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Superfluidity of fermionic pairs in a harmonic trap. Comparative studies: Local Density Approximation and Bogoliubov-de Gennes solutions

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Abstract

Experiments with ultracold gases on the lattice give the opportunity to realize superfluid fermionic mixtures in a trapping potential. The external trap modifies the chemical potential locally. Moreover, this trap also introduces non-homogeneity in the superconducting order parameter. There are, among other approaches, two methods which can be used to describe the system of two-component mixtures loaded into an optical lattice: the Local Density Approximation (LDA) and the self-consistent Bogoliubov–de Gennes equations. Here, we compare results obtained within these two methods. We conclude that the results can be distinguishable only in the case of a small value of the pairing interaction.

1. Introduction

Recent progress in experimental techniques in ultracold quantum gases gives ground to believe that they are good candidates for realization of *quantum simulators* [1–5]. This progress gives the opportunity to study different types of quantum models, well established already in many-body physics [5–7].

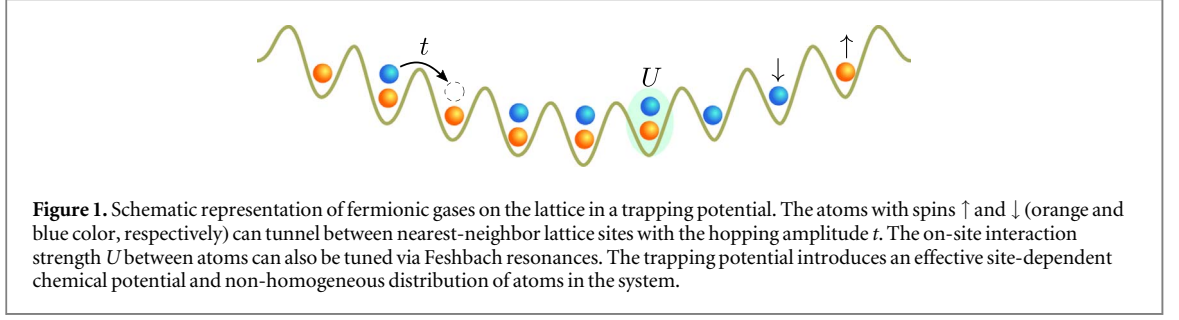
Parameters such as the depth of the periodic trapping potential or the lattice geometry can be tuned with a high level of control in experiments. Moreover, the interaction strengths can also be fully controlled via so-called Feshbach resonances [8], giving the possibility of realization of repulsively and attractively interacting systems [9]. The latter allows for an experimental study of superfluid states [10–12].

Typically, a system of ultracold atoms is located in an external potential, for instance in a harmonic trap. This potential introduces some effective site-dependent chemical potential and non-homogeneous distribution of the particles in the system. As a consequence, non-uniform superconducting order parameter is expected. The system can be studied theoretically via several methods. In this paper, we compare the results obtained within the Local Density Approximation (LDA) and the self-consistent Bogoliubov–de Gennes (BdG) equations, for a system of an ultracold attractive fermionic gas loaded into a one-dimensional (1D) optical lattice, put in a harmonic trap.

The paper is organized as follows: first, we shortly introduce the model as well as the above mentioned methods (section 2). In section 3, we present and discuss numerical results. Finally, we summarize in section 4.

2. Model and techniques

We investigate a fermionic gas loaded onto a one-dimensional lattice, in a harmonic trap, which is schematically illustrated in figure 1. The system under consideration can be described by the Hamiltonian:



$$\mathcal{H} = \sum_{i,j,\sigma} (-t_{ij} - \mu_i \delta_{ij}) c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) describes the creation (annihilation) operator of a particle in the site i and of spin $\sigma = \{\uparrow, \downarrow\}$. For simplification, we assume only hopping between the nearest-neighbor sites, i.e., $t_{(i,j)} \equiv t$. $U < 0$ is the on-site pairing interaction. μ_0 is the chemical potential of the trapped gases, determining the total number of particles in the system, while $\mu_i = \mu_0 + V(r_i)$ is an effective on-site chemical potential. $V(r_i)$ is the trapping potential, typically given in harmonic form, i.e., $V \sim (r_0 - r_i)^2$, where r_0 is the center of the trap. The interaction term is treated within the mean-field approximation:

