Upper critical field for anisotropic superconductivity: A tight-binding approach

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We study the problem of the upper critical field (H_{c2}) for tight-binding electrons in a two-dimensional lattice. The external magnetic field is introduced into the model Hamiltonian both via the Peierls substitution and the Zeeman term. Carrying out calculations for finite systems we analyze the influence of the external field in the commensurable and incommensurable case on an equal footing. The upper critical field has been investigated for intrasite as well as anisotropic intersite pairing that, in the absence of magnetic field, has a $d_{x^2-y^2}$ symmetry. We also briefly discuss the symmetry of the superconducting order parameter in the presence of magnetic field and the role of the next-nearest-neighbor hopping. A comparison of H_{c2} determined for different symmetries shows that for nested Fermi surface the on-site pairing is more affected by the external field, i.e., the critical temperature for the on-site pairing decreases with the increase of the magnetic field faster than in the anisotropic case. Moreover, we have shown that the tight-binding form of the Bloch energy can lead to the upward curvature of H_{c2}, provided that the Fermi level is close enough to the van Hove singularity.

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I. INTRODUCTION

One of many striking properties of high-temperature superconductors is related to the field-induced transition from superconducting to normal state. Magnetic properties of high-T_c compounds give rise to both quantitative and qualitative differences with respect to the conventional superconductors. The systems under consideration are characterized by extremely high values of the upper critical and its unusual temperature dependence. For optimally doped samples experimental investigation of the critical field is limited only to temperatures close to T_c,[1] whereas at lower temperatures the magnitude of H_{c2} is far beyond the reach of laboratory magnetic fields. The measurements carried out in a wide range of temperature for underdoped superconductors clearly indicate the positive curvature of $H_{c2}(T)$ even at genuinely low temperatures.[1–4] Theoretical approaches do not provide a unique, complete description of these phenomena. Most unconventional properties of high-temperature superconductors, like narrow quasiparticle bands, lifetime effects of states close to the Fermi level, and linear temperature dependence of the normal-state resistivity, are usually attributed to strong Coulomb correlations. However, upward curvature of the upper critical field is observed also in overdoped compounds, where the temperature dependence of resistivity changes gradually from linear to quadratic behavior.[5,6] This feature suggests that the positive curvature of $H_{c2}(T)$ could originate from, e.g., symmetry of the superconducting order parameter or details of the density of states and may be explained without a sophisticated treatment of the most difficult problem that is related to the presence of strong electronic correlations. In particular, the upward curvature of the upper critical field can be explained within the Josephson tunneling between some superconducting clusters with a transition temperature higher than T_c for the bulk superconductor.[7,8]

It is believed that the symmetry of the superconducting state can be closely related to the pairing mechanism. There are a lot of node-sensitive experiments, based on the angle-resolved photoemission spectroscopy,[9] London penetration depth,[10] NMR,[11] and quasiparticle tunneling,[12] which indicate that the energy gap is strongly anisotropic and vanishes in particular directions in the Brillouin zone. Moreover, the phase-sensitive superconducting interference device experiments[13] demonstrated the sign change of the order parameter between the x and y directions. Generally, these results are consistent with the $d_{x^2-y^2}$ pairing scenario. On the other hand, there are experimental indications, which had questioned the pure $d_{x^2-y^2}$ symmetry of the energy gap and suggest mixed pairing symmetry with a dominant d-wave component (e.g., $d\pm s$ or $d\pm is$).[14–17]

The measurement of the upper critical field can give insight into the microscopic parameters of a relevant model. For example, the coherence length ξ is usually derived indirectly from the expression $H_{c2}(0)=\phi_0/2\pi\xi^2$,[18] where $H_{c2}(0)$ is the upper critical field determined at $T=0$, and ϕ_0 is the magnetic flux quantum. The theoretical investigation of the upper critical field for different pairing symmetries is predominantly based on the Ginzburg–Landau (GL) (Ref. 19) theory or the Lawrence-Doniach[20] approach in case of layered superconductors. With the help of linearized GL equations Won and Maki[21] have shown that H_{c2} in a model with repulsive on-site interaction depends linearly on temperature near T_c and saturates at $T\rightarrow 0$. They have not found any sign of the upward behavior. There are also calculations for H_{c2} in systems with mixed symmetries, especially for superconductors in which the dominant d-wave order parameter coexists with a subdominant s-wave component. However, in most of these approaches $H_{c2}(T)$ exhibits negative curvature. On the other hand, results obtained in Ref. 22 suggest that the upward curvature of the critical field could be a characteristic feature of a d-wave superconductor. The positive curvature of $H_{c2}(T)$ can also originate from the presence of magnetic impurities.[23,24]

A separate problem, that is usually neglected in the above approaches, is the influence of the periodic lattice potential on the upper critical field.[25] Application of magnetic field to the two-dimensional (2D) electron system in a tight-binding approximation leads to a fractal energy spectrum known as Hofstadter's butterfly, where even very small changes in magnetic field can result in a drastic change of the spectrum.[26–28] In this paper we investigate the upper critical field for electrons described by the two-dimensional tight-binding model with intra- and intersite pairing. We show that anisotropic superconductivity is less affected by the external magnetic field then the isotropic one, especially for the nested Fermi surface. We also demonstrate that the lattice effects can give rise to important corrections with respect to the Helfand-Werthamer[29,23] solution of the Gor'kov equations.[30] This effect is of particular importance in the vicinity of the van Hove singularity and at low temperatures.

