Exercise 1. ***Free Electron Gas.***

The Hamiltonian of a gas of N free electrons is written in the second quantization formalism as

$$H = \sum_{\boldsymbol{k},s} \xi_k \, c^\dagger_{\boldsymbol{k},s} c_{\boldsymbol{k},s} \;, \tag{1}$$

where $c_{\boldsymbol{k},s}$ (resp. $c^\dagger_{\boldsymbol{k},s}$) is the annihilation (resp. creation) operator of the electron mode $\boldsymbol{k}, s$ of energy $\xi_k = \epsilon_k - \mu$. (Here $\varepsilon_k = \hbar^2 k^2/(2m)$ and μ is the chemical potential, $\mu = E_F$ at $T = 0$.) The index s distinguishes the two spin components.

Let's look at excitations that are holes under the Fermi level and electrons above the Fermi level. We would like to rewrite the Hamiltonian in a form which involves explicitly only these excitations. We define the creation and annihilation operators of an excitation $\alpha^\dagger_{\boldsymbol{k},s}$, $\alpha_{\boldsymbol{k},s}$ by

$$\alpha_{\boldsymbol{k},\uparrow} = \begin{cases} c_{\boldsymbol{k},\uparrow} & \text{for } k > k_F \\ c^\dagger_{-\boldsymbol{k},\downarrow} & \text{for } k < k_F \end{cases} \quad ; \quad \alpha_{\boldsymbol{k},\downarrow} = \begin{cases} c_{\boldsymbol{k},\downarrow} & \text{for } k > k_F \\ c^\dagger_{-\boldsymbol{k},\uparrow} & \text{for } k < k_F \end{cases} \;. \tag{2}$$

(a) Show that the α, $\alpha^\dagger$'s obey fermionic commutation relations.

(b) Argue that eq. (2) is a unitary transformation of the creation and annihilation operators. Such a transformation is also called a *Bogoliubov transformation.* What happens if you act with the annihilators $c_{\boldsymbol{k},s}$ and $\alpha_{\boldsymbol{k},s}$ on the ground state of the gas?

(c) Rewrite the Hamiltonian (1) in the form

$$H = \sum_{\boldsymbol{k}} |\xi_k| \left(\alpha^\dagger_{\boldsymbol{k}\uparrow} \alpha_{\boldsymbol{k}\uparrow} + \alpha^\dagger_{\boldsymbol{k}\downarrow} \alpha_{\boldsymbol{k}\downarrow} \right) + E_G \quad ; \quad E_G = 2 \sum_{k<k_F} \xi_k \;. \tag{3}$$

Solution.

(a) First assume $k < k_F < k'$. Then

$$\{\alpha_{\boldsymbol{k},s}, \alpha_{\boldsymbol{k}',s'}\} = \{\alpha^\dagger_{\boldsymbol{k},s}, \alpha^\dagger_{\boldsymbol{k}',s'}\} = \{\alpha_{\boldsymbol{k},s}, \alpha^\dagger_{\boldsymbol{k}',s'}\} = 0 \tag{L.1}$$

simply because the expressions of $\alpha, \alpha^\dagger$ only involve $c, c^\dagger$'s with the same value of k (resp. k'), and the $c, c^\dagger$'s involved anticommute because $k \neq k'$.
Similarly, if $k, k' > k_F$, then the $\alpha, \alpha^\dagger$'s are exactly equal to the $c, c^\dagger$'s and the anticommutation relations hold.
If $k, k' < k_F$, then $\alpha_{\boldsymbol{k},s} = c^\dagger_{-\boldsymbol{k},-s}$ and thus

$$\{\alpha_{\boldsymbol{k},s}, \alpha_{\boldsymbol{k}',s'}\} = \{c^\dagger_{-\boldsymbol{k},-s}, c^\dagger_{-\boldsymbol{k}',-s'}\} = 0 \quad ; \quad \{\alpha^\dagger_{\boldsymbol{k},s}, \alpha^\dagger_{\boldsymbol{k}',s'}\} = \{c_{-\boldsymbol{k},-s}, c_{-\boldsymbol{k}',-s'}\} = 0 \quad ;$$
$$\{\alpha_{\boldsymbol{k},s}, \alpha^\dagger_{\boldsymbol{k}',s'}\} = \{c^\dagger_{-\boldsymbol{k},-s}, c_{-\boldsymbol{k}',-s'}\} = \{c_{-\boldsymbol{k}',-s'}, c^\dagger_{-\boldsymbol{k},-s}\} = \delta_{\boldsymbol{k},\boldsymbol{k}'} \delta_{s,s'} \;.$$