$$n_{i\uparrow} n_{i\downarrow} = \Delta_i^* c_{i\downarrow} c_{i\uparrow} + \Delta_i c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger - |\Delta_i|^2, \quad (2)$$

where $\Delta_i = \langle c_{i\downarrow} c_{i\uparrow} \rangle$ is the s -wave superconducting order parameter (SOP). Hence, the mean-field Hamiltonian in real space takes the form:

$$\mathcal{H}^{MF} = \sum_{i,j,\sigma} (t_{ij} - \mu_i \delta_{ij}) c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i (\Delta_i^* c_{i\downarrow} c_{i\uparrow} + H.c.) - U \sum_i |\Delta_i|^2. \quad (3)$$

2.1. Local density approximation solution

The LDA method is based on an assumption that, locally, the system behaves like a uniform gas [1, 2]. The parameters of the system depend solely on the value of the particle density $n_i = n_{i\uparrow} + n_{i\downarrow}$ (i.e. the average number of particles), at each point i of space [13, 14]. Hence, the local SOP is defined only by $n_i = n(\mu_i)$. In the presence of the trapping potential, local lattice potential is given by $\mu_i = \mu_0(n_i) + V(r_i)$, called *Thomas–Fermi equation* [1, 2]. The chemical potential μ_0 is fixed by the condition $\sum_i n_i = N$, where N is the total number of particles in the system. In a general case, the functional $\Delta_i \equiv \Delta(n_i) = \Delta(\mu_i)$ can be found starting from the solution for the homogeneous system, i.e., $\Delta_i = \Delta(n = n_i)$, which gives $\Delta_i = \Delta(\mu = \mu_i)$.

First, let us shortly describe derivation of the equations which are useful in the LDA method [15, 16]. In the case of a homogeneous system ($\mu_i \equiv \mu$ and $\Delta_i \equiv \Delta$), the Hamiltonian (3) takes the following form in momentum space:

$$\mathcal{H}^{MF} = \sum_{k\sigma} \mathcal{E}_k c_{k\sigma}^\dagger c_{k\sigma} + U \sum_k (\Delta^* c_{k\uparrow} c_{-k\downarrow} + h.c.) - U \sum_k |\Delta|^2, \quad (4)$$

where $\mathcal{E}_k = -2t \cos(k) - \mu$ is the single-particle dispersion relation of the one-dimensional system. Here, it should be noticed that the presented derivations do not depend on the lattice dimensionality. Using anti-commutation relation, the first term can be rewritten as:

$$\sum_{k\sigma} \mathcal{E}_k c_{k\sigma}^\dagger c_{k\sigma} = \sum_k [\mathcal{E}_k c_{k\uparrow}^\dagger c_{k\uparrow} + \mathcal{E}_k (1 - c_{k\downarrow} c_{k\downarrow}^\dagger)]. \quad (5)$$

This allows us to write down the Hamiltonian \mathcal{H}^{MF} in the Nambu notation:

$$\mathcal{H}^{MF} = \sum_k \Phi_k^\dagger \mathbb{H}_k \Phi_k + \sum_k (\mathcal{E}_k - U|\Delta|^2), \quad (6)$$

$$\mathbb{H}_k = \begin{pmatrix} \mathcal{E}_k & \Delta \\ \Delta^* & -\mathcal{E}_k \end{pmatrix},$$

where $\Phi_k^\dagger = (c_{k\uparrow}^\dagger, c_{-k\downarrow})$ are the Nambu spinors. The system can be solved using the Bogoliubov transformation:

$$\begin{pmatrix} c_{k\uparrow}^\dagger \\ c_{-k\downarrow} \end{pmatrix} = \begin{pmatrix} u_k & v_k \\ -v_k & u_k \end{pmatrix} \begin{pmatrix} \gamma_k^\dagger \\ \gamma_k \end{pmatrix}, \quad (7)$$

where γ^\dagger and γ are the quasiparticle operators. The spectrum of the Hamiltonian is given by $\lambda_\pm = \pm \sqrt{\mathcal{E}_k^2 + \Delta^2}$, while

$$\left. \begin{matrix} u_k^2 \\ v_k^2 \end{matrix} \right\} = \frac{1}{2} \left(1 \pm \frac{\mathcal{E}_k}{\sqrt{\mathcal{E}_k^2 + \Delta^2}} \right). \quad (8)$$

