(\varepsilon,k) \sum_{\sigma_1,\sigma_2,\sigma_3} \delta_{\sigma,\sigma_1}\delta_{\sigma',\sigma_2}\delta_{\sigma_2,\sigma_3}\delta_{\sigma_1,\sigma_2} \tag{24}$$

$$= \lambda n_0^2 G^2(\varepsilon,k)\delta_{\sigma,\sigma'} \tag{25}$$

$$J_{4,\sigma,\sigma'}(\varepsilon,k) = -\lambda n_0^2 G^2(\varepsilon,k)\delta_{\sigma,\sigma'}(2S+1) \tag{26}$$

$$J_{5,\sigma,\sigma'}(\varepsilon,k) = -\lambda n_0^2 G^2(\varepsilon,k)\delta_{\sigma,\sigma'}(2S+1) \tag{27}$$

$$J_{6,\sigma,\sigma'}(\varepsilon,k) = \lambda n_0^2 G^2(\varepsilon,k)\delta_{\sigma,\sigma'} \tag{28}$$

The result is

$$G^{(1)}_{\sigma,\sigma'}(\varepsilon,k) = 3\lambda n_0^2 G^2(\varepsilon,k)\delta_{\sigma,\sigma'}(2+(2S+1)^2-3(2S+1)) \tag{29}$$

$$= 6\lambda n_0^2 G^2(\varepsilon,k)\delta_{\sigma,\sigma'}S(2S-1). \tag{30}$$

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

Solution:
From the lecture we know, that the ground state energy is related to the sum of connected vacuum diagrams (lecture equation (3.204)). To lowest order we need to consider connected diagrams with one interaction vertex

$$\Delta E = (E - E_0) \approx \frac{\mathrm{i}}{T}(\text{connected vacuum diagrams with one interaction vertex}) \tag{31}$$

We can construct the following topologically different diagrams:

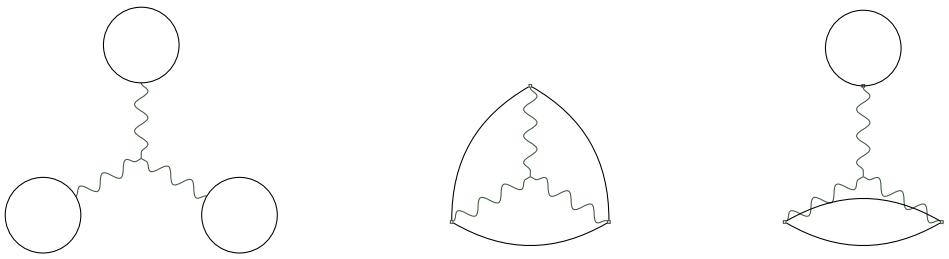

Figure 2: Topologically different diagrams I_1, I_2, I_3.

These diagrams are derived from the expression

$$-\mathrm{i}\lambda \sum_{\sigma_1,\sigma_2,\sigma_3} \int \mathrm{d}t \int \mathrm{d}r \, \langle 0| \, \mathcal{T} \left[\psi^\dagger_{0,\sigma_1}(r,t+0)\psi^\dagger_{0,\sigma_2}(r,t+0)\psi^\dagger_{0,\sigma_3}(r,t+0) \times \right. \tag{32}$$

$$\left. \times \, \psi_{0,\sigma_1}(r,t)\psi_{0,\sigma_2}(r,t)\psi_{0,\sigma_3}(r,t) \right] |0\rangle \tag{33}$$

There is one series of contraction that gets the first expression, 2 for the second diagram, and 3 for the third diagram. We obtain for the diagrams

$$I_1 = -\mathrm{i}\lambda \int \mathrm{d}t \int \mathrm{d}x \sum_{\sigma_1,\sigma_2,\sigma_3} (\mathrm{i}G(0,0))^3 = -\lambda(\mathrm{i}n_0)^3(2S+1)^3 VT \tag{34}$$

$$= \mathrm{i}\lambda n_0^3 (2S+1)^3 VT \tag{35}$$

$$I_2 = -\mathrm{i}\lambda(-n_0)^3 \int \mathrm{d}t \int \mathrm{d}x \sum_{\sigma_1,\sigma_2,\sigma_3} \delta_{\sigma_1,\sigma_2}\delta_{\sigma_2,\sigma_3} = \mathrm{i}\lambda n_0^3 (2S+1) VT \tag{36}$$

$$I_3 = -\mathrm{i}\lambda n_0^3 (2S+1)^2 VT \tag{37}$$

Summing up the contributions (taking into account the factors 1, 2, and 3 arising from different contractions to obtain respective diagrams), we find

$$\Delta E = \frac{\mathrm{i}}{T}(I_1 + 2I_2 + 3I_3) \tag{38}$$

$$= V\lambda n_0^3 (2S+1) \left[3 - 2(2S+1) - (2S+1)^2 \right]. \tag{39}$$

2. Hartree-Fock energy in real space (10 + 10 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

$$\hat{V} = \frac{1}{2}\sum_{\sigma\sigma}\int \mathrm{d}^3\mathbf{x}\int \mathrm{d}^3\mathbf{x}' U(|\mathbf{x}-\mathbf{x}'|)\psi^\dagger_\sigma(\mathbf{x})\psi^\dagger_{\sigma'}(\mathbf{x}')\psi_{\sigma'}(\mathbf{x}')\psi_\sigma(\mathbf{x}), \tag{40}$$

with $U(r) > 0$.

