PHY635, I-Semester 2019/20, Assignment 6 solution

Instructor: Sebastian Wüster
Due-date: TA-Class, 15.11.2019

(1) Degenerate Fermi gases
(a) Following the procedure of the lecture, calculate the energy of hole or particle excitations in a Fermi liquid (homogeneous system as in lecture) to first order perturbation theory in the interaction between different spin Fermion. Then take their energy relative to the unperturbed Fermi sea. Make a graph of particle/hole energy as a function of k and discuss your results. [*5 points*]
Solution: The Hamiltonian in momentum space is (see Eq. (4.30) lecture),

$$\hat{H} = \sum_{\mathbf{k},s} \frac{\hbar^2 \mathbf{k}^2}{2m} \hat{a}^\dagger_{\mathbf{k},s} \hat{a}_{\mathbf{k},s} + \frac{U_0}{\mathcal{V}} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} \hat{a}^\dagger_{\mathbf{k}_3,\uparrow} \hat{a}^\dagger_{\mathbf{k}_4,\downarrow} \hat{a}_{\mathbf{k}_2,\downarrow} \hat{a}_{\mathbf{k}_1,\uparrow} \delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4} \tag{1}$$

where $s \in \{\uparrow, \downarrow\}$. We do perturbation theory in the interaction term, let's call it $\hat{V}$.

For a particle or hole excitation the unperturbed energy is $E_k^{(0)} = \hbar^2(k^2 - k_f^2)/2/m$ (see below Eq. 4.29). The first order energy correction is

$$\Delta E^{(1)} = \langle\, (\mathbf{k}^p \uparrow) \,|\hat{V}|\, (\mathbf{k}^p \uparrow) \,\rangle, \tag{2}$$

where we used the notation (4.39) and concentrate on a particle state with spin-up only, for now.

Thus

$$\begin{aligned} \Delta E^{(1)} &= \frac{U_0}{\mathcal{V}} \langle\, (\mathbf{k}^p \uparrow) \,| \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} \hat{a}^\dagger_{\mathbf{k}_3,\uparrow} \hat{a}^\dagger_{\mathbf{k}_4,\downarrow} \hat{a}_{\mathbf{k}_2,\downarrow} \hat{a}_{\mathbf{k}_1,\uparrow} \delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4} |\, (\mathbf{k}^p \uparrow) \,\rangle \\ &= \frac{U_0}{\mathcal{V}} \langle\, (\mathbf{k}^p \uparrow) \,| \sum_{|\mathbf{k}_1|<k_f, \{|\mathbf{k}_2|<k_f \text{ or } \mathbf{k}_2=\mathbf{k}_p\}, \mathbf{k}_3=\mathbf{k}_1, \mathbf{k}_4=\mathbf{k}_2} \hat{a}^\dagger_{\mathbf{k}_3,\uparrow} \hat{a}^\dagger_{\mathbf{k}_4,\downarrow} \hat{a}_{\mathbf{k}_2,\downarrow} \hat{a}_{\mathbf{k}_1,\uparrow} |\, (\mathbf{k}^p \uparrow) \,\rangle, \end{aligned} \tag{3}$$

The constraints on the sum has come about as follows: The destruction operators $\hat{a}_{\mathbf{k}_2,\downarrow} \hat{a}_{\mathbf{k}_1,\uparrow}$ have to act on a filled state, thus within the Fermi sea, or onto the particle excitation. Then the creation operators have to act on exactly the same single body state, for the result (rhs. ket after acting with all operators onto it) to be non-orthogonal to the bra. The quantum state is a product of Fock states for spin-up and for spin-down, which allows us to write (with using $k_3 = k_1$, $k_4 = k_2$):

