Semimetal–superfluid quantum phase transitions in 2D and 3D lattices with Dirac points

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Abstract

We study the superfluid properties of attractively interacting fermions hopping in a family of 2D and 3D lattices in the presence of synthetic gauge fields having $\pi$-flux per plaquette. The reason for such a choice is that the $\pi$-flux cubic lattice displays Dirac points and that decreasing the hopping coefficient in a spatial direction (say, $t_z$), these Dirac points are unaltered: it is then possible to study the 3D–2D interpolation towards the $\pi$-flux square lattice. We also consider the lattice configuration providing the continuous interpolation between the 2D $\pi$-flux square lattice and the honeycomb geometry. We investigate by a mean-field analysis the effects of interaction and dimensionality on the superfluid gap, chemical potential and critical temperature, showing that these quantities continuously vary along the patterns of interpolation. In the two-dimensional cases at zero temperature and half-filling, there is a quantum phase transition occurring at a critical (negative) interaction $U_c$ presenting a linear critical exponent for the gap as a function of $|U - U_c|$. We show that in three dimensions, this quantum phase transition is again retrieved, pointing out that the critical exponent for the gap changes from 1 to $1/2$ for each finite value of $t_z$.

(Some figures may appear in colour only in the online journal)

1. Introduction

Trapped ultracold atoms provide an ideal system to implement quantum simulations of interacting lattice systems [1]: a key tool is given by the use of optical lattices [2], which are used, for instance, to study Josephson dynamics [3] and Mott-superfluid transitions [4]. The low-energy dynamics of ultracold bosons or/and fermions in deep optical lattices is described by Bose or/and Fermi–Hubbard-like models [5, 7]. In this way, a two-component Fermi mixture in a deep optical lattice allows for the physical implementation of Fermi–Hubbard physics with ultracold fermions [6] since the ratio between the tunnelling rate and the on-site energy can be controlled with high precision [8, 1]. The dimensionality, the shape of the lattice and the anisotropy of the system can be as well tailored: e.g., optical lattices with different strengths in each direction can be synthesized.

A further boost for the field of quantum simulations with ultracold atoms has been given by the possibility to simulate Abelian and non-Abelian gauge fields [9], which are the main subject of the present Journal of Physics B special issue. The synthesis of gauge fields very much enlarges the versatility of the use of ultracold atoms, allowing in perspective to explore new types of topological phases.
and to implement strongly correlated states relevant for the topological quantum computation [10]. Synthetic magnetic and electric fields acting on neutral atoms have already been implemented using spatially dependent optical couplings between internal states of the atoms [11, 12]. This technique has been applied to single-component Bose gases [11–13] and to Bose–Einstein condensates with two components [14, 15]. Spin–orbit-coupled Fermi gases were as well recently realized [16, 17].

Artificial gauge potentials can also be studied in the presence of optical lattices. As discussed in [18], by suitably engineering external laser fields, one can control the phase accumulated by an atom tunnelling across a plaquette, resulting in a non-vanishing artificial magnetic field: a gauge potential amounts in general to complex hopping rates on the bonds. Proposals for implementing non-Abelian gauge potentials in optical lattices were also discussed [19]. In the non-Abelian case, the internal degrees of freedom where the gauge potential is acting on are generally hyperfine levels of suitably chosen atoms: e.g., an advantageous choice could be provided by earth alkaline atoms as Yb [20].

Experimental results have been recently obtained for the simulation of magnetic fields for ultracold atoms in optical lattices. Using Raman-assisted tunnelling in an optical superlattice, a large tunable effective magnetic field for ultracold atoms was generated and the ground state of the system studied [21]. A one-dimensional lattice with a controllable complex tunnelling matrix element was obtained from a combination of Raman coupling and radio-frequency magnetic fields in [22], while in [23], a method basis on a shaken spin-dependent square lattice was used to create strong non-Abelian gauge potentials.

A promising and challenging application of synthetic gauge fields is to the tunable experimental realization of systems relevant for high-energy physics and quantum gauge theories [24–35]: in perspective, new developments could permit to study in a controllable experimental setup part of the phase diagrams of gauge theories even strongly coupled, like QCD [36, 34]. Clearly, gauge fields are a basic ingredient required: from the point of view of ultracold atoms, proposals, including ultracold fermions on a square lattice and eventually merged, open the possibility to study graphene physics with the tunable interaction and geometry in ultracold atom setups.

