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A method of studying the Bogoliubov–de Gennes equations for the superconducting vortex lattice state

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Abstract

In this paper, we present a method to construct the eigenspace of the tight-binding electrons moving on a 2D square lattice with nearest-neighbor hopping in the presence of a perpendicular uniform magnetic field which imposes (quasi-)periodic boundary conditions for the wavefunctions in the magnetic unit cell. Exact unitary transformations are put forward to correlate the discrete eigenvectors of the 2D electrons with those of the Harper equation. The cyclic tridiagonal matrix associated with the Harper equation is then tridiagonalized by another unitary transformation. The obtained truncated eigenbasis is utilized to expand the Bogoliubov–de Gennes equations for the superconducting vortex lattice state, which shows the merit of our method in studying large-sized systems. To test our method, we have applied our results to study the vortex lattice state of an s-wave superconductor.

1. Introduction

Vortex states of type-II superconductors have received great attention in recent years. The theoretical formalism describing this effect is the Bogoliubov–de Gennes (BdG) approach [1], which can be viewed as a real-space extension of Bardeen–Cooper–Schrieffer (BCS) theory. This method allows one to reveal effects of imperfections in superconductors, such as impurities, surfaces, as well as the field-induced vortices which we are concerned with in this paper. In recent years there have been numerous studies on the superconducting vortex lattice state by solving the discrete BdG equations via either the numerical diagonalization of the BdG mean-field Hamiltonian on a two-dimensional tight-binding lattice [2–6] or the recursion method [7] generalized to the superconducting state [8, 9]. However, the size of the unit cell of the vortex lattice, which is inversely proportional to the amplitude of the magnetic field, is limited by computer resources since the dimension of the BdG equations grows with system size. Therefore, early numerical works on small-size unit cells have been limited to high magnetic fields over ten Tesla, which is stronger than used in most experiments, and no remarkable progress has been made over the past decade due to the time consumption of full diagonalization (i.e. all eigenvalues and eigenvectors) of the mean-field BdG Hamiltonian. In fact, in BCS-type superconductors, electrons near the Fermi level bind into Cooper pairs by exchanging virtual bosons such as phonons, excitons or plasmons etc. Therefore, there exists an energy cutoff, which equals approximately the characteristic energy of the bosons, such as the Debye phonon frequency of conventional superconductors, and correspondingly only the electronic states lying near the Fermi surface within an energy shell are necessary to explore. For the vortex problem, the most appropriate starting point is to find the relevant electronic states which participate in BCS pairing and forming of the superconducting vortex lattice when an external magnetic field is applied. The eigenequation describing this state is a 2D difference equation formulated on a magnetic unit cell which is twice the size of that of the superconducting vortex lattice. This eigenvalue problem is also demanding when the system size is large, even though only a truncated eigenspace is desired.

In this paper we present an exact reduction of the Hermitian matrix associated with the 2D discrete equation into a tridiagonal matrix, which composed of two consecutive unitary transformations. First we reduce the 2D discrete equation that describes electrons moving in a magnetic unit cell into the famous Harper equation [10–13]. Algebraically, this unitary transformation reduces the Hermitian matrix into a cyclic tridiagonal matrix corresponding to the Harper equation. Then by another exact transformation the cyclic tridiagonal

matrix is further reduced into a tridiagonal form. The exact reduction greatly lessens the computational burden in numerical methods. Ultimately we diagonalize the tridiagonal matrix utilizing available standard software packages to find the appropriate eigenstates near the Fermi level, i.e. the truncated eigenspace, and then expand and diagonalize the BdG equations in this truncated eigenbasis.

This paper is organized as follows. In section 2, we derive the BdG equations expanded in terms of the truncated eigenbasis of the normal-state electrons in the magnetic field. The Hermitian matrix associated with the 2D tight-binding electrons on a 2D square lattice in a magnetic field is reduced into a tridiagonal form in section 3. In section 4, the vortex lattice state of an s-wave superconductor is studied as a test of our method. Section 5 gives the concluding remarks.