(b) Eq. (2) may be rewritten as

$$\alpha_{\boldsymbol{k},\uparrow} = \begin{cases} c_{\boldsymbol{k},\uparrow} & \text{for } k > k_F \\ c^\dagger_{-\boldsymbol{k},\downarrow} & \text{for } k < k_F \end{cases} \quad ; \quad \alpha^\dagger_{-\boldsymbol{k},\downarrow} = \begin{cases} c^\dagger_{-\boldsymbol{k},\downarrow} & \text{for } k > k_F \\ c_{\boldsymbol{k},\uparrow} & \text{for } k < k_F \end{cases} \;, \tag{L.2}$$

which in turn may be expressed as the Bogoliubov transformation

$$\begin{pmatrix} c_{\boldsymbol{k}\uparrow} \\ c^\dagger_{-\boldsymbol{k}\downarrow} \end{pmatrix} = U_{\boldsymbol{k}} \begin{pmatrix} \alpha_{\boldsymbol{k}\uparrow} \\ \alpha^\dagger_{-\boldsymbol{k}\downarrow} \end{pmatrix} \;, \tag{L.3}$$

where $U_{\boldsymbol{k}}$ is a 2×2 unitary matrix defined as follows:

$$U_{\boldsymbol{k}} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \text{ if } k > k_F; \qquad U_{\boldsymbol{k}} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \text{ if } k < k_F. \tag{L.4}$$

Note that the combination of operators with reversal of $\boldsymbol{k}$ and s comes from the study of Cooper pairs in superconductivity.

Acting on the ground state with $c_{\boldsymbol{k},s}$ yields zero for $k > k_F$ but annihilates an electron for $k < k_F$. However, acting with $\alpha_{\boldsymbol{k},s}$ yields zero for any $\boldsymbol{k}, s$ because for $k < k_F$ $\alpha_{\boldsymbol{k},s}$ is actually a creation operator $c^\dagger$ which gives zero on an already occupied state. This can also be understood as α annihilating excitations: for $k > k_F$, excitations are electrons, and in the ground state there are no such electrons to annihilate, and for $k < k_F$ excitations are holes, yet in the ground state there are no holes under the Fermi level. So α corresponds to an annihilation operator that yields zero when acting on the ground state, this is what one usually wants.

(c) Eq. (3) represents a different way of counting the energy of the system. Instead of counting all electrons and their energies, we count the holes for $k < k_F$ and the electrons for $k > k_F$. Here it is important that the energies ξ_k are scaled such that at the Fermi level $\xi_{k=k_F} = 0$. Note that we could not have just counted the electrons above the Fermi energy and multiplied by two, because we wouldn't know by how much energy such an electron would have been excited.

The transformation (2) effectively means $c_{\boldsymbol{k},s} = \alpha_{\boldsymbol{k},s}$ for $k > k_F$ and $c_{\boldsymbol{k},s} = \alpha^\dagger_{-\boldsymbol{k},-s}$ for $k < k_F$. Now write

$$\begin{aligned} H &= \sum_{k<k_F,\, s} \xi_k\, c^\dagger_{\boldsymbol{k},s} c_{\boldsymbol{k},s} + \sum_{k>k_F,\, s} \xi_k\, c^\dagger_{\boldsymbol{k},s} c_{\boldsymbol{k},s} = \sum_{k<k_F,\, s} \xi_k\, \alpha_{-\boldsymbol{k},-s} \alpha^\dagger_{-\boldsymbol{k},-s} + \sum_{k>k_F,\, s} \xi_k \alpha^\dagger_{\boldsymbol{k},s} \alpha_{\boldsymbol{k},s} \\ &= \sum_{k<k_F,\, s} \xi_k \left(1 - \alpha^\dagger_{-\boldsymbol{k},-s} \alpha_{-\boldsymbol{k},-s}\right) + \sum_{k>k_F,\, s} \xi_k\, \alpha^\dagger_{\boldsymbol{k},s} \alpha_{\boldsymbol{k},s} \\ &= 2 \sum_{k<k_F} \xi_k + \sum_{k<k_F,\, s} |\xi_k|\, \alpha^\dagger_{\boldsymbol{k},s} \alpha_{\boldsymbol{k},s} + \sum_{k>k_F,\, s} |\xi_k|\, \alpha^\dagger_{\boldsymbol{k},s} \alpha_{\boldsymbol{k},s} \ , \end{aligned}$$