In the light of the obtained progresses and ongoing perspectives, a relevant future achievement appears to be the synthesis of semimetallic systems hosting in 3D Dirac fermions. Graphene is not an immediate candidate for 3D generalizations: stacking up graphene sheets, because of the in-plane hopping along the z-direction, Dirac cones are destroyed [50]. The problem of the existence of Dirac points in 3D lattices has been studied [51, 52] by analysing the required symmetries required: from the point of view of ultracold atoms, a setup with a low number of hopping connections (possibly, only hoppings between nearest neighbours) is required for a practical reason. A relatively simple alternative is offered by the use of gauge potentials: it is indeed possible to show that a square lattice with a constant magnetic field having a $\pi$-flux (half of the elementary flux) on each plaquette has a single-particle energy spectrum displaying Dirac points [53]. This observation has been translated in proposals to realize massless $(2 + 1)$ Dirac fermions using external gauge proposals, including ultracold fermions on a square lattice coupled with properly chosen Rabi fields [54], interacting bosons in a 2D lattice produced by a bichromatic light-shift potential with an additional effective magnetic field [55] and bosons with internal energy levels in a tripod configuration [56].

The 2D setup of a square lattice with $\pi$-flux can be generalized to three dimensions [57, 58] considering a cubic lattice with $\pi$-flux per plaquette, obtained via a magnetic field oriented along the diagonal of the cube: this scheme was the starting point for work about chiral spin liquids [58] and topological insulators and superconductors [59]. The energy spectrum still shows Dirac points and 3D Dirac fermions [28]. Therefore, using two-component Fermi gas in a constant magnetic field acting on both the components, one can have a semimetallic behaviour at half-filling: adding an attractive interaction, one obtains a 3D version of the semimetal–superfluid transition studied in 2D [44–48].

This paper aims to analyse at a mean-field level the superfluidity in a family of 2D and 3D lattice systems with Dirac points and in the presence of attractive point-like
interactions between the two species of atoms. Since the Dirac points are unaltered by varying the hopping coefficient in a spatial direction (say, \(t_z\)), it is possible to study in this system the 3D–2D interpolation between the \(\pi\)-flux cubic lattice the \(\pi\)-flux square lattice. We also consider the lattice configuration providing the continuous interpolation between the 2D \(\pi\)-flux square lattice and the honeycomb geometry. Among these patterns of interpolations, the mean-field equations are solved, studying the behaviour of the superfluid gap, the critical temperature and the chemical potential.

2. The models

In this section, we introduce the attractive Hubbard model and the lattices studied in the rest of this paper; we also briefly summarize the mean-field treatment, writing down the equations for the gap and the number of particles studied in the following sections. The attractive Hubbard Hamiltonian is written as

\[ \hat{H} = - \sum_{\langle i,j \rangle, \sigma} \left( t_{ij} c_{i \sigma}^\dagger c_{j \sigma} + \text{h.c.} \right) - U \sum_i c_{i \uparrow}^\dagger c_{i \downarrow}^\dagger c_{i \downarrow} c_{i \uparrow}. \]  

(1)

In equation (1), \(c_{i \sigma}\) is the fermionic operator destroying a particle in the site \(i\) of the lattice with (pseudo)spin \(\sigma = \uparrow, \downarrow\); the sum in the first term of equation (1) is on distinct pairs of nearest neighbours and \(U\) will be assumed to be positive corresponding to on-site attractions. The total number of particles is denoted by \(N\) and \(n\) is the filling (number of particles per lattice site): denoting the number of lattice sites by \(\Omega\), it is \(n = N/\Omega\). Within the grand canonical ensemble, it is necessary to introduce the chemical potential \(\mu\) and consider the operator \(\hat{\mathcal{H}} = \mu \hat{N}\) for describing the system.

The hopping rates \(t_{ij}\) entering equation (1) are in general complex: in the presence of a synthetic field \(\mathbf{B} = \nabla \times \mathbf{A}\) acting on both the Fermi species, through the Peierls substitution, one introduces complex hopping rates in the kinetic term of the Hubbard Hamiltonian. We will assume that the synthetic gauge potential \(\mathbf{A}\) is acting on both species in the same way, corresponding to a \(U(1) \times U(1)\) gauge potential. In particular, the hopping rate from the site \(i\) to the site \(j\) reads

\[ t_{ij} = |t_{ij}| \exp \left( -i \int_0^t \mathbf{A} \cdot \mathbf{d}t \right). \]

(2)

We consider in section 3 a magnetic field along \(\hat{z}\), while in section 4, the magnetic field is taken along the direction \((1, 1, 1)\). In section 4, we also consider the possibility that \(|t_{ij}|\) depends on the direction, having \(|t_{ij}| \equiv t\) along the directions \(\hat{x}\), \(\hat{y}\) and \(|t_{ij}| \equiv t_z\) along \(\hat{z}\): this can be obtained by using optical lattices of a different strength in the \(\hat{z}\)-directions [60].