2. The BdG equations for vortex lattice states

In this work, we adopt a BCS-type mean-field Hamiltonian defined on a two-dimensional(2D) square lattice,

$$\hat{H} = \hat{H}_0 + \hat{H}_\Delta = \sum_{\mathbf{i},\mathbf{j},\sigma}(t_{\mathbf{ij}} - \mu\delta_{\mathbf{i},\mathbf{j}})c^\dagger_{\mathbf{i}\sigma}c_{\mathbf{j}\sigma} + \sum_{\mathbf{i},\mathbf{j}}(\Delta_{\mathbf{ij}}c^\dagger_{\mathbf{i}\uparrow}c^\dagger_{\mathbf{j}\downarrow} + \text{H.c.}), \tag{1}$$

where $\Delta_{\mathbf{ij}} = \frac{V}{2}\langle c_{\mathbf{i}\uparrow}c_{\mathbf{j}\downarrow} - c_{\mathbf{i}\downarrow}c_{\mathbf{j}\uparrow}\rangle$ for spin-singlet pairing[1]. In an external uniform magnetic field applied in the z-direction, the hopping integral acquires the Peierls phase factor as

$$t_{\mathbf{ij}} = -t\exp\left(\mathrm{i}\frac{2\pi}{\phi_0}\int_{\mathbf{j}}^{\mathbf{i}}\mathbf{A}\cdot\mathrm{d}\mathbf{l}\right) \tag{2}$$

$$= \begin{cases} -t, \\ \quad \mathbf{i} = (m_x, m_y),\ \mathbf{j} = (m_x+1, m_y) \\ -t\exp\left(\mathrm{i}\dfrac{2\pi Ba^2}{\phi_0}m_x\right), \\ \quad \mathbf{i} = (m_x, m_y),\ \mathbf{j} = (m_x, m_y+1). \end{cases} \tag{3}$$

Here t denotes the nearest-neighbor hopping integral. We choose the Landau gauge with $\mathbf{A} = B(0, x, 0)$ and the screening field induced by the supercurrent is neglected for extreme type-II superconductors. $\phi_0 = h/e$ is the electronic flux quantum. Hereafter we use a pair of integers $\mathbf{i} \equiv (m_x, m_y)$ as the index of the site in the square lattice to denote the x and y coordinates. In the Nambu representation, the above Hamiltonian can be written as

$$\hat{H} = \sum_{\mathbf{i},\mathbf{j}}(c^\dagger_{\mathbf{i}\uparrow}, c_{\mathbf{i}\downarrow})\begin{pmatrix} t_{\mathbf{ij}} - \mu\delta_{\mathbf{ij}} & \Delta_{\mathbf{ij}} \\ \Delta^*_{\mathbf{ij}} & -t^*_{\mathbf{ij}} + \mu\delta_{\mathbf{ij}}\end{pmatrix}\begin{pmatrix} c_{\mathbf{j}\uparrow} \\ c^\dagger_{\mathbf{j}\downarrow}\end{pmatrix} \tag{4}$$

$$= \hat{\Psi}^\dagger\begin{pmatrix} \check{h} - \mu\check{I} & \check{\Delta} \\ \check{\Delta}^* & -\check{h}^* + \mu\check{I}\end{pmatrix}\hat{\Psi}, \tag{5}$$

where $\hat{\Psi}^\dagger(\hat{\Psi})$ is the Nambu creation (annihilation) operator defined as $\hat{\Psi}^\dagger = (c^\dagger_{\mathbf{1}\uparrow}, c^\dagger_{\mathbf{2}\uparrow}, \cdots, c^\dagger_{K\uparrow}; c_{\mathbf{1}\downarrow}, c_{\mathbf{2}\downarrow}, \cdots, c_{K\downarrow})$ with K the total number of lattice sites. $\check{h}$ and $\check{\Delta}$ are $K\times K$ matrices with elements $(\check{h})_{\mathbf{ij}} = t_{\mathbf{ij}}$ and $(\check{\Delta})_{\mathbf{ij}} = \Delta_{\mathbf{ij}}$, respectively. $\check{I}$ is the $K\times K$ identity matrix. The mean-field Hamiltonian can be diagonalized by solving the following BdG equations,

$$\sum_{\mathbf{j}}\begin{pmatrix} t_{\mathbf{ij}} - \mu\delta_{\mathbf{ij}} & \Delta_{\mathbf{ij}} \\ \Delta^*_{\mathbf{ij}} & -t^*_{\mathbf{ij}} + \mu\delta_{\mathbf{ij}}\end{pmatrix}\begin{pmatrix} u_n(\mathbf{j}) \\ v_n(\mathbf{j})\end{pmatrix} = E_n\begin{pmatrix} u_n(\mathbf{i}) \\ v_n(\mathbf{i})\end{pmatrix} \tag{6}$$