where we have anticommutated $\alpha_{-\boldsymbol{k},-s}$ with $\alpha^\dagger_{-\boldsymbol{k},-s}$, cancelled the minus sign with the sign of ξ_k (remember: $\xi_k < 0$ for $k < k_F$ and $\xi_k > 0$ for $k > k_F$), relabeled $\boldsymbol{k} \to -\boldsymbol{k}$, $s \to -s$ in the second sum on the last line, and obtained a factor 2 in the first term from the summation over the index s.

Eventually,

$$H = 2 \sum_{k<k_F} \xi_k + \sum_{\boldsymbol{k},s} |\xi_k|\, \alpha^\dagger_{\boldsymbol{k},s} \alpha_{\boldsymbol{k},s} \ . \tag{L.5}$$

Exercise 2. *Correlation Functions in a Fermi Sea.*

Consider a gas of N identical fermions with spin $1/2$. The fermions are free and non-interacting. The ground state is then given by

$$|\Phi_0\rangle = \prod_{|\boldsymbol{k}| \leqslant k_F,\, s} a^\dagger_{\boldsymbol{k}\, s} \ |0\rangle \ . \tag{4}$$

One defines the *one-particle correlation function* $G_s(\boldsymbol{x} - \boldsymbol{y})$ as

$$G_s(\boldsymbol{x} - \boldsymbol{y}) = \frac{n}{2}\, g_s(\boldsymbol{x} - \boldsymbol{y}) = \langle \Phi_0 | \Psi^\dagger_s(\boldsymbol{x}) \Psi_s(\boldsymbol{y}) | \Phi_0 \rangle \ . \tag{5}$$

This is the amplitude of recreating a fermion of spin s at position $\boldsymbol{x}$ when one was annihilated at position $\boldsymbol{y}$ with same spin.

(a) Using explicit expressions for the field operators $\Psi_s(\boldsymbol{x})$, calculate $G_s(\boldsymbol{x} - \boldsymbol{y})$ and sketch its graph as function of $|\boldsymbol{x} - \boldsymbol{y}|$. Show that $\lim_{\boldsymbol{r} \to 0} G_s(\boldsymbol{r}) = \frac{n}{2}$ and $\lim_{r \to \infty} G_s(\boldsymbol{r}) = 0$.

Solution. Recall the definition of the field operators $\Psi_s(\boldsymbol{x})$,

$$\Psi_s(\boldsymbol{x}) = \sum_{\text{modes}} \phi_i(\boldsymbol{x})\, a_i \ . \tag{L.6}$$

For free fermions we choose to consider the momentum modes designated by $\boldsymbol{k}$, for which the wave functions are plane waves,

$$\phi_{\boldsymbol{k}}(\boldsymbol{x}) = \frac{1}{\sqrt{V}}\, \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{x}} \ . \tag{L.7}$$