$$\begin{aligned} \Delta E^{(1)} &= \frac{U_0}{\mathcal{V}} \sum_{|\mathbf{k}_1|<k_f} \sum_{\{|\mathbf{k}_2|<k_f \text{ or } \mathbf{k}_2=\mathbf{k}_p\}} \langle\, (\mathbf{k}^p \uparrow) \,| \hat{a}^\dagger_{\mathbf{k}_1,\uparrow} \hat{a}^\dagger_{\mathbf{k}_2,\downarrow} \hat{a}_{\mathbf{k}_2,\downarrow} \hat{a}_{\mathbf{k}_1,\uparrow} |\, (\mathbf{k}^p \uparrow) \,\rangle, \\ &= \frac{U_0}{\mathcal{V}} \sum_{|\mathbf{k}_1|<k_f} \sum_{\{|\mathbf{k}_2|<k_f \text{ or } \mathbf{k}_2=\mathbf{k}_p\}} \langle\, (\mathbf{k}^p \uparrow) \,| \hat{a}^\dagger_{\mathbf{k}_2,\downarrow} \hat{a}_{\mathbf{k}_2,\downarrow} |\, (\mathbf{k}^p \uparrow) \,\rangle \langle\, (\mathbf{k}^p \uparrow) \,| \hat{a}^\dagger_{\mathbf{k}_1,\uparrow} \hat{a}_{\mathbf{k}_1,\uparrow} |\, (\mathbf{k}^p \uparrow) \,\rangle, \end{aligned} \tag{4}$$

In the second line we have used that operators for opposite spin states anti-commute and the state is a simple tensor product $|\, (\mathbf{k}^p \uparrow) \,\rangle = |\, \mathbf{N}_\uparrow \,\rangle \otimes |\, \mathbf{N}_\downarrow \,\rangle$. Here $\mathbf{N}_\uparrow$ is a vector of occupation numbers for all spin up particles (which includes the excitation) and $\mathbf{N}_\downarrow$ one for the spin down particles (with no excitation, only filled Fermi sea). This tensor product structure allows us to factor the average into one pertaining to spin-up and one to spin-down.

We can write the last line simply as $\Delta E^{(1)} = U_0 N_\uparrow N_\downarrow/\mathcal{V}$, exactly as for the energy shift of the Fermi sea itself (see Eq. (4.35)).

If we always compare particles and holes with a Fermi sea of equal particle numbers, we thus get the same dispersion relation as without interactions: $E_k = \hbar^2(k^2 - k_f^2)/2/m$.

(b) Consider a homogeneous attractively interacting balanced spin mixture of Fermions as in chapter 4.10. Assuming the many-body quantum state is given by a thermal density matrix at temperature T for *quasi-particles* (represented by the operators in (4.62), (4.64)), show that the (constant) Fock field vanishes, $F = U_0\langle\hat{\Psi}_\uparrow^\dagger(\mathbf{x})\hat{\Psi}_\downarrow(\mathbf{x})\rangle = 0$. We had used this in the actual derivation of the quasi-particles, so you have now shown that also this was self-consistent. [*Hint: Start as we did when deriving the gap-equation. Also re-read section 3.4.4. for some similar manipulations, there for Bosons and trap-states instead of momentum states*]. [*5 points*]

Solution: First we realize that in a homogeneous system F is independent of position. We can thus look at the spatially averaged value, which will simplify things: $F = \int d^3x F(\mathbf{x})\ /\mathrm{V}$.