which can be viewed as Schrödinger-like equations for the electron and hole amplitudes of a BdG quasiparticle. The pairing potential $\Delta_{\mathbf{ij}}$ couples the u and v components and satisfies the self-consistent condition

$$\Delta_{\mathbf{ij}} = V\sum_{|E_n|<E_D}u_n(\mathbf{i})v^*_n(\mathbf{j})\tanh\left(\frac{E_n}{2k_\mathrm{B}T}\right), \tag{7}$$

where E_D is the Debye-type cutoff energy of the pairing interaction. The BdG equation (6) can be expressed compactly in a matrix form

$$\begin{pmatrix} \check{h} - \mu\check{I} & \check{\Delta} \\ \check{\Delta}^* & -\check{h}^* + \mu\check{I}\end{pmatrix}\begin{pmatrix} u \\ v\end{pmatrix} = E\begin{pmatrix} u \\ v\end{pmatrix}, \tag{8}$$

with u and v K-dimensional vectors.

Abrikosov vortices, each of which carries one superconducting flux quantum $\Phi_0 = h/2e$, are created and form a lattice structure in a type-II superconductor if one applies a magnetic field ($B_{c1} \leqslant B \leqslant B_{c2}$). The vortex lattice causes periodic modulation of the pairing potential and accordingly yields energy bands of BdG quasiparticles. To study this effect in our study we adopt the concept of a magnetic unit cell (MUC) the size of which is twice that of the unit cell of the vortex lattice, and accordingly each MUC accommodates one electronic flux quantum $\phi_0 = 2\Phi_0$. Here for illumination of our method, we study the square vortex lattice which is aligned with the underlying crystalline lattice. The unit cell size of the vortex lattice is $N_x \times N_x$, corresponding to a uniform magnetic field $B = \Phi_0/(N_x a)^2$. Each MUC accommodates two adjacent vortices in the y direction. Therefore the MUC is of size $N_x \times N_y$ with $N_y = 2N_x$. The whole system is composed of $M_x \times M_y$ MUC's. Thus the whole system has $M_xM_yN_xN_y$ lattice sites. For later convenience, we introduce a dimensionless parameter $\alpha \equiv Ba^2/\phi_0 = 1/(N_xN_y)$ denoting the ratio of magnetic flux per plaquette to the electronic flux quantum ϕ_0.

In the Abrikosov vortex lattice state, the BdG equations (6) are symmetric under magnetic translation, with the translation vector $\mathbf{R} = l_xN_x\mathbf{e}_x + l_yN_y\mathbf{e}_y$. Due to this magnetic translational symmetry in the x and y direction, the quasiparticle amplitudes can be expressed in the magnetic Bloch form as

$$\begin{pmatrix} u(\mathbf{i}) \\ v(\mathbf{i})\end{pmatrix} = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{i}}\begin{pmatrix} u^{\mathbf{k}}(\mathbf{i}) \\ v^{\mathbf{k}}(\mathbf{i})\end{pmatrix}, \tag{9}$$

where the magnetic Bloch wavevector $\mathbf{k} = \frac{2\pi l_x}{M_xN_x}\mathbf{e}_x + \frac{2\pi l_y}{M_yN_y}\mathbf{e}_y$ with $l_{x,y} = 0, 1, \cdots, M_{x,y} - 1$. This transformation reduces equation (8) to the new BdG equations for $u^{\mathbf{k}}$ and $v^{\mathbf{k}}$

$$\begin{bmatrix} \check{h}^{\mathbf{k}} - \mu\check{I} & \check{\Delta}^{\mathbf{k}} \\ (\check{\Delta}^{-\mathbf{k}})^* & -(\check{h}^{-\mathbf{k}})^* + \mu\check{I}\end{bmatrix}\begin{pmatrix} u^{\mathbf{k}}_n \\ v^{\mathbf{k}}_n\end{pmatrix} = E^{\mathbf{k}}_n\begin{pmatrix} u^{\mathbf{k}}_n \\ v^{\mathbf{k}}_n\end{pmatrix}, \tag{10}$$

where the matrix elements of the $\mathbf{k}$-dependent matrices $\check{h}^{\mathbf{k}}$ and $\check{\Delta}^{\mathbf{k}}$ are $(\check{h}^{\mathbf{k}})_{\mathbf{ij}} = t_{\mathbf{ij}}\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot(\mathbf{i}-\mathbf{j})}$, $(\check{\Delta}^{\mathbf{k}})_{\mathbf{ij}} = \Delta_{\mathbf{ij}}\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot(\mathbf{i}-\mathbf{j})}$. The