Now insert the expression for the Ψ's into (5),

$$\begin{aligned}\frac{n}{2}\, g_s(\boldsymbol{x}-\boldsymbol{y}) &= \frac{1}{V}\sum_{\boldsymbol{k}_1\,\boldsymbol{k}_2} \mathrm{e}^{-i\boldsymbol{k}_1\boldsymbol{x}+i\boldsymbol{k}_2\boldsymbol{y}}\, \langle\Phi_0|\, a^\dagger_{\boldsymbol{k}_1,s} a_{\boldsymbol{k}_2,s}\,|\Phi_0\rangle = \frac{1}{V}\sum_{\boldsymbol{k}_1\,\boldsymbol{k}_2} \mathrm{e}^{-i\boldsymbol{k}_1\boldsymbol{x}+i\boldsymbol{k}_2\boldsymbol{y}}\, \langle\Phi_0|\, n_{\boldsymbol{k}_1,s}\,|\Phi_0\rangle\, \delta_{\boldsymbol{k}_1\boldsymbol{k}_2} \\ &= \frac{1}{V}\sum_{\boldsymbol{k}} \mathrm{e}^{-i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{y})}\, \langle\Phi_0|\, n_{\boldsymbol{k},s}\,|\Phi_0\rangle = \frac{1}{V}\sum_{k\leqslant k_F} \mathrm{e}^{-i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{y})}\end{aligned} \tag{L.8}$$

Indeed, because Φ_0 is a number basis element, any annihilated fermion has to be recreated to give a nonzero matrix element; in the ground state, all levels under the Fermi level are occupied, such that $\langle\Phi_0|\, n_{\boldsymbol{k},s}\,|\Phi_0\rangle = 1$ for $k < k_F$ and $\langle\Phi_0|\, n_{\boldsymbol{k},s}\,|\Phi_0\rangle = 0$ for $k > k_F$. Pursuing the calculation,

$$\begin{aligned}\text{(L.8)} &= \frac{1}{V}\sum_{k\leqslant k_F} \mathrm{e}^{-i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{y})} \approx \int_{k\leqslant k_F} \frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3}\, \mathrm{e}^{-i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{y})} = \frac{1}{(2\pi)^3}\int_0^{2\pi}\mathrm{d}\phi \int_0^{k_F}\mathrm{d}k\, k^2 \int_{-1}^{+1}\mathrm{d}\cos\theta\ \mathrm{e}^{ik|\boldsymbol{x}-\boldsymbol{y}|\cos\theta} \\ &= \frac{1}{(2\pi)^2}\int_0^{k_F}\mathrm{d}k\, k^2\, \frac{1}{i\,k\,|\boldsymbol{x}-\boldsymbol{y}|}\, 2i\sin\left(k|\boldsymbol{x}-\boldsymbol{y}|\right) = \frac{1}{2\pi^2\,|\boldsymbol{x}-\boldsymbol{y}|}\int_0^{k_F}\mathrm{d}k\, k\sin\left(k|\boldsymbol{x}-\boldsymbol{y}|\right) \\ &= \frac{n}{2}\cdot 3\cdot \left.\frac{\sin x - x\cos x}{x^3}\right|_{x=k_F|\boldsymbol{x}-\boldsymbol{y}|} \ .\end{aligned} \tag{L.9}$$

In the last step one calculates using elementary analysis

$$\int_0^{k_F}\mathrm{d}k\, k\sin\left(k|\boldsymbol{x}-\boldsymbol{y}|\right) = \frac{1}{|\boldsymbol{x}-\boldsymbol{y}|^2}\Big[\sin\left(k_F|\boldsymbol{x}-\boldsymbol{y}|\right) - k_F|\boldsymbol{x}-\boldsymbol{y}|\cos\left(k_F|\boldsymbol{x}-\boldsymbol{y}|\right)\Big] \ , \tag{L.10}$$

and applies the relation $k_F = \left[3\pi^2\, n\right]^{1/3}$ (Eq. (5.1.4) in the lecture notes).

We have replaced the sum by an integral in the previous calculation by sending $V \to \infty$. There the distribution $\frac{1}{V}\,\mathrm{e}^{-i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{y})}$ is replaced by $\frac{1}{(2\pi)^3}\,\mathrm{e}^{-i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{y})}$.