We then write field operators in F in momentum space and obtain

$$
\begin{aligned}
F &= \int d^3x \frac{U_0}{\mathcal{V}}\langle\hat{\Psi}_\uparrow^\dagger(\mathbf{x})\hat{\Psi}_\downarrow(\mathbf{x})\rangle \overset{(4.32)}{=} \frac{U_0}{\sqrt{2\pi}^3\mathcal{V}^2}\sum_{k,k'}\underbrace{\left[\int d^3x \exp\left[i(k'-k)x\right]\right]}_{=(2\pi)^3\delta^{(3)}(k'-k)}\langle\hat{a}_{k,\uparrow}^\dagger\hat{a}_{k',\downarrow}\rangle \\
&= \frac{\sqrt{2\pi}^3 U_0}{\mathcal{V}}\sum_k \mathrm{Tr}[\,\hat{\rho}\,\hat{a}_{k,\uparrow}^\dagger\hat{a}_{k,\downarrow}] \\
&= \frac{\sqrt{2\pi}^3 U_0}{\mathcal{V}}\sum_k \mathrm{Tr}[\,\hat{\rho}\,(u_k^*\hat{\alpha}_{\uparrow,k}^\dagger - v_k^*\hat{\alpha}_{\downarrow,-k})(u_k\hat{\alpha}_{\downarrow,k} - v_k\hat{\alpha}_{\uparrow,-k}^\dagger)] \\
&= \frac{\sqrt{2\pi}^3 U_0}{\mathcal{V}}\sum_k \times\mathrm{Tr}[\,\hat{\rho}\,(u_k^*u_k\hat{\alpha}_{\uparrow,k}^\dagger\hat{\alpha}_{\downarrow,k} - u_k^*v_k\hat{\alpha}_{\uparrow,k}^\dagger\hat{\alpha}_{\uparrow,-k}^\dagger - v_k^*u_k\hat{\alpha}_{\downarrow,-k}\hat{\alpha}_{\downarrow,k} + v_k^*v_k\hat{\alpha}_{\downarrow,-k}\hat{\alpha}_{\uparrow,-k}^\dagger)].
\end{aligned}
\tag{5}
$$

In the third line we used the inverse Bogoliubov transform Eq. (4.49).

Since $\hat{\rho}$ is given as mixture of Fock states for quasi particle occupation numbers, all off-diagonal terms vanish, which means non-vanishing terms need the same spin-index, one α and one $\alpha^\dagger$ with same momentum index.

This disqualifies all terms so we proof the result $F = 0$. [*Disclaimer: The derivation above has issued with factors of $\sqrt{2\pi}, \mathcal{V}$ due to the joint use of integrals and sums over continuous modes. These will be fixed in a future release, but cannot affect the present result.*

(2) BCS State and Cooper pairs. Explore the relation ship between the BCS many-body state and cooper pairs. [*Some of the answers to the following questions can be found in the lecture notes. This question is supposed to encourage you to go through that I detail. I suggest you do it from scratch without looking at the notes, and only use them if you get stuck or to confirm your results. For you hand-in, it is then of course even more important that you write a lot of text to show that you understood everything. Copying the lecture notes will not be sufficient*]

(a) In the lecture we defined the Cooper pair creation operator:

$$\hat{c}^\dagger = \int d^3\mathbf{x} \int d^3\mathbf{y}\, \psi_0(\mathbf{x},\mathbf{y}) \hat{\Psi}^\dagger_\uparrow(\mathbf{x}) \hat{\Psi}^\dagger_\downarrow(\mathbf{y}), \tag{6}$$

Write explicitly the state $\hat{c}^\dagger |\, 0\, \rangle$, where $|\, 0\, \rangle$ is the vaccuum state, in first quantized representation. Use that the spatial wave-function is symmetric $\psi_0(\mathbf{x},\mathbf{y}) = \psi_0(\mathbf{y},\mathbf{x})$. [*3 points*]

(b) Express $\hat{c}^\dagger$ in terms of momentum creation operators, instead of position space field operators. [*3 points*]

(c) Show that the coherent state of Cooper pairs $|\, \gamma\, \rangle = \mathcal{N} \exp[\gamma \hat{c}^\dagger] |\, 0\, \rangle$ is the same as $|\, \psi BCS\, \rangle = \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}} \hat{a}^\dagger_{\uparrow\mathbf{k}} \hat{a}^\dagger_{\downarrow\mathbf{k}}\right) |\, 0\, \rangle$. [*4 points*]

Solution:

(a) The state $\hat{c}^\dagger |\, 0\, \rangle$ in the position space representation can be given as:

$$\begin{aligned}
\langle\, \mathbf{x}'\mathbf{y}'\, |\hat{c}^\dagger |\, 0\, \rangle &= \langle\, \mathbf{x}\mathbf{y}\, | \int d^3\mathbf{x} \int d^3\mathbf{y}\, \psi_0(\mathbf{x},\mathbf{y}) \hat{\Psi}^\dagger_\uparrow(\mathbf{x}) \hat{\Psi}^\dagger_\downarrow(\mathbf{y}) |\, 0\, \rangle \\
&= \int d^3\mathbf{x} \int d^3\mathbf{y}\, \psi_0(\mathbf{x},\mathbf{y}) \langle\, \mathbf{x}'\mathbf{y}'\, |\, \mathbf{y} \downarrow; \mathbf{x} \uparrow\, \rangle, \qquad (7)
\end{aligned}$$

where we have invented a position space ket according to $\hat{\Psi}^\dagger_\uparrow(\mathbf{x}) \hat{\Psi}^\dagger_\downarrow(\mathbf{y}) |\, 0\, \rangle = |\, \mathbf{y} \downarrow; \mathbf{x} \uparrow\, \rangle$, which means “a particle at y with spin down and another one at x with spin up”, see discussion after Eq. (2.27). We can split the state into single-particles states, taking into account that Fermionic many-body states are always implied to be anti-symmetric!

$$\langle\, \mathbf{x}'\mathbf{y}'\, |\hat{c}^\dagger |\, 0\, \rangle = \int d^3\mathbf{x} \int d^3\mathbf{y}\, \psi_0(\mathbf{x},\mathbf{y}) \langle\, \mathbf{x}'\mathbf{y}'\, | \frac{1}{\sqrt{2}} (|\, \mathbf{y} \downarrow\, \rangle \otimes |\, \mathbf{x} \uparrow\, \rangle - |\, \mathbf{x} \uparrow\, \rangle \otimes |\, \mathbf{y} \downarrow\, \rangle). \tag{8}$$

Now the pieces before and after the $\otimes$ symbol denote particle 1, particle 2. Now we consider the first term only, and in that rename integration variables $\mathbf{x} \leftrightarrow \mathbf{y}$. Thanks to the symmetry of ψ_0, we then reach

$$\begin{aligned}
&= \int d^3\mathbf{x} \int d^3\mathbf{y}\, \psi_0(\mathbf{x},\mathbf{y}) \langle\, \mathbf{x}'\mathbf{y}'\, | \frac{1}{\sqrt{2}} (|\, \mathbf{x} \downarrow\, \rangle \otimes |\, \mathbf{y} \uparrow\, \rangle - |\, \mathbf{x} \uparrow\, \rangle \otimes |\, \mathbf{y} \downarrow\, \rangle) \\
&= \int d^3\mathbf{x} \int d^3\mathbf{y}\, \psi_0(\mathbf{x},\mathbf{y}) \underbrace{\langle\, \mathbf{x}'\mathbf{y}'\, |\, \mathbf{x}\mathbf{y}\, \rangle}_{\delta(\mathbf{x}-\mathbf{x}')\delta(\mathbf{y}-\mathbf{y}')} \otimes \frac{1}{\sqrt{2}} (|\downarrow\uparrow\rangle - |\uparrow\downarrow\rangle). \qquad (9)
\end{aligned}$$

$$= \psi_0(\mathbf{x}', \mathbf{y}') \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle). \quad (10)$$

(b) See discussion in lecture notes after Eq. (4.73).

(c) See discussion in lecture notes after Eq. (4.73).

(3) Superconductivity and Superfluidity Write a short (about one page) essay about superconductivity and Fermion superfluidity based on what you learnt in this lecture and/or read elsewhere. Use google also. Focus on the essentials only. Make sure to touch the points below. [*10 points*][*Make sure this is your own text. Plagiarism will strictly not be tolerated*]