We denote by \(\epsilon(\mathbf{k})\) the single-particle energy spectrum of Hamiltonian (1) with \(U = 0\), denoted by \(\hat{H}_0:\)

\[ \hat{H}_0 = - \sum_{\langle i,j \rangle, \sigma} \left( t_{ij} c_{i \sigma}^\dagger c_{j \sigma} + \text{h.c.} \right). \]

(3)

For a \(D\)-dimensional cubic lattice (lattice spacing is taken equal to 1) and with \(\mathbf{A} = 0\) and \(|t_{ij}| \equiv t\), it is \(\epsilon(\mathbf{k}) = -2t \sum_{\sigma} \cos k_{\sigma\sigma}\). The single-particle spectrum and the corresponding BZs of the \(\pi\)-flux square and cubic lattices will be discussed, respectively, in sections 3 and 4.

In the Hartree–Fock approximation, the interaction term \(c_{i \uparrow}^\dagger c_{i \downarrow}^\dagger c_{i \downarrow} c_{i \uparrow}\) is replaced by the two-particle operator

\[ \langle c_{i \uparrow}^\dagger c_{i \downarrow}^\dagger c_{i \downarrow} c_{i \uparrow} + \langle c_{i \downarrow}^\dagger c_{i \uparrow}^\dagger c_{i \uparrow} c_{i \downarrow} + \langle c_{i \uparrow}^\dagger c_{i \downarrow}^\dagger c_{i \downarrow} c_{i \uparrow} - \langle c_{i \downarrow}^\dagger c_{i \uparrow}^\dagger c_{i \uparrow} c_{i \downarrow} - \langle c_{i \uparrow}^\dagger c_{i \downarrow}^\dagger c_{i \downarrow} c_{i \uparrow} \rangle. \]

(4)

where \(\langle \ldots \rangle\) is the grand canonical average computed with the (non-interacting) Hartree–Fock Hamiltonians [61]. Thanks to translational invariance, we can drop the \(i\)-dependence on the mean values in equation (4): moreover by spin-rotational symmetry, it is \(\langle c_{i \uparrow}^\dagger c_{i \downarrow} \rangle = \langle c_{i \downarrow}^\dagger c_{i \uparrow} \rangle = 0\), \(\langle \sigma \rangle = \langle c_{i \uparrow} c_{i \downarrow} \rangle = \langle c_{i \downarrow}^\dagger c_{i \uparrow} \rangle\).

The gap parameter is as usual defined by \(U(c_{i \uparrow} c_{i \downarrow}) = \Delta\) [61]. The Hartree–Fock–Hamiltonian is then given by

\[ \hat{H}_HF = - \mu \hat{N} = - \sum_{\langle i,j \rangle, \sigma} \left( t_{ij} c_{i \sigma}^\dagger c_{j \sigma} + \text{h.c.} \right) - \mu \sum_i c_{i \sigma}^\dagger c_{i \sigma} + \Delta \sum_i (c_{i \uparrow}^\dagger c_{i \downarrow} + c_{i \downarrow}^\dagger c_{i \uparrow}). \]

(5)

Diagonalizing equation (6) and minimizing the free energy [61], one obtains at temperature \(T\)

\[ \begin{aligned}
\frac{1}{\bar{U}} &= \frac{1}{2\Omega} \sum_{k \in \text{BZ}} \frac{1}{E(k)} \tanh \left( \frac{\beta E(k)}{2} \right) \\
\bar{n} &= \frac{1}{\Omega} \sum_{k \in \text{BZ}} \left[ 1 - \frac{\epsilon_0(k)}{E(k)} \tanh \left( \frac{\beta E(k)}{2} \right) \right] 
\end{aligned} \]

(7)

where \(\beta = 1/k_B T\), \(\epsilon_0(k) = \epsilon(k) - \bar{\mu}\) and

\[ E(k) = \sqrt{\epsilon_0^2(k) + \Delta^2} \]

(8)

is the excitation spectrum.

The solutions of equations (7) reveal in general that by increasing the strength of the attractive interaction \(U\), a BCS–BEC crossover takes place: the chemical potential \(\mu\) decreases with \(U\) increasing [62–64]. Studies of the BCS–BEC crossover for the attractive Hubbard model in cubic lattices are available in the literature [65–69, 60]. Note that a qualitatively correct estimation of the critical temperature (at which \(\Delta = 0\)) requires—far from the BCS limit—the Gaussian fluctuation to be used around the mean-field saddle point [70].

Solutions of the mean-field equations (7) on various 2D and 3D lattices with Dirac points will be presented in the following sections.