Express $\langle g|\hat{V}|g\rangle$ in terms of the equal-time correlation function

$$C_{\sigma\sigma'}(\mathbf{x}-\mathbf{x}') = \langle g|\psi^\dagger_\sigma(\mathbf{x})\psi^\dagger_{\sigma'}(\mathbf{x}')\psi_{\sigma'}(\mathbf{x}')\psi_\sigma(\mathbf{x})|g\rangle. \tag{41}$$

and identify the Hartree and Fock contributions. Calculate the spatial dependence of $C_{\sigma\sigma'}(\mathbf{x}-\mathbf{x}')$ for different spin combinations.

Solution:

$$\langle g|\hat{V}|g\rangle = \frac{1}{2}\sum_{\sigma\sigma'}\int \mathrm{d}^3\mathbf{x}\int \mathrm{d}^3\mathbf{x}' U(|\mathbf{x}-\mathbf{x}'|)\langle g|\psi^\dagger_\sigma(\mathbf{x})\psi^\dagger_{\sigma'}(\mathbf{x}')\psi_{\sigma'}(\mathbf{x}')\psi_\sigma(\mathbf{x})|g\rangle \tag{42}$$

$$= \frac{1}{2}\sum_{\sigma\sigma'}\int \mathrm{d}^3\mathbf{x}\int \mathrm{d}^3\mathbf{x}' U(|\mathbf{x}-\mathbf{x}'|)C_{\sigma\sigma'}(\mathbf{x}-\mathbf{x}') \tag{43}$$

We can express the equal-time correlation function as a time-ordered product

$$C_{\sigma\sigma'}(\mathbf{x}-\mathbf{x}') = \langle g|\mathcal{T}\psi_{0,\sigma'}(\mathbf{x}',0)\psi_{0,\sigma}(\mathbf{x},0)\psi^\dagger_{0,\sigma}(\mathbf{x},0^+)\psi^\dagger_{0,\sigma'}(\mathbf{x}',0^+)|g\rangle \tag{44}$$

$$= \langle g|\mathcal{T}U(t)\psi_{0,\sigma'}(\mathbf{x}',0)U^\dagger(t)U(t)\psi_{0,\sigma}(\mathbf{x},0)U^\dagger(t) \tag{45}$$

$$\times U(t)\psi^\dagger_{0,\sigma}(\mathbf{x},0^+)U^\dagger(t)U(t)\psi^\dagger_{0,\sigma'}(\mathbf{x}',0^+)U^\dagger(t)|g\rangle \tag{46}$$

$$= \langle g|\mathcal{T}\psi_{0,\sigma'}(\mathbf{x}',t)\psi_{0,\sigma}(\mathbf{x},t)\psi^\dagger_{0,\sigma}(\mathbf{x},t+0^+)\psi^\dagger_{0,\sigma'}(\mathbf{x}',t+0^+)|g\rangle, \tag{47}$$

where on the first line we have inserted trivial time-evolution operators and changed into the interaction picture. On the second line we add time-evolution operators U and translate them to time t. U's acting on $|g\rangle$ and $\langle g|$ give scalars which cancel each other.

Then we use Wick's theorem to evaluate the expectation value in terms of non-interacting Green's functions:

$$C_{\sigma\sigma'}(\mathbf{x}-\mathbf{x}') = \langle\mathcal{T}\psi_{0,\sigma}(\mathbf{x},t)\psi^\dagger_{0,\sigma}(\mathbf{x},t+0^+)\rangle\langle\mathcal{T}\psi_{0,\sigma'}(\mathbf{x}',t)\psi^\dagger_{0,\sigma'}(\mathbf{x}',t+0^+)\rangle \tag{48}$$

$$- \langle\mathcal{T}\psi_{0,\sigma'}(\mathbf{x}',t)\psi^\dagger_{0,\sigma}(\mathbf{x},t+0^+)\rangle\langle\mathcal{T}\psi_{0,\sigma}(\mathbf{x},t)\psi^\dagger_{0,\sigma'}(\mathbf{x}',t+0^+)\rangle \tag{49}$$

$$= [\mathrm{i}G(0,0)]^2 - \delta_{\sigma\sigma'}[\mathrm{i}G(\mathbf{x}-\mathbf{x}',0)][\mathrm{i}G(\mathbf{x}'-\mathbf{x},0)] \tag{50}$$

$$= n_0^2 + \delta_{\sigma\sigma'}G(|\mathbf{x}-\mathbf{x}'|,0)^2, \tag{51}$$

where we used the fact that equal-time GF at a single point is in_0, with electron density n_0. The first term, which does not depend on spin, gives the Hartree term when combined with the interaction potential. The second term, which does depend on spin, gives the Fock term.