Solution: see lecture notes

(4) Bosonic versus Fermionic 2D Scattering
The template file `Assignment6_phy635_program_draft_v2.xmds` is set up to solve the Schrödinger equation for the relative coordinate $\mathbf{r} = [r_x, r_y]$ for a pair of distinguishable particles of mass m undergoing a scattering process in 2D, interacting with a Gaussian potential $U(\mathbf{r}) = A \exp\left(-\mathbf{r}^2/2/\sigma_{\text{int}}^2\right)$. We use dimensionless units where $\hbar = 1$. The particles are initialised in a wavepacket $\psi(\mathbf{r}) = \mathcal{N} \exp(-(\mathbf{r} - \mathbf{r}_0)^2/(2\sigma^2)) \exp[i\mathbf{k}_{\text{ini}}\mathbf{r}]$, such that they collide (reach $\mathbf{r} = 0$) at half the simulation time. [*Note:* $\sigma \neq \sigma_{int}$].
(4a) The range of the interaction potential set up in the code initially is $\sigma_{\text{int}} = 0.002$. Calculate the impact parameter $d_{l=1}$ for which the particles, considered classically, would have angular momentum corresponding to the quantum mechanical $l = 1$ ($|L| = \hbar\sqrt{l(l+1)}$) and compare with $\sigma_{\text{int}} = 0.002$. For this you need $\mathbf{k}_{\text{ini}} = 100$ from the code. [*2 points*].
Solution: *The impact parameter d and angular momentum are classically linked by $\mathbf{L} = \mathbf{r} \times \mathbf{p} = dp = d\hbar k$. Thus we solve $\hbar\sqrt{l(l+1)} = d\hbar\mathbf{k}_{ini}$ for d at $l = 1$ and get $d = \sqrt{2}/100 \approx 0.015$. This is significantly more than the range of interactions $\sigma_{int} = 0.002$, thus according to the cartoon in the lecture, we should be in the s-wave scattering regime.*

(4b) Run the code and analyse the resultant scattered wave with the attached script `slideshow_ultracold_scattering_v2.m`. This is set up to amplify small intensity features in the matter wave, since scattering is kept weak (small A), so that perturbation theory remains valid. Discuss your findings, relate them to the result of (4a). [*4 points*]
Solution: See figures below discussion is in the captions

(4c) Now modify the code such that it considers the scattering of (i) indistinguishable Bosons, (ii) indistinguishable Fermions. Re-run the scattering of (b) and discuss and interpret your results. [*4 points*]
Solution: For this we just have to change the initial state into a (anti-) symmetrised wavefunction. See figures below discussion is in the captions

(4d, bonus) Explore what happens when you now significantly extend the range of the potential σ_{int}.

Figures:

4a see above

4b Fig. 1, Fig. 2, and Fig. 3 are real and imaginary parts of the wave-function for distinguishable particles with small amplitude of the potential, $A = 200$.

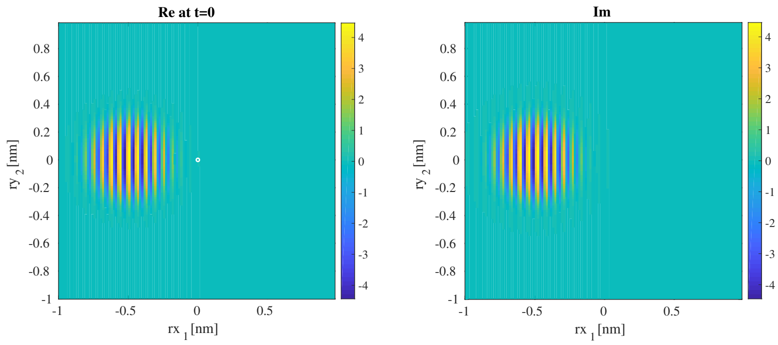

Fig. 1. The real and imaginary parts of the wave-function for the distinguishable particles at $t = 0.0$

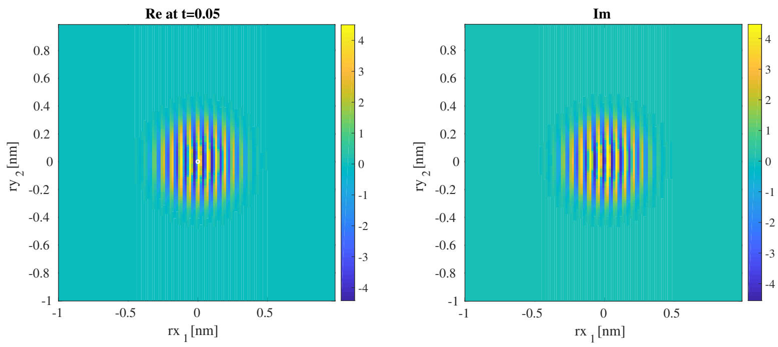

Fig. 2. The real and imaginary parts of the wave-function for the distinguishable particles at the time of interaction.