II. GAP EQUATION CLOSE TO H_{c2}

We consider a two-dimensional square lattice immersed in a uniform, perpendicular, magnetic field. The BCS-type Hamiltonian is of the form

$$\hat{H}=\hat{H}_{\rm kin}+\hat{H}_V-\mu\sum_{i,\sigma} c^\dagger_{i\sigma}c_{i\sigma}+g\mu_B H_z\sum_i (c^\dagger_{i\uparrow}c_{i\uparrow}-c^\dagger_{i\downarrow}c_{i\downarrow}), \tag{1}$$

where $c^\dagger_{i\sigma}$ $(c_{i\sigma})$ creates (annihilates) an electron with spin σ on site i. The chemical potential μ is introduced in order to control the doping level. The last term in the above Hamiltonian describes the paramagnetic Pauli coupling to the external field. Here, g stands for the gyromagnetic ratio, μ_B is the Bohr magneton, and H_z is the z component of the external field. The first ($\hat{H}_{\rm kin}$) and the second ($\hat{H}_V$) term in the Hamiltonian represents the kinetic energy and the pairing interaction, respectively. Within the tight-binding approach

$$\hat{H}_{\rm kin}=\sum_{\langle ij\rangle\sigma} t_{ij}(\mathbf{A})c^\dagger_{i\sigma}c_{j\sigma}. \tag{2}$$

The electrons are gauge-invariantly coupled with local U(1) gauge field by a phase factor in the kinetic-energy hopping term. According to the Peierls substitution[31] in the presence of magnetic field the original hopping integral between sites i and j, t_{ij} acquires an additional factor

$$t_{ij}(\mathbf{A})=t_{ij}\exp\left(\frac{ie}{\hbar c}\int_{\mathbf{R}_j}^{\mathbf{R}_i}\mathbf{A}\cdot d\mathbf{l}\right). \tag{3}$$

In the case of the on-site pairing, which leads to isotropic order parameter, the BCS-type interaction takes on the form

$$\hat{H}_V=-V\sum_i (c^\dagger_{i\uparrow}c^\dagger_{i\downarrow}\Delta_i+c_{i\downarrow}c_{i\uparrow}\Delta^\star_i). \tag{4}$$

Here, we have introduced a local superconducting order parameter, $\Delta_i=\langle c_{i\downarrow}c_{i\uparrow}\rangle$, which in the presence of the magnetic field can change from site to site.[25] We also consider anisotropic superconductivity with the intersite pairing interaction given by

$$\hat{H}_V=-V\sum_{\langle ij\rangle} (c^\dagger_{i\uparrow}c^\dagger_{j\downarrow}\Delta_{ij}+c_{i\downarrow}c_{j\uparrow}\Delta^\star_{ij}). \tag{5}$$

For the sake of simplicity we restrict our considerations only to the nearest-neighbor coupling with the singlet order parameter $\Delta_{ij}=\langle c_{i\downarrow}c_{j\uparrow}-c_{i\uparrow}c_{j\downarrow}\rangle$. As we do not specify the mechanism that is responsible for pairing V is assumed to be field independent. This approximation may be invalid for strong magnetic fields, in particular, when the spin fluctuations (SF) contribute to the pairing correlations. However, results presented in the appendix show that V_{SF} is hardly affected by the weak magnetic field.

We start with the discussion of the normal-state properties. Similarly to Ref. 25 we make use of a unitary transformation U that diagonalizes the kinetic part of the Hamiltonian

$$U^\dagger\hat{H}_{\rm kin}U=\mathcal{H}_{\rm kin}. \tag{6}$$

This transformation defines a new set of fermionic operators $a_{\alpha\sigma}=\Sigma_i U^\dagger_{\alpha i}c_{i\sigma}$, in which the Hamiltonian in the normal state takes on the diagonal form

$$\mathcal{H}=\sum_{\alpha\sigma} (E_\alpha-\mu+\sigma g\mu_B H_z)a^\dagger_{\alpha\sigma}a_{\alpha\sigma}. \tag{7}$$

In the absence of the magnetic field U represents transformation from the Wannier to the Bloch representation. For finite magnetic field and general gauge the quantum number α enumerates eigenstates, although does not represent a reciprocal-lattice vector. We take into account the nearest-neighbor hopping with $t_{\langle ij\rangle}\equiv -t$ and the next-nearest-neighbor hopping with $t_{\langle\langle ij\rangle\rangle}\equiv -t'$. We also assume the type-II limit of superconductors where the magnetic field can be regarded as a spatially uniform object. Choosing the Landau gauge $\mathbf{A}=H_z(0,x,0)$ the hopping integral depends explicitly only on x and the momentum in y direction p_y remains a good quantum number. It is convenient to denote a site on the square lattice by (m,n) in such a way that its position reads $\mathbf{R}=(ma,na)$, where a is the lattice constant.