3. \(\pi\)-flux square lattice model

In this section, we study the solution of the mean-field equation (7) for a 2D square lattice in the presence of a magnetic flux generating a \(\pi\)-flux per plaquette: this model exhibits Dirac points at half-filling. We also consider a continuous interpolation between the \(\pi\)-flux square lattice model and the honeycomb lattice, on which the attractive Hubbard model has been extensively studied [44–48].
Figure 1. \(\pi\)-flux square lattice model (left) and corresponding first BZ (right). Direct and reciprocal lattice vectors are shown. Hopping amplitudes on the central red line in the left figure are complex with phase \(\pi\); the hopping amplitudes on black bonds have instead a real phase equal to 1.

A 2D lattice model having Dirac cones in the energy dispersion was discussed in [53]: this model is formulated on a square lattice with nearest-neighbour hoppings where an orthogonal magnetic field \(B\) is applied such as to have on each plaquette a flux half of the fundamental one \(\Phi_0\) (from now on, we set \(\Phi_0 = 1\)). Using the Peierls substitution, one can implement a magnetic field introducing complex hopping amplitudes according to equation (2), where

\[
A = \pi(-y, 0, 0)
\]

is the vector potential giving rise to \(B\). The scheme of the phases acquired by a particle in a single hopping and with this gauge choice is plotted in figure 1. These quantities are not gauge-invariant, while the total phase acquired around a loop is. Note the doubling of the elementary cell in one space direction and the consequent halving of a reciprocal vector. Indeed, a choice for the first magnetic Brillouin zone is that the lattice vectors are

\[
a_1 = d(1, 0) \quad \text{and} \quad a_2 = 2d(0, 1),
\]

where \(d\) is the lattice constant, with the reciprocal lattice vectors given by

\[
b_1 = \frac{2\pi}{d}(1, 0) \quad \text{and} \quad b_2 = \frac{\pi}{d}(0, 1).
\]

From now on, we will set \(d = 1\). Note that the primitive cell is half with respect to the square lattice with no magnetic flux because in the presence of \(B\), the translations along \(\hat{x}\) and \(\hat{y}\) do not commute with each other any longer and one has to double one of them.

The kinetic Hamiltonian \(\hat{H}_0\), defined by equation (3), reads in momentum space:

\[
\hat{H}_0 = -2t \sum_{k \in BZ, \sigma} (c_{k,a}^\dagger c_{k,a}^\sigma)(\cos k_x - \cos k_y)(\epsilon_{k,a} \epsilon_{k,b})
\]

where the subscript \(a\) or \(b\) is related to the \(A\) or \(B\) sublattices, a sublattice being defined by the set of lattice sites having a given set of hopping phases along the bond starting from them. The Hamiltonian matrix can be easily diagonalized leading to the single-particle spectrum

\[
\epsilon_{\pm}(k) = \pm 2t \sqrt{\cos^2 k_x + \cos^2 k_y}.
\]

Figure 2. Dispersion relation for the tight-binding Hamiltonian \(\hat{H}_0\) on the \(\pi\)-flux square lattice model. The horizontal line represents the Fermi level at half-filling.

Figure 3. Density of states (normalized to 2) for the \(\pi\)-flux square lattice model.

The band structure and the density of states (normalized to 2) are shown in figures 2 and 3. The main property of (13) is the
presence of two inequivalent Dirac points in
\[
\mathbf{K} = \frac{\pi}{2} (1, 1) \quad \text{and} \quad \mathbf{K}' = \frac{\pi}{2} (-1, 1),
\]
with the other two Dirac points at \(\frac{\pi}{2} (1, 1)\) and \(\frac{\pi}{2} (1, 1)\) being related to the previous ones by the translations of the primary vectors of the reciprocal lattice. The dispersion relation near these points is linear:
\[
\epsilon_{\pm}(\mathbf{K} + \mathbf{q}) = \pm 2t|\mathbf{q}| + \mathcal{O}(|\mathbf{q}|^3)
\]
(15)

The \(\pi\)-flux model admits a smooth interpolation with the honeycomb lattice model: notably along this interpolating path, the Dirac points are always present. The path that we consider is realized using an anisotropic honeycomb lattice as in Figure 4. A magnetic field with flux \(\pi\) on each trapezoidal plaquette, being half of the hexagons, is added; on each hexagon the flux instead vanishes. Notice that the eigenvalues of the Hamiltonian depend only on the total magnetic flux on hexagon the flux instead vanishes. Notice that the eigenvalues of the Hamiltonian depend only on the hexagon. 

