

Upper critical field for electrons in a two-dimensional lattice

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We address a problem of the upper critical field in a lattice described by a two-dimensional tight-binding model with the on-site pairing. We develop a finite-system approach which enables investigation of magnetic and superconducting properties of electrons on clusters, consisting of a few thousand sites. We present the temperature dependence of the upper critical field and discuss the reentrance of superconductivity for high magnetic field. We also briefly discuss possible extension of the model to account for the properties of high-temperature superconductors. [S0163-1829(99)05633-7]

The issue of the critical field consists of two different phenomena, namely, the movement of electrons in a periodic potential under the influence of a magnetic field and superconductivity. Each of these phenomena has been investigated for many decades and many solutions in limiting cases are known at present. Concerning the movement of electrons one deals with two limiting cases: free or nearly free electrons in a magnetic field, when Landau levels structure sets on,^{1,2} and electrons in a periodic potential in the absence of magnetic field, when the solutions are Bloch waves which lead to energy bands. Away from these limiting cases the situation is much more complicated. Application of magnetic field to the two-dimensional (2D) electron system in tight-binding approximation leads to a fractal energy spectrum known as Hofstadter's butterfly, where very small changes in magnetic field can result in a completely different spectrum.³⁻⁵ Electrons on a lattice are gauge invariantly coupled with a U(1) gauge field by introducing phase factors in the kinetic-energy hopping term, i.e., the wave function acquires a factor $\exp[(ie/\hbar c)\int_i^j \mathbf{A} \cdot d\mathbf{l}]$, where \mathbf{A} is the external classical vector potential, when an electron hops from site i to site j .⁶ The Zeeman term is neglected. The same energy spectrum can be obtained in a nearly free-electron method with a weak periodic perturbation introduced into the Landau-quantized 2D electron system.^{4,7,8}

On the other hand, the influence of a magnetic field on superconductivity is usually described by phenomenological Ginzburg-Landau theory⁹ (or Lawrence-Doniach theory in the case of layered superconductors¹⁰) where the magnetic field is treated semiclassically. This approach was later justified also at the microscopic level,¹ but the temperature dependence of physical quantities is also of a phenomenological character and therefore its validity is limited.

Although, there is a general agreement that external magnetic field reduces the critical temperature, positive curvature of $H_{c2}(T)$ observed in high-temperature superconductors¹¹ is still a matter at issue. The most important differences between standard BCS type and high-temperature superconductors are related to the presence of strong electronic correlations and specific geometry of high- T_c materials. In this paper we address an important problem concerning the upper critical field for electrons described by the two-dimensional tight-binding model.

Our starting point is a two-dimensional square lattice immersed in a perpendicular, uniform magnetic field. The mean-field Hamiltonian is of the form

$$\hat{H} = \sum_{i,j,\sigma} t_{ij}(\mathbf{A}) c_{i\sigma}^\dagger c_{j\sigma} - V \sum_i (c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger \Delta_i + c_{i\downarrow} c_{i\uparrow} \Delta_i^*). \quad (1)$$

Here, $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) creates (annihilates) an electron with spin σ on site i , V stands for the magnitude of the on-site attraction and \mathbf{A} is the vector potential corresponding to the external magnetic field \mathbf{H} . Similarly to Gor'kov's approach we introduce local superconducting order parameter¹

$$\Delta_i = \langle c_{i\downarrow} c_{i\uparrow} \rangle, \quad (2)$$

which, in general, can be site dependent. According to the Peierls substitution⁶ the original hopping integral t_{ij} is multiplied by a phase factor, which accounts for coupling of electrons to the magnetic field

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

In order to derive the self-consistent equation for the gap-function, we make use of unitary transformation and introduce

$$a_{m\sigma} = \sum_i U_{mi}^\dagger c_{i\sigma}, \quad (4)$$

where the unitary matrix U_{im} consists of eigenvectors of the Hermitian matrix $t_{ij}(\mathbf{A})$

$$\sum_{i,j} U_{mi}^\dagger t_{ij}(\mathbf{A}) U_{jn} = \delta_{mn} E_m. \quad (5)$$

This unitary transformation determines energy spectrum of the system in the normal state in the presence of external magnetic field. In the absence of magnetic field, Eq. (4) represents a transformation to the momentum space, namely, $U_{jm} = N^{-1/2} \exp(i\mathbf{R}_j \cdot \mathbf{k}_m)$. In the case of free electron gas external magnetic field leads to the occurrence of rotationally invariant states corresponding to the Landau orbits.