According to Eq. (3) the hopping integrals to the nearest and next-nearest neighbors are given by

$$t_1=t_5=t,\quad t_2=t'e^{ih(m+1/2)},$$

$$t_3=t_7^*=te^{ihm},\quad t_4=t'e^{ih(m-1/2)},$$

$$t_6=t'e^{-ih(m-1/2)},\quad t_8=t'e^{-ih(m+1/2)},$$

where the meaning of $t_1,\ldots,t_8$ is explained in Fig. 1. Here, we have introduced a reduced dimensionless magnetic field $h=ea^2H_z/(\hbar c)$. This quantity can be expressed with the help of magnetic flux ϕ through lattice cell and flux quantum $(h=2\pi\phi/\phi_0)$.

Due to the plane-wave behavior in y direction the unitary matrix U takes on the form

$$U_{i(\bar{p}_x,p_y)}=U_{(m,n)(\bar{p}_x,p_y)}=N^{-1/4}e^{ip_yna}g(\bar{p}_x,p_y,m), \tag{8}$$

where $(\bar{p}_x,p_y)$ represents the eigenstate α of the Hamiltonian (7). Straightforward calculations[28] show that the x-dependent part of the wave function, $g(\bar{p}_x,p_y,m)$, fulfills a one-dimensional difference equation

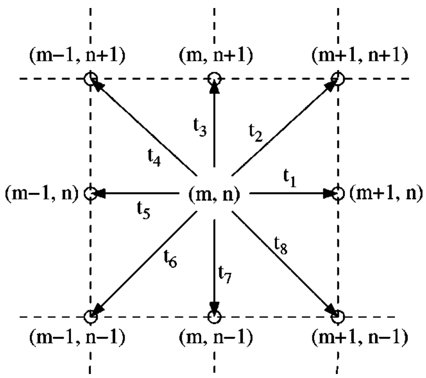

FIG. 1. Hopping integrals $t_1,\ldots,t_8$ for electrons that move from site (m,n) to the nearest and next-nearest neighbors. Their values are given in the text.

$$\begin{aligned}&\left\{t+2t'\cos\left[h\left(m-\tfrac{1}{2}\right)-p_ya\right]\right\}g(\overline{p_x},p_y,m-1)\\&\quad+2t\cos(hm-p_ya)g(\overline{p_x},p_y,m)\\&\quad+\left\{t+2t'\cos\left[h\left(m+\tfrac{1}{2}\right)-p_ya\right]\right\}g(\overline{p_x},p_y,m+1)\\&\quad=E(\overline{p_x},p_y)g(\overline{p_x},p_y,m).\end{aligned}\tag{9}$$

For $t'=0$ Eq. (9) is reduced to the well-known Harper equation[26] which has been extensively studied.[32,33] The Harper equation, derived here within a tight-binding approximation, can also be obtained in a case of weak perturbation of a Landau-quantized two-dimensional electron system.[27,34]

Now, let us take into account the pairing potential H_V. In order to investigate the transition from the superconducting to the normal state we make use of the equation of motion for the anomalous Green function. In the case of the isotropic on-site pairing one obtains

$$\begin{aligned}&[\omega-E(\overline{p_x},p_y)+\mu+g\mu_BH_z]\langle\langle a_{(\overline{p_x},p_y)\uparrow}|a_{(\overline{k_x},k_y)\downarrow}\rangle\rangle\\&\quad=-V\sum_{i,\overline{k'_x},k'_y}\Delta_iU^{\star}_{i(\overline{p_x},p_y)}U^{\star}_{i(\overline{k'_x},k'_y)}\langle\langle a^{\dagger}_{(\overline{k'_x},k'_y)\downarrow}|a_{(\overline{k_x},k_y)\downarrow}\rangle\rangle.\end{aligned}\tag{10}$$

As far as we are close to the phase transition we make use of a linearized gap equation i.e., we calculate the propagator $\langle\langle a^{\dagger}_{(\overline{k'_x},k'_y)\downarrow}|a_{(\overline{k_x},k_y)\downarrow}\rangle\rangle$ in the normal state. Similarly to the standard BCS theory, such approach allows one to determine the critical temperature or, in our case, the upper critical field. However, it is irrelevant for calculations below T_c.