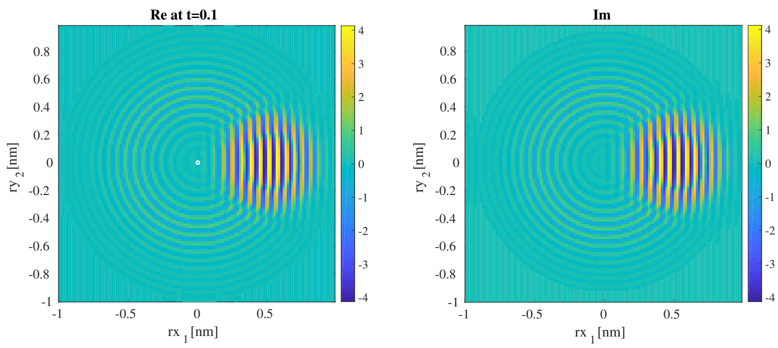

Fig. 3. The real and imaginary parts of the wave-function for the distinguishable particles after the interaction. We can see the isotropic radially outgoing wave from s-wave scattering.

4c Fig. 4, Fig. 5, and Fig. 6 are real and imaginary parts of the wave-function for Bosons with small amplitude of the scattering potential, $A = 200$. *Similarily Fig. 7, Fig. 8, and Fig. 9 are real and imaginary parts of the wave-function for Fermions.*

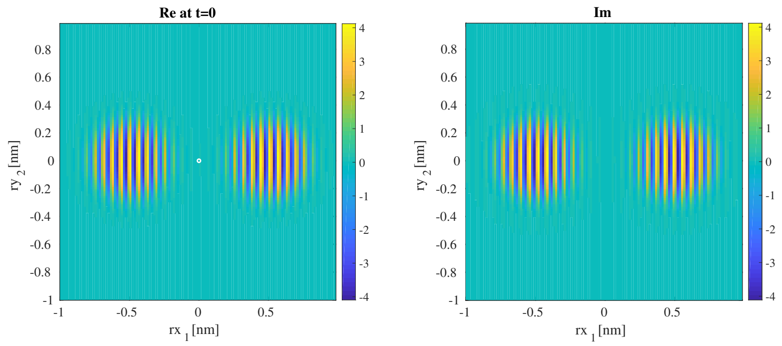

Fig. 4. The real and imaginary parts of the wave-function for the Bosons after at $t = 0.0$.

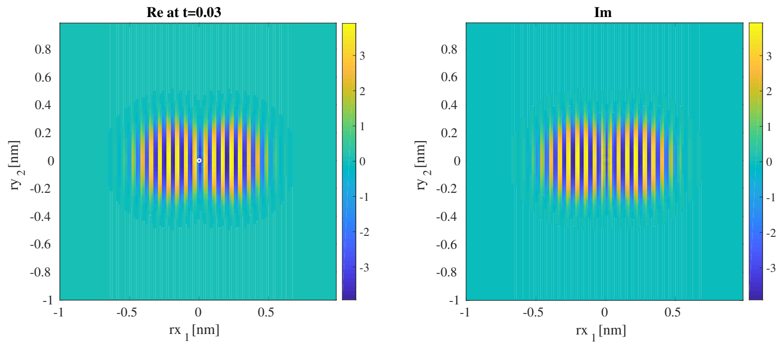

Fig. 5. The real and imaginary parts of the wave-function for the Bosons at the time of interaction.