Equations of motion lead to formally exact expression for the anomalous Green's function

$$(\omega - E_m) \langle \langle a_{m\uparrow} | a_{n\downarrow} \rangle \rangle = -V \sum_{i,n'} \Delta_i U_{im}^* U_{in'}^* \langle \langle a_{n'\uparrow} | a_{n\downarrow} \rangle \rangle. \quad (6)$$

At temperatures close to T_c one can restrict himself only to terms linear in the superconducting order parameter. Therefore, the Green's function $\langle \langle a_{n'\uparrow} | a_{n\downarrow} \rangle \rangle$ which enters the above equation can be calculated in the normal state and one can derive a system of linearized gap equations which determine the upper critical field

$$\Delta_j = V \sum_i \Delta_i \sum_{m,n} U_{jn} U_{jm} U_{im}^* U_{in}^* \times \frac{\tanh(E_m/2k_B T) + \tanh(E_n/2k_B T)}{2(E_m + E_n)}. \quad (7)$$

In the absence of magnetic field one can choose the order parameter as a site-independent quantity ($\Delta_i = \Delta$). Then the above equation can be easily reduced to the standard BCS form. This formula is gauge invariant and is valid for any dispersion relation determined by the hopping integral t_{ij} . However, in order to simplify numerical calculations we restrict ourselves only to the nearest-neighbor hopping with $t_{\langle i,j \rangle} = t$ and choose the Landau gauge $\mathbf{A} = H_z(0, x, 0)$. Such a form of \mathbf{A} neglects the effects of diamagnetic screening supercurrents induced by the applied field what means that the true vector potential should be determined self-consistently. However, close to the transition temperature, i.e., in the limit of infinite London penetration depth, such an approximation is correct. Then, the unitary matrix U_{in} takes on the form

$$U_{in} \equiv U_{x,y}(\bar{p}_x, p_y) = N^{-1/4} e^{ip_y y a} g(\bar{p}_x, p_y, x), \quad (8)$$

where (x, y) enumerate the lattice sites $\mathbf{R}_{x,y} = \mathbf{e}_x a x + \mathbf{e}_y a y$, p_y is the wave vector in the y direction, and a is the lattice constant.

It follows from Eq. (5) that $g(\bar{p}_x, p_y, x)$ must fulfill the Harper equation³

$$g(\bar{p}_x, p_y, x+1) + 2 \cos(hx - p_y a) g(\bar{p}_x, p_y, x) + g(\bar{p}_x, p_y, x-1) = t^{-1} E(\bar{p}_x, p_y) g(\bar{p}_x, p_y, x), \quad (9)$$

where $h = e a^2 H_z / (\hbar c)$. $h/(2\pi)$ can be interpreted as a ratio of the flux through a lattice cell to one flux quantum.⁵ In the absence of magnetic field \bar{p}_x corresponds to the x component of the wave vector \mathbf{p} . As the choice of Landau gauge breaks the translational symmetry along the x axis, for $\mathbf{H} \neq \mathbf{0}$ \bar{p}_x represents a quantum number which, however, cannot be identified as a component of the wave vector. The choice of this gauge allows one to take U_{in} in the form given by Eq. (8) and reduces the original two-dimensional eigenproblem (diagonalization of the kinetic part of the Hamiltonian) to a one-dimensional difference equation. A thorough analysis of Harper's equations can be found in Ref. 5.

Due to the plane-wave behavior in the y direction, there is a solution of Eq. (7) which does not depend explicitly on y :

$$\Delta_i \equiv \Delta_{x,y} = \Delta_x. \quad (10)$$

For the specific form of U_{in} , as given by Eq. (8), the upper critical field is determined by the following equation:

$$\Delta_{x'} = \frac{V}{\sqrt{N}} \sum_x \Delta_x \sum_{p_y, \bar{p}_x, \bar{k}_x} g(\bar{p}_x, p_y, x') g(\bar{k}_x, -p_y, x') \times g(\bar{k}_x, -p_y, x) g(\bar{p}_x, p_y, x) \times \frac{\tanh[E(\bar{p}_x, p_y)/2k_B T] + \tanh[E(\bar{k}_x, -p_y)/2k_B T]}{2[E(\bar{p}_x, p_y) + E(\bar{k}_x, -p_y)]}. \quad (11)$$