The choice of the Landau gauge implies that the isotropic order parameter does not depend on y: $\Delta_i\equiv\Delta_{(m,n)}=\Delta_m$. Then, the linearized gap equation reads

$$\vec{\Delta}=\mathcal{M}\vec{\Delta},\tag{11}$$

where $\vec{\Delta}=(\Delta_1,\Delta_2,\Delta_3,\ldots)$ and

$$\begin{aligned}\mathcal{M}(m,m')=&\frac{V}{\sqrt{N}}\sum_{\overline{p_x},p_y,\overline{k_x}}g(\overline{p_x},p_y,m)g(\overline{k_x},-p_y,m)\\&\times g(\overline{k_x},-p_y,m')g(\overline{p_x},p_y,m')\\&\times\chi(\overline{p_x},p_y;\overline{k_x},-p_y).\end{aligned}\tag{12}$$

In the presence of the magnetic field the Cooper pair susceptibility is given by

$$\begin{aligned}\chi(\overline{p_x},p_y;\overline{k_x},k_y)&\\=&\left[\tanh\frac{E(\overline{p_x},p_y)-\mu+g\mu_BH_z}{2k_BT}\right.\\&\left.+\tanh\frac{E(\overline{k_x},k_y)-\mu-g\mu_BH_z}{2k_BT}\right]\\&\times[2(E(\overline{p_x},p_y)+E(\overline{k_x},k_y)-2\mu)]^{-1}.\end{aligned}\tag{13}$$

In the case of the nearest-neighbor pairing we obtain the gap equation analogous to Eq. (11). Similarly to the isotropic pairing Δ_{ij} does not depend explicitly on y. However, there are two types of order parameters at each site: $\Delta_m^{(x)}$ when sites i and j lay along the x axis, and $\Delta_m^{(y)}$ when sites i and j lay along the y axis. Close to the upper critical field the gap equation for anisotropic superconductivity can be written in a matrix form

$$\begin{pmatrix}\vec{\Delta}^{(x)}\\\vec{\Delta}^{(y)}\end{pmatrix}=\begin{pmatrix}\mathcal{M}^{(x,x)}&\mathcal{M}^{(x,y)}\\\mathcal{M}^{(y,x)}&\mathcal{M}^{(y,y)}\end{pmatrix}\begin{pmatrix}\vec{\Delta}^{(x)}\\\vec{\Delta}^{(y)}\end{pmatrix},\tag{14}$$

where

$$\begin{aligned}\mathcal{M}^{(\alpha,\beta)}(m,m')=&\frac{V}{\sqrt{N}}\sum_{\overline{p_x},p_y,\overline{k_x}}\chi(\overline{p_x},p_y;\overline{k_x},-p_y)\\&\times A^{(\alpha)}(\overline{p_x},\overline{k_x},p_y,m)A^{(\beta)}(\overline{p_x},\overline{k_x},p_y,m'),\end{aligned}\tag{15}$$

and

$$\begin{aligned}A^{(x)}(\overline{p_x},\overline{k_x},p_y,m)=&g(\overline{p_x},p_y,m)g(\overline{k_x},-p_y,m+1)\\&+g(\overline{p_x},p_y,m+1)g(\overline{k_x},-p_y,m),\end{aligned}\tag{16}$$

$$A^{(y)}(\overline{p_x},\overline{k_x},p_y,m)=2\cos(p_ya)g(\overline{p_x},p_y,m)g(\overline{k_x},-p_y,m).\tag{17}$$

Equations (11) and (14) constitute a system of linear equations for the order parameters and the condition for existence of a nonzero solution can be written as

$$\det(\mathcal{M}-I)=0\tag{18}$$

in the case of isotropic pairing, and

$$\det\begin{pmatrix}\mathcal{M}^{(x,x)}-I&\mathcal{M}^{(x,y)}\\\mathcal{M}^{(y,x)}&\mathcal{M}^{(y,y)}-I\end{pmatrix}=0\tag{19}$$

for anisotropic superconductivity, where I is the unit matrix. These equations allow one to obtain the magnitude of the upper critical field perpendicular to the plane. For the two-dimensional square lattice the size of matrices which enter Eqs. (18) and (19) is proportional to the square root of the number of the lattice sites. Analytical solutions of the Harper Eq. (9) are known only in a few cases of commensurable field[33] (in our notation $h=2\pi p/q$, where p and q are relative prime integers), which correspond to unphysically high magnetic field. Therefore in order to investigate H_{c2} we restrict our considerations to a finite lattice, for which we are able to analyze numerically the commensurable and incommensurable magnetic field on an equal footing.