Hence, the coefficients u_k and v_k satisfy the condition: $u_k^2 + v_k^2 = 1$. The energy of the system is determined from the grand-canonical potential $\Omega \equiv -k_B T \ln(\text{Tr}[\exp(-\mathcal{H}^{MF}/k_B T)])$, while the SOP value is determined from its global minimum. In the absence of a discontinuous phase transition, the minimum of energy corresponds to $\partial\Omega/\partial\Delta = 0$ or, equivalently:

$$\Delta = -\frac{U}{N} \sum_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}} [f(\lambda_{\mathbf{k}}^+) - f(\lambda_{\mathbf{k}}^-)]. \quad (9)$$

The above equation is called *the gap equation*. Here, $f(\omega) = [1 + \exp(\omega/k_B T)]^{-1}$ is the Fermi–Dirac distribution at temperature T , while N is the number of states. Similarly, the occupations $n_{k\sigma} = \langle c_{k\sigma}^\dagger c_{k\sigma} \rangle$ can be found as:

$$\left. \begin{matrix} n_{k\uparrow} \\ n_{k\downarrow} \end{matrix} \right\} = u_{\mathbf{k}}^2 f(\lambda_{\mathbf{k}}^\pm) + v_{\mathbf{k}}^2 f(-\lambda_{\mathbf{k}}^\mp), \quad (10)$$

which is equivalent to $\sum_{k\sigma} n_{k\sigma} = -\partial\Omega/\partial\mu$. As a result, one can find values of $\Delta(\mu)$ and $n(\mu)$ within the LDA method.

2.2. Bogoliubov–de Gennes solution

In the case of the non-homogeneous Hamiltonian (3), the system can be solved within the *Bogoliubov–Valatin* transformation:

$$c_{i\sigma} = \sum_n (u_{in\sigma} \gamma_{n\sigma} - \sigma v_{in\sigma}^* \gamma_{n\bar{\sigma}}^\dagger), \quad (11)$$

where $\gamma_{n\sigma}$ and $\gamma_{n\bar{\sigma}}^\dagger$ are the *quasi-particle* fermionic operators and $\bar{\sigma} = -\sigma$. The above transformation can be treated as an extended version of the transformation (7) in real space. If the Hamiltonian is diagonalized under the transformation (11), i.e., $\mathcal{H}^{MF} = \sum_{n\sigma} \mathcal{E}_{n\sigma} \gamma_{n\sigma}^\dagger \gamma_{n\sigma}$, the relations [17]:

$$[\mathcal{H}^{MF}, \gamma_{n\sigma}] = -\mathcal{E}_{n\sigma}, \quad [\mathcal{H}^{MF}, \gamma_{n\bar{\sigma}}^\dagger] = \mathcal{E}_{n\sigma} \gamma_{n\bar{\sigma}}^\dagger \quad (12)$$

hold such that one straightforwardly finds *Bogoliubov–de Gennes equations* [18] (called also *Blonder–Tinkham–Klapwijk equations*):

$$\mathcal{E}_{n\sigma} \begin{pmatrix} u_{in\sigma} \\ v_{in\bar{\sigma}} \end{pmatrix} = \sum_j \begin{pmatrix} H_{ij\sigma} & \Delta_{ij} \\ \Delta_{ij}^* & -H_{ij\bar{\sigma}}^* \end{pmatrix} \begin{pmatrix} u_{jn\sigma} \\ v_{jn\bar{\sigma}} \end{pmatrix}, \quad (13)$$