[1] Our method can be readily extended to the case of spin-triplet pairing.

quasiparticle amplitudes $u^{\mathbf{k}}$ and $v^{\mathbf{k}}$ satisfy the quasi-periodic boundary conditions with period N_x along the x direction

$$u^{\mathbf{k}}(m_x + N_x, m_y) = \mathrm{e}^{-\mathrm{i}2\pi m_y N_x \alpha} u^{\mathbf{k}}(m_x, m_y) \tag{11}$$

$$v^{\mathbf{k}}(m_x + N_x, m_y) = \mathrm{e}^{\mathrm{i}2\pi m_y N_x \alpha} v^{\mathbf{k}}(m_x, m_y) \tag{12}$$

while they are periodic in the y direction with period N_y. The (m_x, m_y) in equations (10)–(12) are restricted to sites within one MUC with $m_{x,y} = 0, 1, \ldots, N_{x,y} - 1$. The above procedure reduces the Hermitian matrix with linear dimension $2M_xM_yN_xN_y$ (equation (8)) into a direct sum of M_xM_y block matrices, each of which is labeled by $\mathbf{k}$ and has linear dimension $2N_xN_y$ (equation (10)). For each quasimomentum $\mathbf{k}$, equation (10) is diagonalized along with the boundary conditions and then the whole solutions of all $\mathbf{k}$ are used by the following equation:

$$\Delta_{\mathbf{ij}} = V \sum_{|E_n^{\mathbf{k}}|<E_{\mathrm{D}}} u_n^{\mathbf{k}}(\mathbf{i})[v_n^{\mathbf{k}}(\mathbf{j})]^* \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{i}-\mathbf{j})} \tanh\left(\frac{E_n^{\mathbf{k}}}{2k_{\mathrm{B}}T}\right), \tag{13}$$

to achieve self-consistence.

In the literature the typical size of the unit cell of the vortex lattice studied by previous works was limited to around 20×20 [2–6]. Such a small unit cell size corresponds to a magnetic field as large as $B = \Phi_0/(20a)^2 \approx 32$ T, which is much higher than used by most experiments, if one assumes a typical lattice constant $a \approx 4$ Å. Therefore one should find a way to diagonalize the BdG Hamiltonian (Hermitian matrix) with a larger scale in order to match numerical calculation with experimental data. Although one can take advantage of the sparse nature of the BdG Hamiltonian $\check{\Omega}$, we think that iterative methods, such as the Lanczos algorithm, are not appropriate for this problem because they are designed to compute a few eigenvalues (eigenvectors) with the largest/smallest magnitudes.

To study the vortex lattice state with a larger unit cell and correspondingly weaker and realistic magnetic field, we re-express the real-space BdG equations (10) in the diagonal representation of $\check{h}^{\mathbf{k}}$, which describes the 2D tight-binding electrons in presence of a magnetic field,

$$\check{h}^{\mathbf{k}}\varphi_q^{\mathbf{k}} = \varepsilon_q^{\mathbf{k}}\varphi_q^{\mathbf{k}}, \tag{14}$$

where $\varphi_q^{\mathbf{k}}$ obeys the same boundary condition as equation (11). According to the BCS theory, only a fraction of electrons in the energy shell E_{D} around the Fermi energy participate in the Cooper pairing. Therefore we should first get the eigenstates $\varphi_q^{\mathbf{k}}$ from equation (14) with energies $|\varepsilon_q^{\mathbf{k}} - \mu| \leqslant E_{\mathrm{D}}$ relative to the Fermi level, which will be addressed in section 3. Here the quasiparticle amplitudes $u^{\mathbf{k}}$ and $v^{\mathbf{k}}$ are expanded in the basis functions $\varphi_q^{\mathbf{k}}$ and $(\varphi_q^{-\mathbf{k}})^*$, respectively,

$$\begin{aligned} u_n^{\mathbf{k}} &= \sum_q a_n^{\mathbf{k}}(q)\varphi_q^{\mathbf{k}} \\ v_n^{\mathbf{k}} &= \sum_q b_n^{\mathbf{k}}(q)(\varphi_q^{-\mathbf{k}})^*. \end{aligned} \tag{15}$$