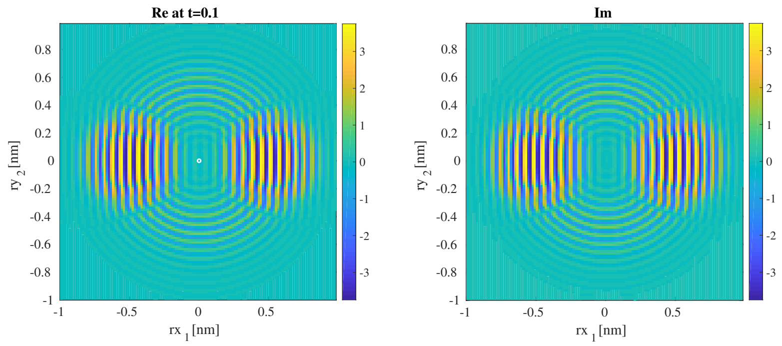

Fig. 6. The real and imaginary parts of the wave-function for the Bosons after the interaction. Also for Bosons we see a radially outgoing wave from s-wave scattering.

4d When increasing the range of the potential, we leave the regime with only s-wave scattering (see 4a). Thus we recover a scattered wave also for Fermions.

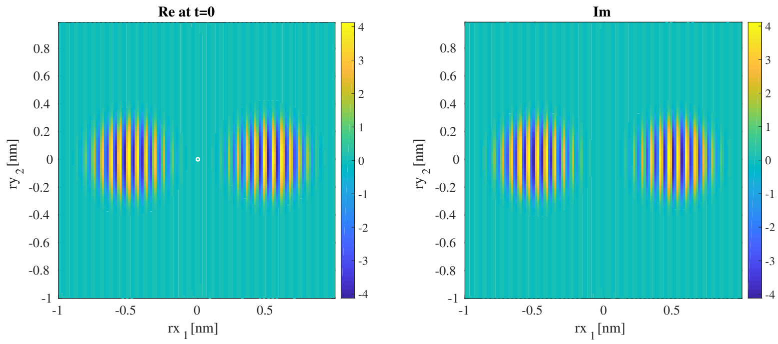

Fig. 7. The real and imaginary parts of the wave-function for the Fermions after at $t = 0.0$.

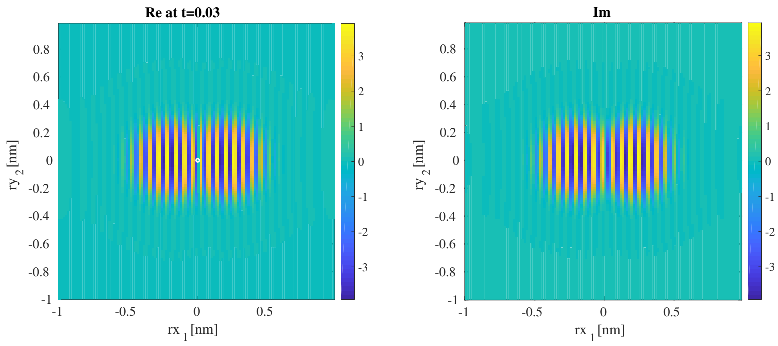

Fig. 8. The real and imaginary parts of the wave-function for the Fermions at the time of interaction.

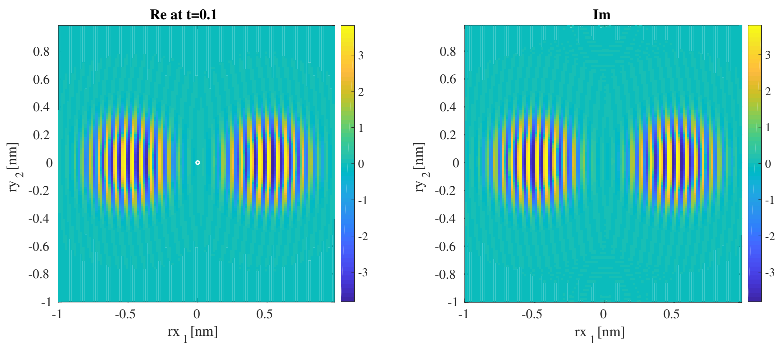

Fig. 9. The real and imaginary parts of the wave-function for the Fermions after the interaction. Here we see no radially outgoing wave. This is because there is no s-wave scattering for Fermions, and p-wave scattering is suppressed. Another way to think of this, is that two radially outgoing scattered waves such as in Fig. 3 from the two “piecesöf the many-body wave function destructively interfere due to the (-1) sign difference between them.