where $H_{ij\sigma} = -t\delta_{(i,j)} - \mu_i \delta_{ij}$ is the single-particle Hamiltonian and $\Delta_{ij} = U \Delta_i \delta_{ij}$ are the on-site SOPs. Due to the symmetry of the BdG equations with respect to spin inversion, we can find an identity relation between eigenpairs:

$$E_{n\sigma} \begin{pmatrix} u_{in\sigma} \\ v_{in\bar{\sigma}} \end{pmatrix} \rightarrow -E_{n\bar{\sigma}} \begin{pmatrix} -v_{in\sigma} \\ u_{in\bar{\sigma}}^* \end{pmatrix}. \quad (14)$$

The SOPs can be found self-consistently as:

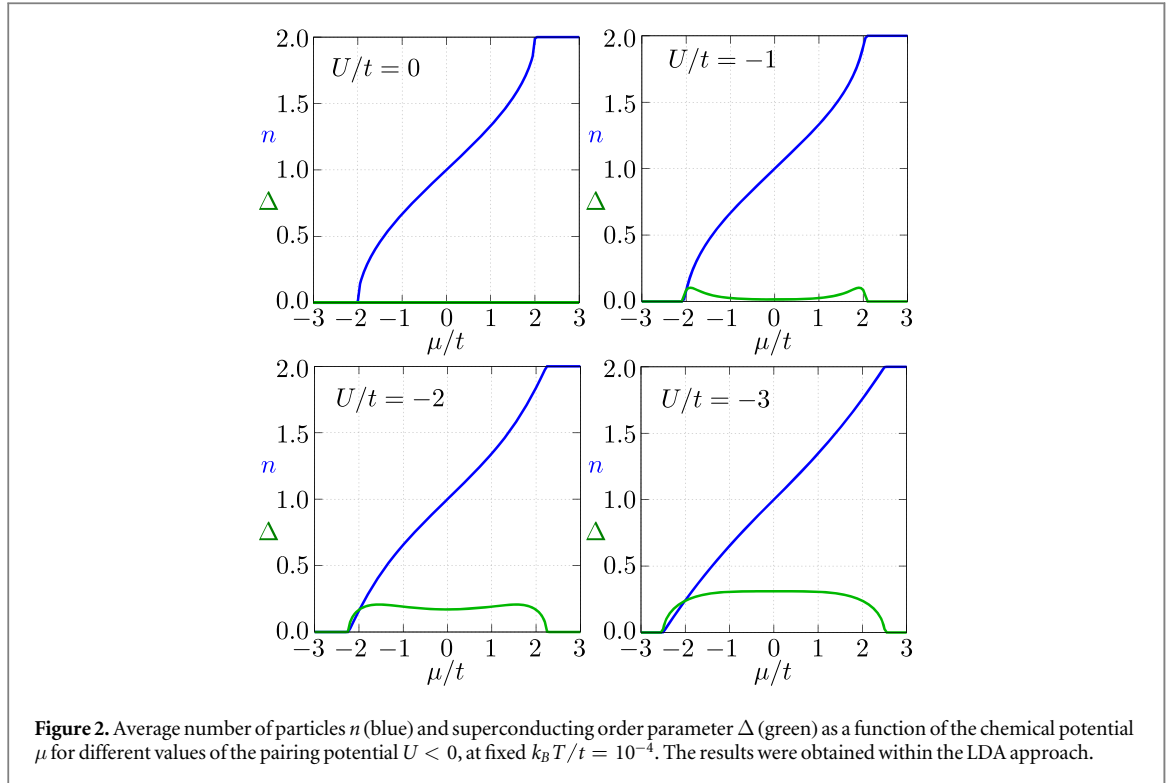
$$\begin{aligned} \Delta_i &= \langle c_{i\downarrow} c_{i\uparrow} \rangle \\ &= \sum_n [u_{in\uparrow} v_{in\downarrow}^* f(\mathcal{E}_{n\uparrow}) - u_{in\downarrow} v_{in\uparrow}^* f(-\mathcal{E}_{n\downarrow})]. \end{aligned} \quad (15)$$