Choosing the distance between nearest neighbours to be unitary, the lattice vectors are given by
\[
a_1 = (1 + \cos \theta, 0) \quad \text{and} \quad a_2 = (0, 2 \sin \theta)
\]
and the reciprocal lattice vectors are
\[
b_1 = \frac{2 \pi}{1 + \cos \theta} (1, 0) \quad \text{and} \quad b_2 = \frac{\pi}{\sin \theta} (0, 1).
\]
Defining
\[
C = \cos \theta \quad \text{and} \quad S = \sin \theta,
\]
(19)

In equation (21), \(0\) is the \(2 \times 2\) zero matrix and the matrix \(A\) is given by
\[
A = \begin{pmatrix}
0 & A \\
A^\dagger & 0
\end{pmatrix}
\]
(21)

Diagonalizing \(M\), one obtains the energy spectrum
\[
\epsilon_{\pm}(\mathbf{k}; a) = \pm \sqrt{\Delta^2 + 2 \cos(2\theta(k_x + k_y) - 4 \alpha_0 \cos(2k_x \sin(k_y) + 1 + \alpha)]}
\]
(23)
\[
\epsilon_{\pm}(\mathbf{k}; a) = \pm \sqrt{\Delta^2 + 2 \cos(2\theta(k_x + k_y) - 4 \alpha_0 \cos(2k_x \sin(k_y) + 1 + \alpha)]}
\]
(24)

Note that equations (23) and (24), using equations (17) and (18), do not depend explicitly on \(\theta\). The results for the \(\pi\)-flux square lattice model can be recovered imposing \(a = 1\), while the honeycomb lattice is defined by setting \(a = 0\). In these two limits, the energy bands are doubly degenerate. In particular, for \(a = 0\) one has that \(\epsilon_{\pm}(\mathbf{k}; 0)\) and \(\epsilon_{\pm}(\mathbf{k}; 0)\) are related by the momentum shift \(k_x \rightarrow k_x + \pi\) or \(k_y \rightarrow k_y + \pi\). This is due to the fact that the cell defined by the vectors in (17) is not a primitive one: selecting correctly the primitive cell, this fictitious degeneration is removed and one obtains two non-degenerate bands. One then finds the spectrum (13) for the \(\pi\)-flux square lattice and \(\epsilon_{\pm}(\mathbf{k}) = \pm t \sqrt{\Delta^2 + f(k)}\)
\[
f(k) = 2 \cos(\sqrt{\Delta} k_x) + 4 \cos(\frac{\sqrt{\Delta}}{2} k_x) \cos(\frac{\sqrt{\Delta}}{2} k_y) + 1 - \Delta
\]
(37)

The mean-field results for the gap, the critical temperature and the critical interaction (at half-filling, \(n = 1\)) are obtained solving equations (7) using the single-particle energy spectrum (23) and (24): the corresponding findings are shown in figures 5–7. In Figure 5, we plot at half-filling the superfluid gap \(\Delta\) versus \(U\) at \(T = 0\) for different values of the interpolating parameter \(a\): a quantum phase transition between a semimetal (for \(U\) smaller than a critical value \(U_c\)) and a superfluid state (for \(U > U_c\)) is clearly visible in Figure 5. The quantum phase transition continuously varies passing from the honeycomb...
Similarly, we expect that the result for the critical value of the interpolating parameter $a$ at half-filling ($n = 1$).

Results across the interpolation are shown in figure 6. For the honeycomb lattice ($a = 0$), the critical value $U_c$ can be evaluated to be $U_c = 2.23 \ t$: this result should be compared with the Monte Carlo calculation giving $U_c = (4.5 \pm 0.5) \ t$ [72, 46]. Similarly, we expect that the result for the critical value of $U_c$ for the $\pi$-flux square lattice is underestimated by the mean field (we find $U_c = 3.12 \ t$ for $a = 1$). Finally in figure 7, we plot the mean-field critical temperature $T_c$ as a function of the interpolating parameter $a$. Notice that $T_c$ becomes non vanishing at the same critical value $U_c$ for which $\Delta$ at $T = 0$ becomes non vanishing.

A property of the quantum phase transition conserved during the interpolation between the honeycomb lattice and the $\pi$-flux square lattice is a linear gap scaling law as a function of $|U - U_c|$:

$$\Delta \propto |U - U_c|.$$  \hspace{1cm} (25)

As occurs in the honeycomb lattice [72], this is due to the presence of $|\Delta|^3$ terms in the Landau–Ginzburg expansion of the Hartree–Fock energy per unit cell at zero temperature, which is given for the $\pi$-flux square lattice by the integral

$$\frac{E_{HF}(\Delta)}{\Omega} = \int_{\epsilon_0}^{E_0} d\epsilon \ g(\epsilon) \sqrt{\epsilon^2 + \Delta^2} + \frac{\Delta^2}{U \Omega},$$  \hspace{1cm} (26)

where $\epsilon_0 = -2\sqrt{2}t$ is the minimum value of the single-particle energy spectrum. Note that (26) is also valid for a general value of the interpolating parameter provided that $\epsilon_0$ is the minimum energy of the spectrum (23), (24). In order to obtain a cubic term in the expansion, it is necessary that, at some point within the integration interval in equation (26), the density of states is linear in $\epsilon$ and $\Delta > \epsilon$ for arbitrary small $\Delta$, then $\epsilon \to 0$. This condition is fulfilled for both the $\pi$-flux square lattice and the honeycomb lattice, as well as across the interpolation.