We need to calculate the Green's function in space-time representation. This is different from what we calculated on sheet 1, where we calculated the retarded GF.

This is the time-ordered GF. The difference is in the positions of the poles.

$$G(\mathbf{k}, t = 0^-) = \int \mathrm{d}\varepsilon \frac{e^{-\mathrm{i}\varepsilon 0^-}}{\varepsilon + \mathrm{i}\mathrm{sgn}(\varepsilon_{\mathbf{k}})0^+ - \varepsilon_{\mathbf{k}}} = \mathrm{i}\theta(\varepsilon_{\mathbf{k}}) \tag{52}$$

$$G(\mathbf{r}, 0^-) = \mathrm{i}\int \frac{\mathrm{d}\mathbf{k}}{(2\pi)^3}\theta(\varepsilon_{\mathbf{k}})e^{\mathrm{i}\mathbf{k}\cdot r} = \frac{\mathrm{i}}{2\pi^2}\int_{-1}^{+1}\mathrm{d}x\int_0^{k_\mathrm{F}}\mathrm{d}k\, k^2 e^{\mathrm{i}krx} \tag{53}$$

$$= \mathrm{i}n_0\frac{3\left[\sin(k_\mathrm{F}r) - k_F r\cos(k_\mathrm{F}r)\right]}{(k_\mathrm{F}r)^3} = \mathrm{i}n_0 P(k_\mathrm{F}r), \tag{54}$$

where $\varepsilon_{\mathbf{k}} = \hbar^2k^2/2m - \mu$ with $\mu = \varepsilon_\mathrm{F}$, electron density is $n_0 = 2\pi^2\hbar^3k_\mathrm{F}^3/3$, and $P(x) = 3[\sin x - x\cos x]/x^3$. We find

$$C_{\sigma\sigma'}(r) = n_0^2(1 - \delta_{\sigma\sigma'}P(k_\mathrm{F}r)^2). \tag{55}$$

At zero $P(0) = 1$ and P decays with Friedel oscillations at the scale of k_F^{-1}. The correlation function behaves differently depending on whether the spins are equal or not:

$$C_{\uparrow\downarrow}(r) = n_0^2. \tag{56}$$

$$C_{\uparrow\uparrow}(r) = n_0^2(1 - P(k_\mathrm{F}r)^2). \tag{57}$$

If the interaction is repulsive, the interaction energy for equal spins is smaller than for same spins because the short range potential is avoided by Pauli repulsion. This creates a tendency towards ferromagnetic state which is explored in the next subtask.

(b) Now assume a short-range interaction

$$U(\mathbf{x} - \mathbf{x}') = U_0\delta(\mathbf{x} - \mathbf{x}') \tag{58}$$

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.

Solution: Here we partially generalize the calculation for part (a) for the case in which the zeroth order GFs for up and down spins are different. We start from Eq. (42) and use the delta-function to simplify the integral:

$$\begin{aligned}
\langle g|\hat{V}|g\rangle &= \frac{U_0}{2}\sum_{\sigma\sigma'}\int \mathrm{d}^3\mathbf{x}\langle g|\psi_\sigma^\dagger(\mathbf{x})\psi_{\sigma'}^\dagger(\mathbf{x})\psi_{\sigma'}(\mathbf{x})\psi_\sigma(\mathbf{x})|g\rangle \\
&= \frac{U_0}{2}\sum_{\sigma\sigma'}(\mathrm{i})^2\left[G_\sigma(\mathbf{x}-\mathbf{x},0)G_{\sigma'}(\mathbf{x}-\mathbf{x},0) - \delta_{\sigma\sigma'}G_\sigma(\mathbf{x}-\mathbf{x},0)G_\sigma(\mathbf{x}-\mathbf{x},0)\right] \\
&= -\frac{U_0}{2}\left[G_\uparrow G_\uparrow + G_\uparrow G_\downarrow + G_\downarrow G_\uparrow + G_\downarrow G_\downarrow - G_\uparrow G_\uparrow - G_\downarrow G_\downarrow\right] \\
&= -U_0 G_\uparrow G_\downarrow = U_0 n_\downarrow n_\uparrow = U_0 n_0^2(1-P)(1+P) = U_0 n_0^2(1-P^2)
\end{aligned} \tag{59}$$

The interaction energy is minimized when the system is completely polarized ($P = \pm 1$). In this case the electrons completely avoid each other by Pauli repulsion, so that they never get close enough to actually interact, and the interaction energy vanishes.

The interaction energy is not the only contribution to the internal energy. One should also consider the kinetic energy of the electrons, given by the non-interacting Hamiltonian:

$$E_{\mathrm{K}} = \langle P|H_0|P\rangle = \left(\sum_{|\mathbf{p}|<p_{\mathrm{F}\uparrow}} + \sum_{|\mathbf{p}|<p_{\mathrm{F}\downarrow}} \right) \frac{p^2}{2m}, \tag{60}$$

where $|P\rangle$ is the spin-polarized (ground) state. Finite polarization will increase the total kinetic energy. If the kinetic energy cost of finite P is smaller than the interaction energy, the system will magnetize spontaneously.