This reduces equation (10) to

$$\sum_q \begin{bmatrix} (\varepsilon_q^{\mathbf{k}} - \mu)\delta_{p,q} & \Delta_{p,q}^{\mathbf{k}} \\ \Delta_{p,q}^{-\mathbf{k}*} & (\mu - \varepsilon_q^{\mathbf{k}})\delta_{p,q} \end{bmatrix} \begin{bmatrix} a_n^{\mathbf{k}}(q) \\ b_n^{\mathbf{k}}(q) \end{bmatrix} = E_n^{\mathbf{k}} \begin{bmatrix} a_n^{\mathbf{k}}(p) \\ b_n^{\mathbf{k}}(p) \end{bmatrix} \tag{16}$$

where the matrix element $\Delta_{p,q}^{\mathbf{k}}$ is calculated according to

$$\Delta_{p,q}^{\mathbf{k}} = (\varphi_p^{\mathbf{k}})^\dagger \check{\Delta}^{\mathbf{k}}(\varphi_q^{-\mathbf{k}})^* = \sum_{\mathbf{i},\mathbf{j}} [\varphi_p^{\mathbf{k}}(\mathbf{i})]^* \Delta_{\mathbf{ij}} \mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot(\mathbf{i}-\mathbf{j})} [\varphi_q^{-\mathbf{k}}(\mathbf{j})]^*, \tag{17}$$

while from equations (13) and (15), we have

$$\Delta_{\mathbf{ij}} = V \sum_{\mathbf{k},p,q,n} \varphi_p^{\mathbf{k}}(\mathbf{i})\varphi_q^{-\mathbf{k}}(\mathbf{j}) a_n^{\mathbf{k}}(p)[b_n^{\mathbf{k}}(q)]^* \tanh\left(\frac{E_n^{\mathbf{k}}}{2k_{\mathrm{B}}T}\right). \tag{18}$$

The equations (16)–(18) are solved iteratively until self-consistence is satisfied. Eventually we can calculate the local density of states, which is proportional to the differential tunneling conductance, from the energy spectrum and wavefunctions,

$$\rho(\mathbf{i}, E) = \sum_{\mathbf{k},n} |u_n^{\mathbf{k}}(\mathbf{i})|^2 \delta(E - E_n^{\mathbf{k}}) + |v_n^{\mathbf{k}}(\mathbf{i})|^2 \delta(E + E_n^{\mathbf{k}}). \tag{19}$$

At the present stage, we have expressed the BdG equations in the truncated eigenbasis of $\check{h}^{\mathbf{k}}$. The issue now is how to compute this truncated eigenbasis, i.e. the eigenstates of $\check{h}^{\mathbf{k}}$ lying within an energy shell E_{D} around the Fermi level.

Utilizing a standard computational algorithm [14], it would be rather time consuming to compute some selected eigenstates of a large matrix as $\check{h}^{\mathbf{k}}$, whose size $N \times N$ grows rapidly with the length scale of the MUC, by tridiagonalizing the matrix *numerically*. Even after taking advantage of the sparse nature of $\check{h}^{\mathbf{k}}$, we find that iterative methods, such as the Lanczos algorithm, are not quite appropriate for this problem because they are most efficient at finding largest/smallest eigenvalues(eigenvectors). In the following sections, we solve this issue by showing that $\check{h}^{\mathbf{k}}$ can be tridiagonalized *exactly* by two unitary transformations. Then we appeal to standard packages such as LAPACK [15] to compute the desired eigenstates of the resulting tridiagonal matrix within an energy range.

The dimension of the truncated eigenspace is approximately equal to $N\gamma$, where $\gamma \equiv E_{\mathrm{D}}/W$ is the ratio of the energy cutoff E_{D} to the width of the electronic band. Therefore the dimension of the BdG equations (16) expressed in the truncated eigenspace is $2N\gamma$, and thus the total labor of the diagonalization is $O((2N\gamma)^3)$. For weak-coupling BCS-type superconductors, in which electron pairing is mediated by boson glue, E_{D} can be chosen as the characteristic Boson energy, which is much smaller than the width of the electronic band. Consequently, computational efforts can be greatly saved for small γ. As a comparison, the standard numerical algorithm [14] of diagonalizing a Hermitian matrix (BdG Hamiltonian) involves first reducing the Hermitian matrix to the real tridiagonal form by Householder reduction and then finding the selected eigenvalues and eigenvectors of the tridiagonal matrix. Although in the second procedure only a fraction of eigenstates is desired and the workload is lessened, the total workload is determined by the tridiagonalization procedure, for which the workload is always $O((2N)^3)$ as long as the Householder reduction is utilized.