In a similar way, the site-dependent average number of particles, $n_i = n_{i\uparrow} + n_{i\downarrow}$ can be determined, where:

$$\begin{aligned} n_{i\sigma} &= \langle c_{i\sigma}^\dagger c_{i\sigma} \rangle \\ &= \sum_n [|u_{in\sigma}|^2 f(\mathcal{E}_{n\sigma}) + |v_{in\bar{\sigma}}|^2 f(-\mathcal{E}_{n\bar{\sigma}})]. \end{aligned} \quad (16)$$

2.3. Numerical implementation

As has been pointed out in the previous paragraph, the chemical potential μ_0 of the system in the trapping potential is fixed by the total number of particles N . Next, the solution of the system within the LDA method is defined by the effective potential μ_i given by the Thomas–Fermi equation. Hence, the corresponding SOP Δ can be found by minimization of $\Omega(\Delta)$ at fixed μ_i [19–21]. In fact, this way is equivalent to the one in which equation (9) should be solved [22]. The huge advantage of this method is based on the fact that it is relatively simple to implement and quite quickly solvable even for a trapped system, due to an efficient procedure of finding the solution for a homogeneous system. For instance, in the two-dimensional (2D) case, the solution (the minimum of the grand canonical potential) can be found for the system with around a thousand sites [21].



In turn, the self-consistent solution Δ_i (15) and $n_{i\sigma}$ (16) of the BdG equations (13), in the presence of the trapping potential, can be found only when all eigenpairs are known. Hence, the BdG equations are associated with the exact diagonalization of the Hamiltonian in matrix form, which can be found numerically using one of the available numerical libraries, e.g. LAPACK [23], Intel MKL [24] or MAGMA [25, 26]. However, this method is very computational time-consuming $\sim N^3$ and leads to a limitation in the system size N . This problem can be partially solved by using the sparse matrices storage implemented in some modern softwares, for instance ARPACK [27]. Moreover, there exist some iterative methods for solving the BdG equations [28–32], based on the kernel polynomial method [33]. For instance, in the *Chebyshev–Bogoliubov–de Gennes method*, the Chebyshev expansion of Green’s functions is implemented. This type of methods allows to study the large size systems, even with hundreds or thousands sites [32]. Moreover, in some physical problems, it is reasonable to limit the number of eigenpairs to only few nearest ones to ‘zero energy’ (i.e. the Fermi level). This issue is implemented, e.g., in FEAST [34] and it can be applicable to topological edge states investigations, for instance.