III. DISCUSSION OF RESULTS

We consider square $M\times M$ cluster with periodic boundary conditions (BC) along the y axis. As the Landau gauge breaks the translation invariance along x axis we use fixed BC in this direction. An additional advantage originating from such a mixed BC is the absence of the unphysical degeneracy of states at the Fermi level, which occurs for the half filled band in cluster calculations with fixed or periodic BC taken in both directions.[35] In order to estimate the finite-size effects we have carried out numerical calculations for clusters of different sizes. We have found that in the case of the isotropic pairing and small concentration of holes ($\delta<0.2$) there are no significant differences between results obtained on 150×150 and 200×200 clusters. For anisotropic pairing already 120×120 clusters give convergent results. The results presented in our previous paper[25] have been obtained for much smaller clusters. Although we have properly reproduced the Hofstadter energy spectrum and the critical temperature in the absence of magnetic field, the slope of $H_{c2}(T)$ calculated for $H\rightarrow 0$ has been strongly overestimated. In the case of weak magnetic field classical radiuses of the Landau orbits become large and the finite-size effects can be of significant importance. Let us start with a discussion of the upper critical field for $t'=0$, when the Fermi surface is perfectly nested.

Figures 2 and 3 show the reduced critical field, $h_{c2}=ea^2H_{c2}/(\hbar c)$, for different concentrations of holes. Independently on the symmetry of the superconducting order parameter, i.e., for isotropic (Fig. 2) as well as anisotropic pairing (Fig. 3), the slope of $H_{c2}(T)$ strongly decreases with increasing doping. This result can be easily understood within the standard Gor'kov equations. Namely, the increment of doping corresponds to the reduction of the average Fermi velocity and the critical temperature T_{c0} calculated in the absence of magnetic field.

Note that our cluster results exactly reproduce the BCS transition temperature when the magnetic field tends to zero. In the case of intersite pairing the arrows indicate BCS solutions for $d_{x^2-y^2}$ superconductivity. However, the external magnetic field affects the relative phases of the order parameter in the x and y directions, which can change from site to site. Therefore it is difficult to investigate the type of the symmetry of the energy gap in the presence of magnetic field. This problem will be discussed at the end of this chapter.

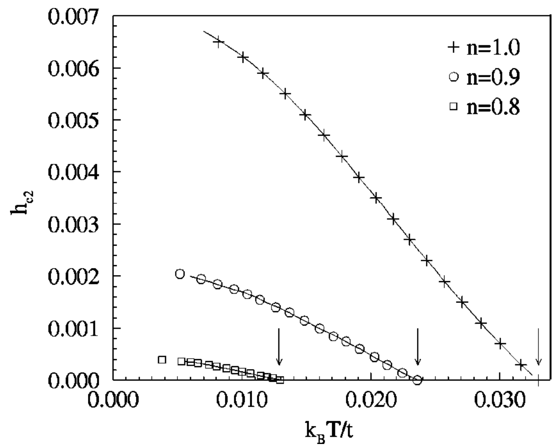

FIG. 2. Temperature dependence of the reduced upper critical field for isotropic pairing and different occupation numbers n. The cross, circle, and square marks indicate results obtained on the 150×150 cluster, whereas the solid lines correspond to the 200×200 cluster. The arrows show the superconducting transition temperature for an infinite system calculated from the BCS gap equation in the absence of magnetic field. $V=t$ and $t'=0$ have been assumed.

Contrary to the conclusion presented in Ref. 22, our results (Figs. 2 and 3) do not indicate that the upward curvature of $H_{c2}(T)$ can emerge as a direct consequence of the symmetry of the superconducting state. However, the anisotropy of the order parameter can significantly influence the magnitude of the upper critical field. In order to investigate this relationship we have directly compared results obtained for on-site and intersite pairing. We have chosen the magnitudes of the pairing potentials V, which, in the absence of magnetic field, lead to the same superconducting transition

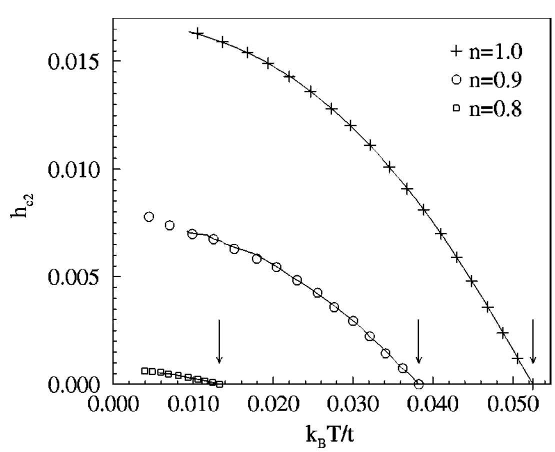

FIG. 3. The same as in Fig. 2, but for anisotropic pairing. The cross, circle, and square marks indicate results obtained on the 120×120 cluster, whereas the solid lines correspond to the 150×150 cluster. The arrows show the d-wave superconducting transition temperature for an infinite system calculated from the BCS gap equation in the absence of magnetic field. Here, $V=0.3t$ and $t'=0$ have been assumed.