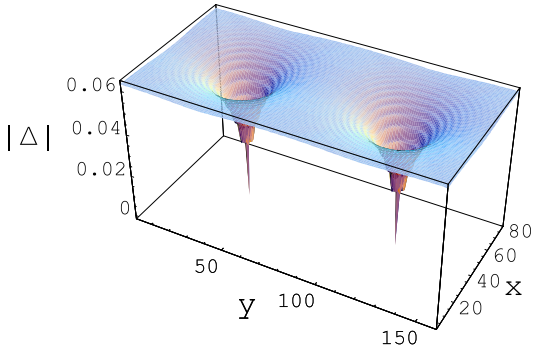

Figure 1. Spatial distribution of the magnitude of the s-wave pairing potential $|\Delta|$ in one magnetic unit cell of size 80×160. The x- and y-axis are in units of the lattice constant a. $|\Delta|$ is in units of the hopping integral t.

(This figure is in colour only in the electronic version)

3. 2D tight-binding electrons in a magnetic unit cell

In this section, we show in detail the method of exactly reducing the matrix $\check{h}^{\mathbf{k}}$ to a tridiagonal matrix. The eigenequation of $\varphi_n^{\mathbf{k}}$ (equation (14)), i.e. the discrete Schrödinger equation describing a 2D free electron moving in a perpendicular uniform magnetic field in a square lattice, can be written in an explicit form

$$\begin{aligned} &\mathrm{e}^{\mathrm{i}k_x}\varphi_n^{\mathbf{k}}(m_x+1,m_y)+\mathrm{e}^{-\mathrm{i}k_x}\varphi_n^{\mathbf{k}}(m_x-1,m_y)\\ &\quad+\mathrm{e}^{\mathrm{i}(2\pi m_x\alpha+k_y)}\varphi_n^{\mathbf{k}}(m_x,m_y+1)\\ &\quad+\mathrm{e}^{-\mathrm{i}(2\pi m_x\alpha+k_y)}\varphi_n^{\mathbf{k}}(m_x,m_y-1)=\tilde{\varepsilon}_n^{\mathbf{k}}\varphi_n^{\mathbf{k}}(m_x,m_y), \end{aligned} \tag{20}$$

where $\tilde{\varepsilon}_n^{\mathbf{k}}=\varepsilon_n^{\mathbf{k}}/(-t)$ and $\varphi^{\mathbf{k}}$ obeys the quasi-periodic boundary condition along the x direction and a periodic boundary condition along the y direction

$$\begin{aligned} \varphi^{\mathbf{k}}(m_x+N_x,m_y)&=\mathrm{e}^{-\mathrm{i}2\pi m_y N_x\alpha}\varphi^{\mathbf{k}}(m_x,m_y),\\ \varphi^{\mathbf{k}}(m_x,m_y+N_y)&=\varphi^{\mathbf{k}}(m_x,m_y). \end{aligned} \tag{21}$$

First we find that the eigenfunction $\varphi^{\mathbf{k}}$ is related to the eigenfunction $g^{\mathbf{k}}$ of the Harper equation by a unitary transformation. Explicitly,

$$\varphi_n^{\mathbf{k}}(m_x,m_y)=\frac{1}{\sqrt{N_y}}\sum_{l=0}^{N_y-1}\mathrm{e}^{\mathrm{i}2\pi m_y l N_x\alpha}g_n^{\mathbf{k}}(m_x+lN_x). \tag{22}$$

Substituting the above equation into equation (20), one readily find that $g_n^{\mathbf{k}}$ satisfies the Harper equation

$$\begin{aligned} &\mathrm{e}^{\mathrm{i}k_x}g_n^{\mathbf{k}}(m+1)+\mathrm{e}^{-\mathrm{i}k_x}g_n^{\mathbf{k}}(m-1)+2\cos(2\pi m\alpha+k_y)g_n^{\mathbf{k}}(m)\\ &\quad=\tilde{\varepsilon}_n^{\mathbf{k}}g_n^{\mathbf{k}}(m), \end{aligned} \tag{23}$$