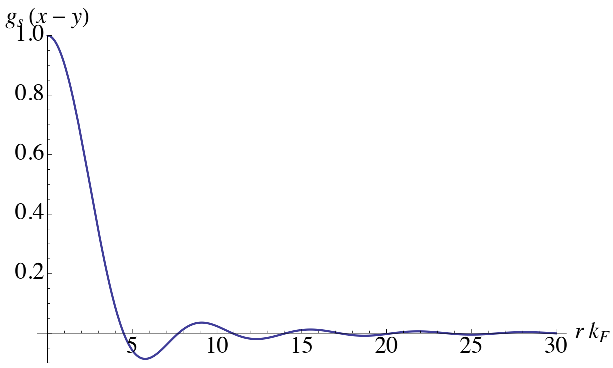
If $\boldsymbol{r}\to 0$, then

$$\frac{n}{2}\, g_s\left(\boldsymbol{r}\right) = \frac{n}{2}\cdot 3\cdot \left.\frac{x - \frac{1}{3!}\,x^3 + O(x^5) - x + \frac{1}{2}\,x^3 + O(x^5)}{x^3}\right|_{x=k_F|\boldsymbol{r}|} = \frac{n}{2}\cdot 3\cdot \left.\frac{\frac{1}{3}\,x^3 + O(x^5)}{x^3}\right|_{x=k_F|\boldsymbol{r}|} \longrightarrow \frac{n}{2} \ . \tag{L.11}$$

Likewise, if $r\to\infty$, then

$$\left|\frac{n}{2}\, g_s\left(\boldsymbol{r}\right)\right| = \frac{n}{2}\cdot 3\left|\frac{\sin x}{x^3} - \frac{x\cos x}{x^3}\right| \leqslant \frac{n}{2}\cdot 3\left[\frac{1}{x^3} + \frac{x}{x^3}\right] \longrightarrow 0 \ . \tag{L.12}$$

A plot of $g_s\left(\boldsymbol{r}\right)$ is given in the following figure.



Likewise, one can define the *pair correlation function* $g_{ss'}(\boldsymbol{x}-\boldsymbol{y})$ by

$$\left(\frac{n}{2}\right)^2 g_{ss'}(\boldsymbol{x}-\boldsymbol{y}) = \langle\Phi_0|\Psi_s^\dagger(\boldsymbol{x})\Psi_{s'}^\dagger(\boldsymbol{y})\Psi_{s'}(\boldsymbol{y})\Psi_s(\boldsymbol{x})|\Phi_0\rangle\ . \tag{6}$$

(b) Rewrite Eq. (6) in the form

$$\left(\frac{n}{2}\right)^2 g_{ss'}(\boldsymbol{x}-\boldsymbol{y}) = \frac{1}{V^2}\sum_{\boldsymbol{k}_1\,\boldsymbol{k}_2\,\boldsymbol{q}_1\,\boldsymbol{q}_2} \mathrm{e}^{-i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot\boldsymbol{x}}\,\mathrm{e}^{-i(\boldsymbol{q}_1-\boldsymbol{q}_2)\cdot\boldsymbol{y}}\,\langle\Phi_0|a_{\boldsymbol{k}_1,s}^\dagger a_{\boldsymbol{q}_1,s'}^\dagger a_{\boldsymbol{q}_2,s'}a_{\boldsymbol{k}_2,s}|\Phi_0\rangle\ . \tag{7}$$

Solution. This follows directly by inserting explicit expressions of $\Psi_s(\boldsymbol{x})$, analogously to point (a).

(c) Assume first that $s \neq s'$. Calculate $g_{ss'}(\boldsymbol{x}-\boldsymbol{y})$.

Solution. Considering (7) and assuming $s \neq s'$, we must have $\boldsymbol{k}_1 = \boldsymbol{k}_2$ and $\boldsymbol{q}_1 = \boldsymbol{q}_2$, or the matrix element is zero because we would fail to recreate the particle that we annihilated and we would end up with a state orthogonal to the ground state. (This argument holds since $|\Phi_0\rangle$ is a number eigenstate.) So

$$\left(\frac{n}{2}\right)^2 g_{ss'}(\boldsymbol{x}-\boldsymbol{y}) = \frac{1}{V^2}\sum_{\boldsymbol{k}\,\boldsymbol{q}}\langle\Phi_0|n_{\boldsymbol{k},s}n_{\boldsymbol{q},s'}|\Phi_0\rangle = \left(\frac{n}{2}\right)^2\ , \tag{L.13}$$

because $\frac{1}{V}\sum_{k<k_F} 1 = \frac{n}{2}$ (the factor $\frac{1}{2}$ is due to spin degeneracy). Finally

$$g_{s\neq s'}\,(\boldsymbol{x}-\boldsymbol{y}) = 1\ . \tag{L.14}$$

(d) Now consider the case where $s = s'$ and calculate $g_{ss}(\boldsymbol{x}-\boldsymbol{y})$. Plot the quantity $g_{ss}(\boldsymbol{x}-\boldsymbol{y})$ as a function of $|\boldsymbol{x}-\boldsymbol{y}|$.