In order to evaluate the upper critical field one has to start with solving the Harper equation. The corresponding energy spectrum $E(\bar{p}_x, p_y)$ was obtained for the first time by Hofstadter and constitutes a self-similar, fractal structure known as the Hofstadter butterfly.⁵ In the thermodynamic limit Eq. (11) is actually an infinite system of equations and cannot be solved exactly. Therefore, in order to get the first insight into the properties of the system under consideration, we have performed numerical calculations for finite systems. In particular, we have investigated square clusters which consist of a few thousand lattice sites. Due to the broken translational symmetry, we have introduced periodic boundary conditions only along the y axis and fixed boundary conditions in x direction. It means that for the $M \times M$ cluster we have taken into account M points along x axis and M values of the wave vector $p_y \in (-\pi/a, \pi/a]$. Making use of the fixed boundary conditions in the x direction the Harper equation (9) simplifies to an eigenproblem of a tridiagonal matrix with all the off-diagonal elements equal unity. An additional effect originating from such specific boundary conditions is the absence of unphysical degeneracy of states at the Fermi level which occurs in cluster calculations with fixed and periodic boundary conditions taken in both directions.¹²

To check the influence of finite size effects we have calculated the density of states of 2D electron lattice gas in the normal state. We have found that the density of states calculated for clusters reproduces very well the results obtained on the basis of Hofstadter's procedure for an infinite system.⁵ Figure 1 shows a comparison of results obtained within these two approaches for rather unrealistically high magnetic field $h = 2\pi/10$ ($\sim 4000T$). This agreement takes place also for much weaker field, however, small distances between the energy levels would make the presentation unreadable. As a further verification of our cluster approach we have compared the critical temperature calculated without the external magnetic field with exact results for the 2D lattice obtained from the BCS-type gap equation (see the inset in Fig. 1). The critical temperature obtained from the cluster calculations is always a bit lower than the exact value simply due to the absence of van Hove singularity in finite cluster.

Since our method works well in both limiting cases, i.e., in the normal state influenced by external magnetic field and in superconducting state analyzed without the field, we have used this approach to tackle the problem which is fundamental in the intermediate region, namely, the influence of the external field on superconductivity. Numerical solutions of Eq. (11) are shown in Fig. 2.

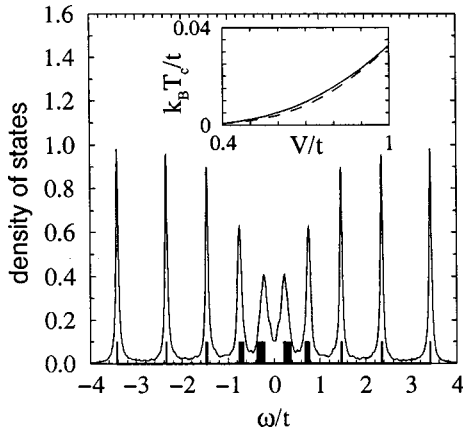


FIG. 1. Density of states obtained for a 50×50 cluster and $h = 2\pi/10$. Vertical bars show the energy spectrum obtained for infinite system (Hofstadter's butterfly). Energy levels obtained from the cluster calculations are represented by the Lorentz function with a width equal to $0.03t$. The inset shows the superconducting transition temperature calculated in the absence of magnetic field versus the magnitude of pairing potential. Here, continuous and dashed lines show exact result for infinite lattice and solution for the 40×40 cluster, respectively.

However, one has to bear in mind that our cluster calculations are not valid in genuinely low temperatures when the Cooper pair susceptibility accounts only for very few poles of the Green's function $[E(\bar{p}_x, p_y)]$ instead of a continuous density of states. The simplest criterion of validity for a $M \times M$ cluster is an assumption that temperature ($k_B T$) must be larger than an average distance between different quasiparticle energies ($\approx 8t/M^2$). We have found that, similarly to the free electron gas described by Gor'kov equations,^{1,2} also in the tight-binding model $H_{c2}(T)$ exhibits the negative curvature. It is remarkable that the critical temperature is a smooth function of applied magnetic field despite the fact that the energy spectrum is strongly affected even by small changes of the field.⁵ However, for realistic values of magnetic field, $h \sim 10^{-4} - 10^{-3}$, the band splits into a huge number of subbands ($\propto h^{-1}$) with the gaps between them much smaller