Here $m=0,1,\ldots,N-1$ with $N=N_xN_y$. g satisfies the periodic boundary condition $g_n^{\mathbf{k}}(m+N)=g_n^{\mathbf{k}}(m)$. In the matrix form, the Harper equation can be expressed as

$$\check{P}^{\mathbf{k}}g_n^{\mathbf{k}}=\tilde{\varepsilon}_n^{\mathbf{k}}g_n^{\mathbf{k}}, \tag{24}$$

where

$$\check{P}^{\mathbf{k}}=\begin{pmatrix} a_0 & \mathrm{e}^{\mathrm{i}k_x} & & & \mathrm{e}^{-\mathrm{i}k_x}\\ \mathrm{e}^{-\mathrm{i}k_x} & a_1 & \mathrm{e}^{\mathrm{i}k_x} & & \\ & \mathrm{e}^{-\mathrm{i}k_x} & \cdot & \cdot & \\ & & \cdot & \cdot & \cdot\\ & & & \cdot & \cdot & \mathrm{e}^{\mathrm{i}k_x}\\ \mathrm{e}^{\mathrm{i}k_x} & & & \mathrm{e}^{-\mathrm{i}k_x} & a_{N-1} \end{pmatrix}, \tag{25}$$

with $a_m=2\cos(2\pi m\alpha+k_y)$. In addition, the eigenvector $g_n^{\mathbf{k}}=(g_n^{\mathbf{k}}(0),\ldots,g_n^{\mathbf{k}}(N-1))^{\mathrm{T}}$. As a special case of the almost Mathieu equation, where the anisotropy parameter equals unity, the Harper equation (23) is also known as the Azbel–Hofstadter problem [11, 12] and can be viewed as a discrete Schrödinger equation describing tight-binding electrons moving on a one-dimensional lattice subject to a commensurate (in this paper, $\alpha=1/N_xN_y$ is rational) potential.

The periodic tridiagonal matrix $\check{P}^{\mathbf{k}}$ can be further reduced to a tridiagonal matrix by another unitary transformation. For simplicity, we only show the procedure for the $k_y=0$ case and the following discussion can be readily generalized for $k_y\neq 0$. The transformation of wavevectors from g to f is as follows:

$$\begin{aligned} f(0)&=g(0),\\ f(1)&=\frac{\mathrm{e}^{\mathrm{i}k_x}g(1)+\mathrm{e}^{-\mathrm{i}k_x}g(N-1)}{\sqrt{2}},\\ f(2)&=\frac{\mathrm{e}^{2\mathrm{i}k_x}g(2)+\mathrm{e}^{-2\mathrm{i}k_x}g(N-2)}{\sqrt{2}},\\ &\cdots\\ f\left(\frac{N}{2}-1\right)&=\frac{\mathrm{e}^{\mathrm{i}(\frac{N}{2}-1)k_x}g(\frac{N}{2}-1)+\mathrm{e}^{-\mathrm{i}(\frac{N}{2}-1)k_x}g(\frac{N}{2}+1)}{\sqrt{2}},\\ f\left(\frac{N}{2}\right)&=g\left(\frac{N}{2}\right),\\ f\left(\frac{N}{2}+1\right)&=\frac{\mathrm{e}^{\mathrm{i}(N/2-1)k_x}g(\frac{N}{2}-1)-\mathrm{e}^{-\mathrm{i}(\frac{N}{2}-1)k_x}g(\frac{N}{2}+1)}{\sqrt{2}},\\ &\cdots\\ f(N-2)&=\frac{e^{2ik_x}g(2)-e^{-2ik_x}g(N-2)}{\sqrt{2}},\\ f(N-1)&=\frac{\mathrm{e}^{\mathrm{i}k_x}g(1)-\mathrm{e}^{-\mathrm{i}k_x}g(N-1)}{\sqrt{2}}. \end{aligned} \tag{26}$$

