Upper critical field for electrons in 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 discuss how the quasiparticle density of states changes with the applied external magnetic field and present the temperature dependence of the upper critical field. We also briefly discuss possible extension of the model to account for the properties of high–temperature superconductors.

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The issue of the critical field consists of two different phenomena, namely a movement of electrons in a periodic potential under influence of a magnetic field and superconductivity. Each of these phenomena has been investigated since 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 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. 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(iec∫A·dl), where A is the external classical vector potential, when an electron hops from site i to site j. 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. On the other hand, the influence of a magnetic field on superconductivity is usually described by phenomenological Ginzburg–Landau theory, (or Lawrence–Doniach theory in the case of layered superconductors) where the magnetic field is treated semiclassically. This approach was later justified also at the microscopic level, 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 Hc2(T) observed in high–temperature superconductors 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–Tc 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 two-dimensional square lattice immersed in a perpendicular, uniform magnetic field. The mean-field Hamiltonian is of the form

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

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

\[\Delta_i = \langle c_i c_i^\dagger \rangle ,\] (2)

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

\[t_{ij}(A) = t_{ij} \exp \left( \frac{ie}{hc} \int_{R_j} A \cdot dl \right) .\] (3)

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

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

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

\[\sum_{ij} U_{mi}^\dagger t_{ij}(A) U_{jn} = \delta_{mn} E_m ,\] (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 $U_{jm} = 1/N \exp (i \mathbf{R}_j \cdot \mathbf{k}_m)$. In the case of free electron gas external magnetic field leads to the occurrence of rotationally invariant states corresponding to the Landau orbits. In order to visualize the impact of magnetic field on electrons in the 2D lattice we have calculated the resulting current distribution. Within the framework of linear–response theory the current operator 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 $t_{i(i,j)} = t$ and choose the Landau gauge $A = H_\perp (0, x, 0)$. Here, $H_\perp$ denotes a magnitude of external magnetic field perpendicular to the $(x, y)$ plane. Such a form of $A$ 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:

$$U_{in} = U_{x,y} (\tilde{p}_x, p_y) = N^{-1/4} e^{ip_y y_0} g (\tilde{p}_x, p_y, x), \quad (8)$$

where $(x, y)$ enumerate the lattice sites $\mathbf{R}_{x,y} = e_x ax + e_y ay$ and $p_y$ is the wave vector in the $y$ direction.

It follows from Eq. (5) that $g (\tilde{p}_x, p_y, x)$ must fulfill the Harper’s equation $\mathbf{3}$:

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

where $h = e a^2 H_\perp/(hc)$. $h/(2\pi)$ can be interpreted as a ratio of the flux through a lattice cell to one flux quantum $\mathbf{3}$. In the absence of magnetic field $\tilde{p}_x$ 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 $\mathbf{H} \neq 0 \tilde{p}_x$ represents a quantum number which, however, can not 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. $\mathbf{3}$.

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

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

For the specific form of $U_{in}$, as given by Eq. (8), the upper critical field is determined by the following equation:
\[
\Delta_{x'} = \frac{V}{\sqrt{N}} \sum_x \sum_{p_x,p_y,k_x} g(p_x, p_y, x') g(k_x, -p_y, x') \\
\times g(k_x, -p_y, x) \times \frac{\tanh E(p_x, p_y) + \tanh E(k_x, -p_y)}{2[E(p_x, p_y) + E(k_x, -p_y)]}.
\] (11)

In order to evaluate the upper critical field one has to start with solving the Harper’s equation. The corresponding energy spectrum \(E(p_x, p_y)\) has been obtained for the first time by Hofstadter and constitutes a self-similar, fractal structure known as the Hofstadter butterfly [5].

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. 3). 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. 3.

![FIG. 2. Density of states obtained for a 50 x 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 the width equal 0.03\(t\).](image)

Making use of the fixed boundary conditions in the \(x\) direction the Harper equation (9) simplifies to an eigenvalue problem 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 [2].

To check the influence of finite size effects we have calculated the density of states of 2D electron lattice gas in the normal state. Fig. 2 shows that the density of states calculated for a 50 x 50 cluster reproduces very well the results obtained on the basis of Hofstadter’s procedure for infinite systems [5].

FIG. 3. Reduced upper critical field obtained for 40 x 40 and 50 x 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 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 40 x 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 \([E(p_x, p_y)]\) 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 ($\simeq 8t/M^2$). We have found that, similarly to the free electron gas described by Gor’kov equations (1), 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. However, for realistic values of magnetic field, $h \sim 10^{-4} \div 10^{-3}$, the band splits into a huge number of subbands ($\propto h^{-1}$) with the gaps between them much smaller than $k_B T$. Therefore, macroscopic properties of the system remain smooth functions of the magnetic field.

To conclude, we have investigated the relationship between superconductivity and an external magnetic field in a simple model of electron gas in a 2D lattice. The proposed method allows one to analyze such a model on large clusters, of size of the order of a few thousand lattice sites, carrying out exact calculations. The main result is the temperature dependence of the upper critical field (or, equivalently, the applied magnetic field dependence of the critical temperature). We have found that the external magnetic field suppresses superconductivity, what remains in agreement with a general filling, although there are papers where the reentrance of the superconductivity due to Landau quantization in strong magnetic field is analyzed (3). 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. Such a geometry is believed to play a crucial role in high–critical–temperature superconductors. However, in spite of the differences between these two approaches the curvature of the transition curve $H_{c2}(T)$ in both cases is negative. This result suggests 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 and additional factors have to be taken into account. The most important feature of these materials neglected in our approach is the presence of strong on–site repulsion (4). This problem is currently under investigation.

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