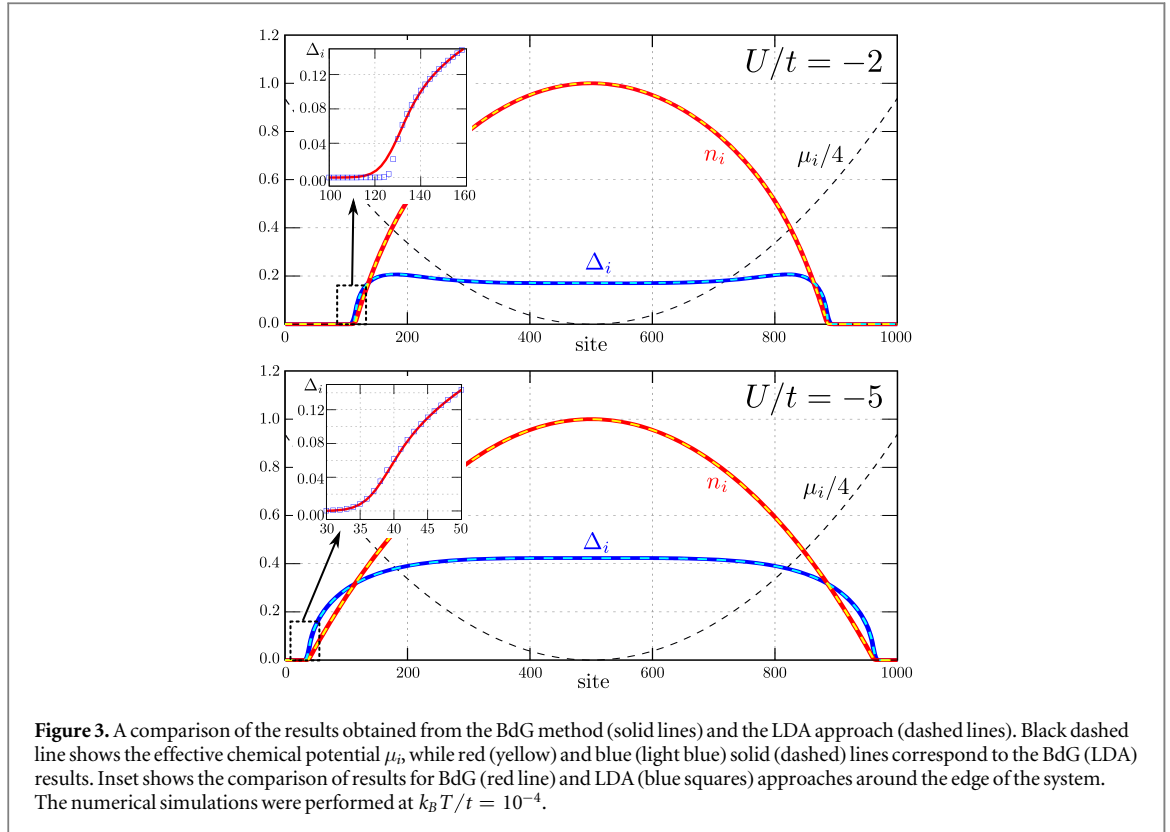
3. Numerical results and discussion

3.1. Spin-balanced system

Here, we describe the balanced system case, which means the average number of particles with opposite spin in each site is equal ($n_{i\uparrow} = n_{i\downarrow}$). Due to the fact that the average number of particles n_i in each site is determined by the effective chemical potential μ_i , to perform the calculation within both methods, the chemical potential is discretized with the parametrization: $\mu_i = \mu + V(r_i)$.

Figure 2 shows n versus μ and Δ versus μ dependences, obtained within LDA calculations. In the case of a one-dimensional system, the band edges are at $\pm\mu = 2t$. At $U/t = 0$, the chemical potential changes from $-2t$ to $2t$, which corresponds to the filling $n = 0$ and $n = 2$ at the band edges. The SOP is equal to zero for the non-interacting system. With increasing on-site interaction, the SOP increases. For intermediate couplings, the chemical potential drops below the lower band edge, which, according to the Leggett criterion [35], indicates the BCS-BEC crossover [36]. Found values of the $n(\mu)$ and $\Delta(\mu)$ can be used as a solution of the system for a given $U < 0$ from the LDA approach.

Figure 3 shows results in the case of the system in a harmonic trap, $V(r_i) = V_0(r_0 - r_i)^2$. We fix $V_0/t = 15 \times 10^{-6}$. The average number of particles n_i , obtained within these two methods, is comparable for the chosen parameters. A similar behavior is observed for the SOP Δ_i in the center of the trap. However, the situation looks differently at the edge of the harmonic trap (insets). Namely, LDA gives significantly different solutions for the SOP from those obtained within the BdG method at relatively small attractive interactions U



(top panel). A similar behavior has been observed in the case of a spin-imbalanced system in which unconventional pairing [37–39] can be realized at the edge of the system.

It is worth emphasizing that the LDA is a reliable approach when the gradient corrections are relatively small. In turn, the BdG solutions in each site depend on the rest of the system via equations (13) and (15). Hence, the BdG method is a better approach to describe the system under consideration. Moreover, the LDA can also fail in the description of the system in a strong anisotropic trap [40].

3.2. Other applications and limitations

The theoretical predictions within the LDA method are in relatively good agreement with experimental results [41–44]. This method was already successfully implemented in the context of trapped ultracold quantum gases [37, 40, 45–47]. However, the LDA method has some limitations which can be lifted by applying the BdG technique. Below, we give two examples of the systems for which the LDA method fails.