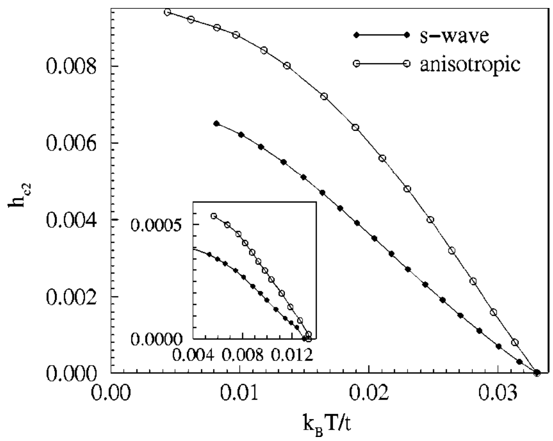

FIG. 4. The temperature dependence of the upper critical field evaluated for the half filled case, $n=1$. The circle and diamond symbols denote results obtained for intersite pairing with $V=0.244t$ and on-site pairing with $V=t$, respectively. $t'=0$ has been assumed. The symbols and continuous lines correspond to the same sizes of clusters as in Figs. 2 and 3. The inset shows the upper critical field obtained for the occupation number $n=0.8$. Here we have taken the intersite pairing potential $V=0.3t$.

temperatures for isotropic and anisotropic superconductivity. Figure 4 shows the temperature dependence of the upper critical field obtained for the half filled case. One can see that the anisotropic superconductivity is less affected by the external field than the isotropic one. An important observation is that this result depends neither on the magnitude of the pairing potential nor on the concentration of holes (see the inset in Fig. 4).

In the absence of magnetic field there is a van Hove singularity in the middle of the band. Although the external field results in a splitting of the Bloch band into a huge number of subbands, the presence of the original van Hove singularity is reflected in the Hofstadter spectrum.[28] In contradistinction to the structure of Landau levels, the Hofstadter spectrum does not consist of uniformly distributed energy levels. In particular, the average distance between the energy levels close to the Fermi energy achieves its minimum when the chemical potential is in the middle of the Bloch band. It can be considered as a remnant of the original van Hove singularity.

The question which arises concerns the impact of this feature on the upper critical field. In order to analyze this problem we have fitted $H_{c2}(T)$ obtained for isotropic superconductivity to the results obtained for the two-dimensional version[23] of the Helfand–Werthamer approach to the Gor'kov equations. Figure 5 shows the numerical results. Away from the half filled case the qualitative temperature dependence of the upper critical field can be very well approximated by the solution of the Gor'kov equations. It suggests that the complicated Hofstadter spectrum does not influence qualitatively the temperature dependence of the critical field, provided that the Fermi level is far enough from the original van Hove singularity. Although, the Cooper-pair susceptibility is strongly peaked at the Fermi level, eigenstates with energies of the order of kT give a comparable contribution to the gap equation. Therefore small modifica-

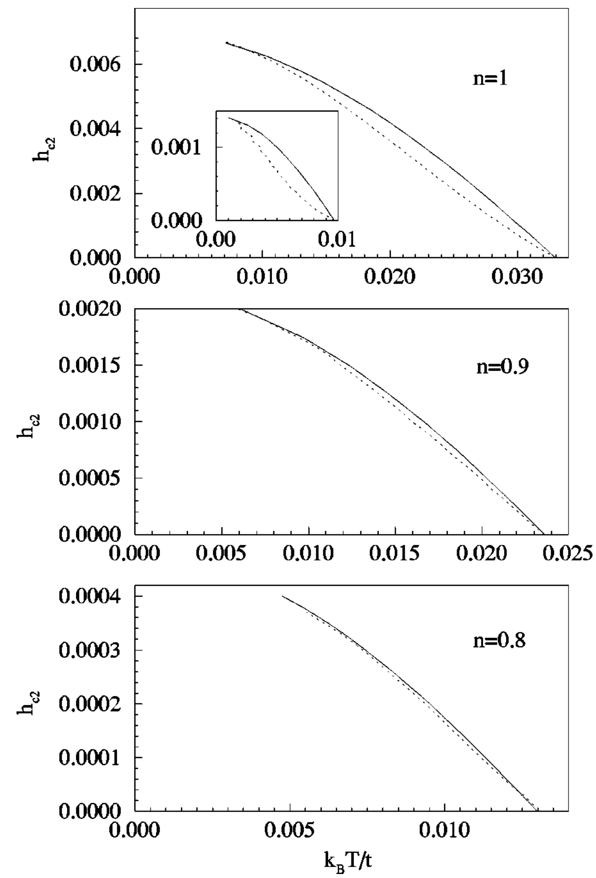

FIG. 5. The upper critical field obtained for the on-site pairing with $t'=0$ (dashed lines) fitted to the results obtained for the two-dimensional version of the Helfand-Werthamer approach to the Gor'kov equations (continuous lines). We have chosen the pairing potential $V=t$, for different values of the occupation number n, indicated in the figures. The inset shows results obtained for $V=0.7t$ and $n=1$.

tions of the Hofstadter butterfly ($\ll kT$) do not affect the upper critical field, whereas a smeared energy spectrum changes smoothly with the magnetic field.[28] However, in the vicinity of the van Hove singularity the second derivative of $H_{c2}(T)$ is significantly enhanced, when compared to the results obtained from the Gor'kov equations. It is of particular importance for small values of the pairing potential, when the system remains in superconducting state only at relatively low temperatures and the Cooper-pair susceptibility is strongly peaked at the Fermi level. Then, the curvature of $H_{c2}(T)$ can gradually change from negative to positive, as depicted in the inset of Fig. 5. This effect takes place for isotropic as well as for anisotropic pairing. Similar results have been reported in Refs. 36 and 37.