We observe that in the presence of a mass term, the linear critical exponent of the gap is changed: the critical exponent becomes $1/2$ and this again occurs across the whole interpolation from the honeycomb lattice to the $\pi$-flux square lattice. This can be seen by analysing how the coefficient of the $|\Delta|^3$ terms in the Landau–Ginzburg energy changes in the presence of a mass: we consider for simplicity the honeycomb lattice. Let us consider an on-site energy $+m$ for the sublattice $A$ and $-m$ for the sublattice $B$ [73]; the single-particle spectrum becomes $\epsilon_{\pm}(k) = \pm t \sqrt{3 + f(k)} + m^2$. The resulting density of states shows a gap of amplitude $2m$ around $\epsilon = 0$: the position of the Van Hove singularities changes introducing the mass term, and the density of states diverges for $\epsilon = \pm \sqrt{t + m^2}$. Since the density of states is gapped around $\epsilon = 0$, so (26) becomes for the honeycomb lattice:

$$\frac{E_{HF}(\Delta)}{\Omega} = \int_{-\epsilon_0(m)}^{-mg} d\epsilon \ g(\epsilon) \sqrt{\epsilon^2 + \Delta^2} + \frac{\Delta^2}{U \Omega},$$  \hspace{1cm} (27)

$\epsilon_0(m)$ being the minimum of the spectrum in the presence of the mass term. Therefore, choosing $\Delta > mt$, it is not possible to fulfill the required condition for the cubic term in the expansion discussed above, so that we recover the usual critical exponent ($1/2$).

The previous results for the critical temperature and the gap have been found at the mean-field level and the inclusion of
quantum fluctuations on top of it is expected to quantitatively modify such results: in particular in [44], the case of the honeycomb lattice was investigated, finding that the critical temperature is rather considerably lowered by the inclusion of quantum fluctuations (it is found that $T_c^{\text{max}} \sim 0.1 \ T_c$ [44]). Proceeding as in [44], we performed for $a = 1$ an estimate of the Kosterlitz–Thouless critical temperature $T_{KT}$: we found a decrease of the critical temperature induced by quantum fluctuations less pronounced than for the honeycomb at $a = 0$ (e.g., for $a = 1$ and $U \sim 1.5 T_c$ we found $T_{KT} \sim 0.5 T_c$, where $T_c$ is the mean-field critical temperature). Given the smoothness exhibited by the considered model across the interpolating path, we expect the presented results for the gap and the critical temperature will be quantitatively modified of a similar amount (but qualitatively robust) passing from $a = 0$ to $a = 1$. A qualitative difference is anyway expected to be induced by the quantum fluctuations for the specific values of the critical exponents for the gap near $T_c$. More importantly, time-dependent fluctuations around mean-field coupling amplitude and phase fluctuations are required to study the collective modes, as the Leggett and the Goldstone modes.

4. 3D lattice with Dirac points: $\pi$-flux cubic lattice model

The discussion presented in the previous section shows that at the mean-field level, the superfluid properties of the attractive Hubbard model on the honeycomb lattice and on the $\pi$-flux square lattice are qualitatively equivalent, with only quantitative differences. In order to study the corresponding problem in 3D, it is then natural to consider the cubic $\pi$-flux lattice, which has the desired structure of the Dirac points (we remind that stacking up layers of graphene leads to the graphite geometrical structure, with Dirac cones destroyed [50]). We consider a cubic lattice with the magnetic field $B$ along the direction $d = (1, 1, 1)$ as such to generate a $\pi$-flux on each plaquette. This can be obtained using the Peierls substitution with the vector potentials [57]:

$$ A(r) = \pi (0, x - y, y - x). $$

Notably enough, tuning the hopping amplitude along the $z$-direction, it is possible to investigate a crossover between 2D and 3D lattice having the same Dirac points: this can be done considering hopping amplitudes with the absolute value $t$ along $\hat{x}$- and $\hat{y}$-directions and $t_0 \equiv at$ along $\hat{z}$. $a$ is an interpolation parameter ($0 \leq a \leq 1$) characterizing how much the layers of the system are connected: changing the value of the parameter $a$, one can explore the bidimensional $\pi$-flux square lattice model ($a = 0$) and the isotropic 3D $\pi$-flux square lattice model ($a = 1$).