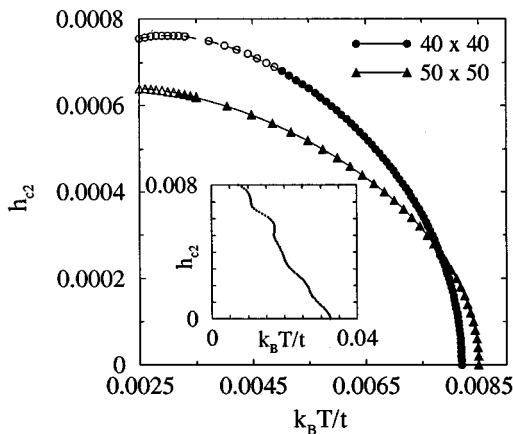


FIG. 2. Reduced upper critical field obtained for 40×40 and 50×50 clusters plotted as a function of temperature. $V = 0.7t$ has been used. Filled circles and triangles denote results which fulfill the criterion $k_B T > 8t/M^2$. The inset shows $H_{c2}(T)$ for $V = t$ obtained for 40×40 cluster.

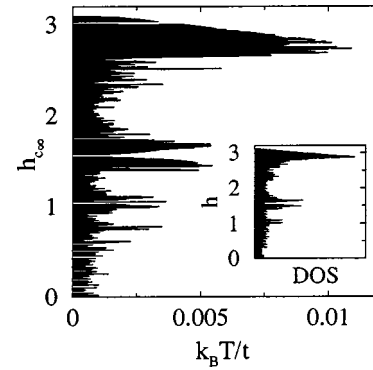


FIG. 3. The phase diagram for the reentrant superconductivity in the T - H plane. The filled area shows the superconducting phase. The inset presents the density of states at the Fermi level as a function of magnetic field.

than $k_B T$. Therefore, macroscopic properties of the system remain smooth functions of the magnetic field. For stronger magnetic fields and at lower temperature, oscillations, which occur due to the discrete energy spectrum, should be visible. However, the above mentioned criterion restricts the region of temperatures which is available in our cluster approach. Therefore, in order to see the impact of these oscillations on the upper critical field we have considered higher values of the local pairing potential. The inset in Fig. 2 shows the temperature dependence of the upper critical field calculated with $V = t$. As the system remains in superconducting state for much higher values of magnetic field ($\sim 50T$), H_{c2} strongly depends on the structure of Hofstadter's spectrum.

Realistic magnetic field suppresses superconductivity, what remains in agreement with a general feeling (in the case of free electron gas it can be attributed to the orbital frustration of the order parameter¹³). However, as presented in Fig. 3, for genuinely strong magnetic field the reentrance of superconducting phase takes place. A possibility of such an unusual behavior has recently attracted a lot of interest.^{13,14} For free electron gas this effect originates from the high degeneracy of Landau levels in strong magnetic field, namely when only a few lowest levels are occupied the orbital frustration of the order parameter is reduced and the only pair-breaking mechanism corresponds to a Zeeman splitting (for singlet superconductivity) and impurity scattering. In the case of lattice gas, the presence of strong magnetic field results in a small number of narrow subbands with strongly peaked density of states (see Fig. 1). Consequently, any time the chemical potential is in the region of finite density of states there is Cooper singularity in the kernel determining the critical temperature (Eq. 7) and T_c is finite.¹⁵ Therefore, the density of states is the most important quantity, which determines the temperature dependence of the critical field in the reentrant phase. It can be justified by a comparison of the curve $H_{c2}(T)$ and the density of states shown in the inset in Fig. 3.

To conclude, we have investigated the relationship between superconductivity and an external magnetic field in a model of electron gas in a 2D lattice. The proposed method allows one to analyze such a model on large clusters, of the order of a few thousand lattice sites, carrying out exact calculations. In contradistinction to the Gor'kov approach, which is valid for free electron gas, we have carried out

calculations for a system with different geometry, i.e., for the 2D electron gas on a square lattice. We have obtained three qualitatively different solutions for $H_{c2}(T)$: an Abrikosov-Gor'kov-type solution for weak magnetic field, the reentrance of superconductivity for strong magnetic field (quantum limit), and small oscillations in the intermediate region. Our results suggest that the lattice geometry itself is insufficient to explain the origin of the positive curvature of the upper critical field observed in the copper-oxide high- T_c superconductors. The most important feature of these materials neglected in our approach is the presence of strong correlations resulting from the on-site repulsion on the copper sites. On the other hand, in order to analyze the influence of these

correlations on the upper critical field one has to diagonalize the full Hamiltonian with the interaction term, which is possible only for very small clusters for which the finite size effects play a much more important role. In the framework of the proposed approach one can take into account not only local, but also nonlocal pairing. Such an extension would lead to an anisotropic superconductivity, which can survive in spite of the presence of strong on-site repulsion.¹⁶

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