Results presented in Figs. 2–5 have been obtained for a rather unrealistic dispersion relation with $t'=0$ when the Fermi surface is perfectly nested for the half filled band. This shortcoming can be significantly improved when accounting for the next-nearest-neighbor hopping. Figure 6 shows the upper critical field calculated for $t'=-0.45t$ that is commonly used to simulate the actual Fermi surface of high-T_c compounds.[38] Despite a serious modification of the band

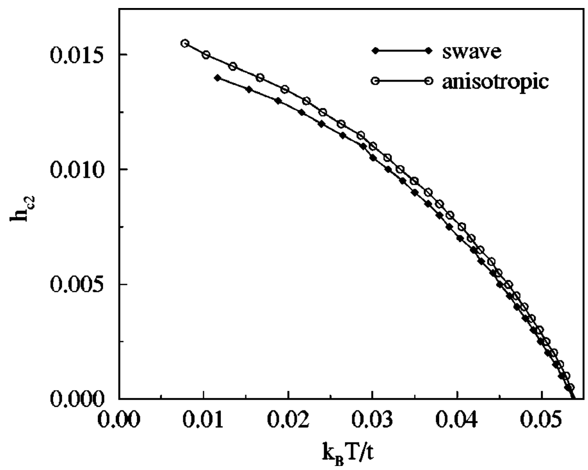

FIG. 6. The same as in Fig. 4, but for $t' = -0.45t$ and occupation number $n = 0.7$. The circle and diamond symbols denote results obtained for intersite pairing with $V = 0.3t$ and on-site pairing with $V = 0.9t$, respectively.

structure, the qualitative features of $H_{c2}(T)$ remain unchanged. Here, contrary to the results presented in Fig. 4, the difference between H_{c2} obtained for isotropic and anisotropic superconductivity is much smaller. These results clearly show the importance of the shape of Fermi surface for the upper critical field, as pointed out in Ref. 36.

To get the first insight into the symmetry of the superconducting order parameter we have calculated $\det[\mathcal{M}^{(x,x)} - \mathcal{M}^{(x,y)} - I]$ and $\det[\mathcal{M}^{(x,x)} + \mathcal{M}^{(x,y)} - I]$ for $H \to H_{c2}$, where $\mathcal{M}^{(\alpha,\beta)}$ are given by Eq. (15) and I is the unit matrix. These quantities should vanish when the solution of Eq. (14) would be of purely d-wave ($\vec{\Delta}^{(x)} = -\vec{\Delta}^{(y)}$) or extended s-wave symmetry ($\vec{\Delta}^{(x)} = \vec{\Delta}^{(y)}$). We have found that for a 120×120 cluster the ratio of these quantities increases with the magnetic field, however, it is always less than 10^{-6}. One should keep in mind that none of these quantities can be exactly zero, due to the mixed boundary conditions in x and y directions. Our results suggest that also in the presence of the magnetic field the extended s-wave symmetry is of minor importance. However, as we have restricted our consideration to the nearest-neighbor pairing, we cannot discuss the possibility of the field-induced phase transition to the $d_{x^2-y^2} + id_{xy}$ symmetry recently suggested by Krishana *et al.*[15,39]

IV. CONCLUDING REMARKS

We have investigated the temperature dependence of the upper critical field for the two-dimensional lattice gas. With the help of unitary transformation we have obtained a diagonal form of the Hamiltonian in the normal state and derived gap equations both for isotropic and anisotropic superconductivity. We have discussed influence of the symmetry of the superconducting state and the van Hove singularity on the upper critical field. Our results clearly indicate that the symmetry of the superconducting order parameter itself cannot lead to upward curvature of $H_{c2}(T)$. However, quite pronounced tendency can be observed for the half filled case, when the Fermi energy is close to the original van Hove singularity. In the absence of the external field this singularity occurs in the middle of the band. The enhancement of curvature of $H_{c2}(T)$ takes place for isotropic as well as anisotropic superconductivity and is of particular importance for small values of the pairing potential. Then, the curvature can gradually change from negative to positive. This effect smears out for larger doping where the temperature dependence of the upper critical field can be rendered very well when solving the Gor'kov equations. We have found that in the case of anisotropic pairing the upper critical field exceeds the critical field obtained for isotropic superconductivity. It takes place for small doping ($\delta < 0.2$) and arbitrary magnitude of the pairing potential. These results suggest that in the two-dimensional lattice gas with nested Fermi surface anisotropic superconductivity is less affected by the external field than the isotropic one.