Figure 8 draws a schematic plot of the layered $\pi$-flux cubic lattice. The lattice vectors in units of the lattice spacing (assumed to be equal in all three directions) are given by

$$ a_1 = (2, 0, 0) \quad a_2 = (0, 2, 0) \quad a_3 = (0, 0, 1) \quad (28) $$

so the reciprocal lattice vectors are

$$ b_1 = \pi (1, 0, 0) \quad b_2 = \pi (0, 1, 0) \quad b_3 = 2\pi (0, 0, 1). \quad (29) $$

The Hamiltonian $\hat{H}_0$ in the Fourier space is given by

$$ \hat{H}_0 = 2t \sum_{k \in \text{MBZ},\sigma} \left( \begin{array}{cc} \alpha \cos(k_x + \pi) & 2 \cos k_x + 2e^{-i\pi} \cos k_y \\ 2 \cos k_x + 2e^{i\pi} \cos k_y & \alpha \cos k_y \end{array} \right) \left( \begin{array}{c} \psi_{\sigma, A} \\ \psi_{\sigma, B} \end{array} \right) \quad (30) $$

where the subscripts $a$ and $b$ indicate, respectively, the $A$ and $B$ sublattices shown in figure 8. This Hamiltonian can be diagonalized exactly, leading to the single-particle energy spectrum

$$ \epsilon_{\pm}(k) = \pm 2t \sqrt{(\cos^2 k_x + \cos^2 k_y + a^2 \cos^2 k_z). \quad (31) $$

The energy spectrum has two inequivalent Dirac points

$$ K = \frac{\pi}{2} (1, 1, 1) \quad \text{and} \quad K' = \frac{\pi}{2} (1, 1, -1); \quad (32) $$

notably, their position does not depend on the layering parameter $a$. The dispersion relation around these points is given by

$$ \epsilon_{\pm}(K + q) = \pm 2t |q| \sqrt{1 + (a^2 - 1) \cos^2 \theta + O(|q|^2)}. \quad (33) $$
The linear-order term depends on the polar angle $\theta = \arcsin(q_z/|q|)$, so the speed of light for the Dirac fermions is not isotropic (unless $a = 1$). Of course, if $a = 0$, this quantity vanishes along the $z$-direction. The band structure and the density of states for different values of the parameter $a$ are shown in figures 10 and 11, respectively. It is also possible to obtain an expansion for the density of states near $\epsilon = 0$ if $0 < a \lesssim 1$:

$$g(\epsilon) \approx \frac{\epsilon^2}{2(\alpha^2 + 1)^3}.$$  \hfill (34)

We solved the BCS mean-field equations at half-filling with the single-particle energy spectrum (31): the various results are shown in figures 12–14. The quantum phase transition between semimetal and superconductor is robust passing from a 2D to a 3D system, as shown in figure 12: at the mean-field level, the change is quantitative, a larger interaction being needed to induce the superfluid phase as shown in figure 13. Consequently, mean-field critical temperature decreases with $a$ increasing, as shown in figure 14.
We observe that the critical exponent $\alpha$ in the law $\Delta \propto |U - U_c|^\alpha$ at $T = 0$ abruptly changes from 1 to 0.5 for finite $a$ because of the different behaviour of the density of states near the Fermi level. In fact, introducing the hopping terms along the $z$-direction, $g(\epsilon)$ is not linear in the neighbourhood of the Fermi energy, as shown in figure 11.

We finally observe that for a quantitative improvement of the results presented in this section, the inclusion of quantum fluctuations is certainly needed, even though we expect on general grounds that such corrections are less pronounced compared to the 2D cases discussed in section 3. For this reason, we think that an interesting line of future work would be to include quantum fluctuations passing from 2D to 3D, i.e. from $a = 0$ to $a = 1$, and possibly to include the effect of charge-density waves on equilibrium properties at half-filling.

5. Conclusions

In this paper, we analysed the superfluidity of attractively interacting fermions in a family of 2D and 3D ultracold lattice systems with Dirac points, focusing in particular on the honeycomb lattice, the $\pi$-flux square lattice, the $\pi$-flux cubic lattice and related interpolating geometries. We studied the effects of interaction and dimensionality on the relevant physical parameters, as the superfluid gap, chemical potential and critical temperature $T_c$: these quantities are found to vary continuously along the patterns of interpolation. In the 2D cases, at zero temperature and at half-filling, there is a quantum phase transition occurring at a critical (negative) interaction $U_c$ presenting a linear critical exponent for the gap as a function of $|U - U_c|$. This behaviour holds for the honeycomb lattice, for the $\pi$-flux square lattice model and for the interpolating schemes. We also observed that across the interpolation between the honeycomb and the $\pi$-flux square lattice, in the presence of an energy offset for the two sublattices (i.e., a mass term), the critical exponent is the usual one ($1/2$). These investigations show that at the mean-field level, there is no qualitative difference between the superfluid properties of the attractive honeycomb model and the $\pi$-flux square lattice. Following [44], we also performed an estimate of the effect of quantum fluctuations on the mean-field critical temperature, finding that the decrease of $T_c$ is less pronounced on the $\pi$-flux square lattice with respect to the honeycomb lattice.