Solution. If $s = s'$, then we must have in (7) either $\boldsymbol{k}_1 = \boldsymbol{k}_2$ and $\boldsymbol{q}_1 = \boldsymbol{q}_2$, or $\boldsymbol{k}_1 = \boldsymbol{q}_2$ and $\boldsymbol{q}_1 = \boldsymbol{k}_2$. This can be written as

$$\langle\Phi_0|a_{\boldsymbol{k}_1,s}^\dagger a_{\boldsymbol{q}_1,s}^\dagger a_{\boldsymbol{q}_2,s}a_{\boldsymbol{k}_2,s}|\Phi_0\rangle = \delta_{\boldsymbol{k}_1,\boldsymbol{k}_2}\delta_{\boldsymbol{q}_1,\boldsymbol{q}_2}\langle\Phi_0|n_{\boldsymbol{k}_1,s}n_{\boldsymbol{q}_1,s}|\Phi_0\rangle - \delta_{\boldsymbol{k}_1,\boldsymbol{q}_2}\delta_{\boldsymbol{q}_1,\boldsymbol{k}_2}\langle\Phi_0|n_{\boldsymbol{k}_1,s}n_{\boldsymbol{q}_1,s}|\Phi_0\rangle\ , \tag{L.15}$$

where the minus sign comes from having anticommuted an odd number of a's to obtain the number operators in the second term.

Recalling Eq. (7), we have

$$\begin{aligned}\left(\frac{n}{2}\right)^2 g_{ss}(\boldsymbol{x}-\boldsymbol{y}) &= \frac{1}{V^2}\sum_{\boldsymbol{k}\,\boldsymbol{q}}\left[1-\mathrm{e}^{-i(\boldsymbol{k}-\boldsymbol{q})\cdot\boldsymbol{x}}\mathrm{e}^{-i(\boldsymbol{q}-\boldsymbol{k})\cdot\boldsymbol{y}}\right]\langle\Phi_0|n_{\boldsymbol{k},s}n_{\boldsymbol{q},s}|\Phi_0\rangle \\ &= \frac{1}{V^2}\sum_{\boldsymbol{k}\,\boldsymbol{q}}\left[1-\mathrm{e}^{-i(\boldsymbol{k}-\boldsymbol{q})\cdot(\boldsymbol{x}-\boldsymbol{y})}\right]\langle\Phi_0|n_{\boldsymbol{k},s}n_{\boldsymbol{q},s}|\Phi_0\rangle \\ &= \frac{1}{V^2}\left[\left(\frac{N}{2}\right)^2 - \sum_{k,q<k_F}\mathrm{e}^{-i\boldsymbol{k}(\boldsymbol{x}-\boldsymbol{y})}\mathrm{e}^{-i\boldsymbol{q}(\boldsymbol{x}-\boldsymbol{y})}\right] = \left(\frac{n}{2}\right)^2\left[1-g_s(\boldsymbol{x}-\boldsymbol{y})^2\right]\ ,\end{aligned} \tag{L.16}$$

where in the last line, the sign in the second exponential was flipped by sending $\boldsymbol{q}\to-\boldsymbol{q}$, and the quantity $g_s(\boldsymbol{x}-\boldsymbol{y})$ appeared by recognizing the expression in (L.8).

Recalling the result for $g_s(\boldsymbol{x}-\boldsymbol{y})$, known from point (a),

$$g_{ss}(\boldsymbol{x}-\boldsymbol{y}) = 1 - 9\cdot\left.\frac{(\sin x - x\cos x)^2}{x^6}\right|_{x=k_F|\boldsymbol{x}-\boldsymbol{y}|}\ . \tag{L.17}$$

A plot of $g_{ss}(\boldsymbol{x}-\boldsymbol{y})$ can be found in the lecture notes, p. 69, Fig. 10.