The proposed method allows one to derive the gap equation in the same way as the standard BCS approach. The only differences are related to the fact that the diagonal form of the normal-state Hamiltonian is obtained numerically and the superconducting order parameter can be a site-dependent quantity. The similarity between our method and the BCS approach allows for straightforward incorporation of the local Coulomb repulsion within any standard approximation. Here, one may expect destructive influence of correlations, in particular in the isotropic channel. This originates from the fact that local repulsion always acts to the detriment of the formation of local Cooper pairs. The impact of Coulomb, Hubbard-like, correlations on anisotropic superconductivity seems to depend on the approximation scheme. This problem is under our current investigation.

It would be also interesting to investigate the relative motion of electrons which form the Cooper pairs and to discuss the vortex lattice (see Ref. 40 for the details of this approach). However, our method is not suitable for investigation of the Abrikosov lattice. We assume the plane-wave behavior in y direction that allows us to reduce the original two-dimensional problem to the one-dimensional one. Therefore we can perform a numerical calculation for much larger clusters. Without this simplification one can look for the solution that is spatially inhomogenous in y direction, e.g., the Abrikosov lattice-type solution, but for much smaller systems.

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APPENDIX: SPIN-FLUCTUATIONS EXCHANGE INTERACTION

The singlet pairing (or depairing) originating from the spin-fluctuation exchange interactions is determined by random-phase approximation–type expression that contains magnitude of local Coulomb repulsion U and zero-frequency susceptibility of the noninteracting band electrons χ_0.[41] In

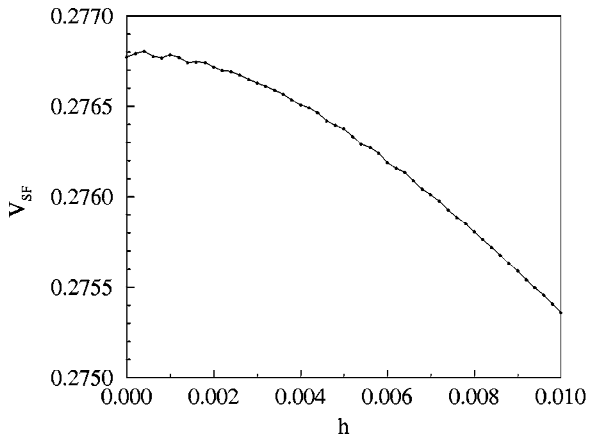

FIG. 7. Magnitude of the on-site interaction (V_{SF}) as a function of the reduced magnetic field for the half filled band with $t'=0$. $k_BT=0.01t$ and $U=t$ have been assumed.

order to investigate the impact of magnetic field on this interaction, we consider only the lowest-order contribution, with respect to U:

$$V_{SF}(\mathbf{p},\mathbf{p}')=U^2\chi_0(\mathbf{p},\mathbf{p}',\omega=0), \tag{A1}$$

where $\mathbf{p}$ and $\mathbf{p}'$ denote momenta of electrons (see Ref. 41 for the notation). We have found that in the presence of magnetic field the spin-fluctuaction-induced interaction for arbitrary situated sites i and j is given by

$$\begin{aligned} V_{SF}(\vec{\rho}) = {} & \frac{U^2}{2N^2}\sum_{m,m'}\sum_{\overline{p}_x,p_y}\sum_{\overline{k}_x,k_y}\exp[-ia\rho_y(p_y+k_y)] \\ & \times g^*(\overline{p}_x,p_y,m)g(\overline{p}_x,p_y,m+\rho_x)g^*(\overline{k}_x,k_y,m' \\ & +\rho_x)g(\overline{k}_x,k_y,m')\left[\tanh\frac{E(\overline{k}_x,k_y)-\mu+g\mu_BH_z}{2k_BT}\right. \\ & \left.-\tanh\frac{E(\overline{p}_x,p_y)-\mu-g\mu_BH_z}{2k_BT}\right] \\ & \times[E(\overline{k}_x,k_y)-E(\overline{p}_x,p_y)+2g\mu_BH_z]^{-1}, \end{aligned} \tag{A2}$$

where $a\vec{\rho}=\vec{R}_i-\vec{R}_j$ (a is the lattice constant). In particular, $\vec{\rho}=(\pm1,0)$ and $\vec{\rho}=(0,\pm1)$ when the neighboring sites are situated along the x and y axis, respectively, and $\vec{\rho}=(0,0)$ for on-site interaction. Figure 7 presents the dependence of the on-site repulsion upon the magnetic field.

Similarly, in the case of intersite attraction, we have found that V_{SF} is hardly affected by weak magnetic field.

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