In three dimensions, the quantum phase transition is again retrieved and it is shown to be continuously varying passing from the $\pi$-flux square lattice to the $\pi$-flux cubic lattice: we point out that, unlike the 2D case, the critical exponent for the gap changes from 1 to 1/2.

We observe that in the two considered interpolations (from the honeycomb to the $\pi$-flux square lattice and from the $\pi$-flux cubic lattice to the $\pi$-flux square lattice), a smooth behaviour for the gap and the critical temperature is found: since the considered lattices all have Dirac points, but different spectra far from them, our obtained results show that most of the contribution to the physical observables come—at the mean-field level—from low-energy excitations around Dirac points.

Our analysis was done at the mean-field level: since the effects of non-mean-field terms are in general relevant—especially for the critical temperature [64]—further investigations for the considered lattices are needed to include the effects of fluctuations, whose effects have been studied in honeycomb lattices at half-filling [44] and estimated for the $\pi$-flux square lattice in this paper. Similarly, it would be very interesting to study the effects on the superfluidity of a general truly non-Abelian synthetic gauge potential for the 3D $\pi$-flux cubic lattice: work in this direction is currently ongoing.

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References

[1] Bloch I, Dalibard J and Zwerger W 2008 Rev. Mod. Phys. 80 885
[2] Lewenstein M, Sanpera A and Ahufinger V 2012 Ultracold Atoms in Optical Lattices: Simulating Quantum Many-Body Systems (Oxford: Oxford University Press)
[3] Cataliotti F S, Burger S, Fort C, Maddaloni P, Minardi F, Trombettoni A, Smerzi A and Inguscio M 2001 Science 293 843
[4] Greiner M, Mandel O, Esslinger T, Hansch T E and Bloch I 2002 Nature 415 39
[5] Jaksh D, Bruder C, Cirac J I, Gardiner C W and Zoller P 1998 Phys. Rev. Lett. 81 3108
[6] Esslinger T 2010 Annu. Rev. Condens. Matter Phys. 1 129
[7] Hofstetter W, Cirac J I, Zoller P, Demler E and Lukin M D 2002 Phys. Rev. Lett. 89 220407
[8] Morsch O and Oberthaler M K 2006 Rev. Mod. Phys. 78 179
[9] Dalibard J, Gerbier F, Juzeliunas G and Ohoberg P 2011 Rev. Mod. Phys. 83 1523
[10] Nayak C, Simon S H, Stern A, Freedman M and Das Sarma S 2008 Rev. Mod. Phys. 80 1083
[11] Lin Y J, Compton R L, Jimenez-Garcia K, Porto J V and Spielman I B 2009 Nature 462 628
[12] Lin Y J, Compton R L, Jimenez-Garcia K, Phillips W D, Porto J V and Spielman I B 2011 Nature Phys. 7 531
[13] Lin Y J, Compton R L, Perry A R, Phillips W D, Porto J V and Spielman I B 2009 Phys. Rev. Lett. 102 130401
[14] Lin Y J, Jimenez-Garcia K and Spielman I B 2011 Nature 471 83
[15] Fu Z, Wang P, Chai S, Huang L and Zhang J 2011 Phys. Rev. A 84 043609
[16] Wang P, Yu Z-Q, Fu Z, Miao J, Huang L, Chai S, Zhai H and Zhang J 2012 Phys. Rev. Lett. 109 095301
[17] Cheuk L W, Sommer A T, Hadzibabic Z, Yefsah T, Bakr W A and Zwierlein M W 2012 Phys. Rev. Lett. 109 095302
[18] Jaksh D and Zoller P 2003 New J. Phys. 5 S6
[19] Osterloh K, Baig M, Santos L, Zoller P and Lewenstein M 2005 Phys. Rev. Lett. 95 010403
[20] Gerbier F and Dalibard J 2012 New J. Phys. 12 033007
[21] Aidelsburger M, Atala M, Nascimbene S, Trotzky S, Chen Y-A and Bloch I 2012 Phys. Rev. Lett. 107 255301
[22] Jimenez-Garcia K, LeBlanc L J, Williams R A, Beerer M C, Perry A R and Spielman I B 2012 Phys. Rev. Lett. 108 225303
[23] Hauke P et al 2012 Phys. Rev. Lett. 109 145301
[24] Zhu S-L, Wang B and Duan L-M 2007 Phys. Rev. Lett. 98 260402