3.2.1. Spin-imbalanced systems

Both methods under consideration can be applied for a spin-imbalanced system, i.e., when $n_{i\uparrow} \neq n_{i\downarrow}$ [13, 48]. This corresponds to the experimental setup with a two-component Fermi mixture, with unequal number of atoms with opposite spins [49–51]. This leads effectively to the substitution $\mathcal{H} \rightarrow \mathcal{H} - h \sum_i (c_{i\uparrow}^\dagger c_{i\uparrow} - c_{i\downarrow}^\dagger c_{i\downarrow})$, where h is the Zeeman magnetic field inducing the spin-imbalance. In the case of the LDA method, this is equivalent to the substitution $\mathcal{E}_k \rightarrow \mathcal{E}_{k\sigma} = \mathcal{E}_k - \sigma h$. Hence, an additional condition is needed in the numerical calculations, i.e. $\delta N = \sum_i (n_{i\uparrow} - n_{i\downarrow})$. Here, the $n_{i\uparrow} - n_{i\downarrow}$ corresponds to the magnetization at i -th site. It is worth mentioning, that the symmetry of the BdG equations, given by equation (14), is preserved.

In the weak coupling limit, at a large spin imbalance (i.e. polarization) [22, 38], the Fulde–Ferrell–Larkin–Ovchinnikov (FFLO) phase [52, 53] can occur. In this case, the SOP is characterized by oscillations in real space and at non-zero local polarization [13, 54]. If the polarization is equal to zero or low, the connection between the phase diagrams of the system without a trapping potential and in the presence of the harmonic trap [55] exists, in the LDA method [22]. Unfortunately, the LDA approach cannot account for the oscillating character of the SOP as well as the oscillations of the average number of particles in the FFLO phase [13, 56]. A similar problem has been observed for the spin-imbalanced gap [57] estimated within the LDA method and the Density Matrix Renormalization Group (DMRG). In this case, the oscillating character of n_i at relatively low polarization has not been reproduced within the LDA method. Moreover, the LDA calculations underestimate critical parameters of the system, with respect to the results obtained within the DMRG [57] or the BdG approach [22].

The situation can be even more complicated in the two dimensional systems. In the case of the harmonic trap, the additional SOP oscillations along the radial direction have been reported [37, 58–60]. However, for the toroidal trap, the oscillations of the SOP can be function of angle, due to rotational symmetry of the system [61–63]. The combination of these two types of oscillations can be expected [64] as well. This case shows an advantage of the BdG technique in the comparison to LDA, i.e. the spin-imbalanced systems with unconventional superconducting phases.

3.2.2. Non-homogeneous systems

The strongly inhomogeneous systems, e.g. systems with long-range magnetic or charge orderings or disordered systems are examples for which the LDA method fails. Apart from the above systems, one should mention ultracold fermionic gases or the condensed matter systems [65]. Here, the impurities [66–68] or vortices [69–71] play the role of inhomogeneity. It is worth mentioning the superconducting systems with spin-density (SDW) or charge-density (CDW) waves coexistence [72–75]. The ‘local’ disorder in the system influences on the properties of the system. Because of the presence of inhomogeneity with ‘long-range’ impact on the system, the LDA method can not be used. In such cases, only the BdG technique is suitable [65].

4. Summary

In this paper, we studied an ultracold fermionic mixture loaded into a one-dimensional lattice, put in a harmonic trap. We briefly compared the Local Density Approximation and the self-consistent Bogoliubov–de Gennes equations—the main assumptions, implementations and limitations of both of these methods. We have shown that both approaches give comparable results in the case of relatively large pairing interactions U . For smaller U , the results for the superconducting order parameter Δ can be significantly different, especially in the case of a small density of particles, i.e. small filling at the edge of the system. Concluding, the results obtained within the LDA method can be treated as a starting point for the more accurate BdG technique. One should be aware of the LDA method limitations. This method is strongly unrecommended to use for spin-imbalanced as well as strongly inhomogeneous systems.

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