Substituting the above relations into equation (23), we have the eigenequation for f, which reads,

$$\check{T}^{\mathbf{k}}f_n^{\mathbf{k}}=\tilde{\varepsilon}_n^{\mathbf{k}}f_n^{\mathbf{k}} \tag{27}$$

where $\check{T}$ is an $N\times N$ tridiagonal matrix,

$$\check{T}^{\mathbf{k}}=\begin{pmatrix}\check{T}_u^{\mathbf{k}} & 0\\ 0 & \check{T}_d^{\mathbf{k}}\end{pmatrix} \tag{28}$$

where the two matrices $\check{T}_u^{\mathbf{k}}$ and $\check{T}_d^{\mathbf{k}}$ are written as

$$\check{T}_u^{\mathbf{k}} = \begin{pmatrix} a_0 & \sqrt{2} & & & & & \\ \sqrt{2} & a_1 & 1 & & & & \\ & 1 & \cdot & \cdot & & & \\ & & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & 1 & \\ & & & 1 & a_{\frac{N}{2}-1} & \sqrt{2}(-1)^{l_x} & \\ & & & & \sqrt{2}(-1)^{l_x} & a_{\frac{N}{2}} & \end{pmatrix} \tag{29}$$

and

$$\check{T}_d^{\mathbf{k}} = \begin{pmatrix} a_{\frac{N}{2}-1} & 1 & & & & & \\ 1 & a_{\frac{N}{2}-2} & 1 & & & & \\ & 1 & \cdot & \cdot & & & \\ & & \cdot & \cdot & \cdot & & \\ & & & \cdot & \cdot & 1 & \\ & & & & 1 & a_1 & \end{pmatrix}. \tag{30}$$

The eigenvector $f_n^{\mathbf{k}} = (f_n^{\mathbf{k}}(0), \cdots, f_n^{\mathbf{k}}(N-1))$.

After the two consecutive unitary transformations, we have successfully reduced the Hermitian matrix $\check{h}^{\mathbf{k}}$ into a tridiagonal matrix $\check{T}^{\mathbf{k}}$. Here we emphasize that the reduction is exact without any numerical assumption and takes no CPU time compared with the numerical reduction. Then the eigenproblem of the tridiagonal matrix $\check{T}^{\mathbf{k}}$ can be solved using standard packages such as LAPACK.

4. An example: vortex lattice states of a type-II s-wave superconductor

In this section, we illustrate how our method is applied in solving the BdG equation for the vortex lattice states of an s-wave superconductor. The microscopic parameters used in this paper are as follows. As a model calculation we set the relevant parameters as follows. $\mu = -3t$, which gives rise to an almost circular Fermi surface with the Fermi wavevector $k_{\mathrm{F}} \approx 1.03a^{-1}$ and Fermi velocity $v_{\mathrm{F}} \approx 1.81ta/\hbar$. The on-site attractive interaction $V = 2t$. The Debye-type energy cutoff $E_{\mathrm{D}} = 0.5t$. This set of parameters results in an s-wave pairing potential $\Delta_0 \approx 0.065t$ in the zero-temperature limit with the estimated coherence length $\xi_0 = \hbar v_{\mathrm{F}}/\pi\Delta_0 \approx 9a$.

The model calculation is carried out for a system composed of $M_x \times M_y = 40 \times 20$ MUCs with each MUC of size $N_x \times N_y = 80 \times 160$, which corresponds to a magnetic field $B = \phi_0/(N_x N_y a)^2 \approx 2.0$ T if the lattice constant is set as 4 Å. Therefore, for each $\mathbf{k}$ of the total 800 quasimomenta, we employ the standard LAPACK routine to diagonalize the 12 800 × 12 800 tridiagonal matrix (equation (28)) and find that there are approximately 1173 eigenstates $\{f_n^{\mathbf{k}}\}$ with eigenenergies lying within the energy range $|\varepsilon^{\mathbf{k}} - \mu| \leqslant E_{\mathrm{D}}$. We can obtain the eigenstates of the Harper equation $\{g_n^{\mathbf{k}}\}$ by the inverse transformation of equation (26). Then substituting $g_n^{\mathbf{k}}$ into equation (22) we successfully obtain the truncated eigenbasis $\{\varphi_n^{\mathbf{k}}\}$, in which the BdG equations (16) are expressed as the 2×1173-dimensional eigenvalue problem and the matrix elements $\Delta_{p,q}^{\mathbf{k}}$ are calculated from equation (17). After the BdG equations are diagonalized for each $\mathbf{k}$, we substitute the quasiparticle amplitudes $a_n^{\mathbf{k}}$ and $b_n^{\mathbf{k}}$ into the self-consistent condition equation (18) to compute the renewed values of the pairing potential. Equations (16)–(18) are solved iteratively until convergence is reached.

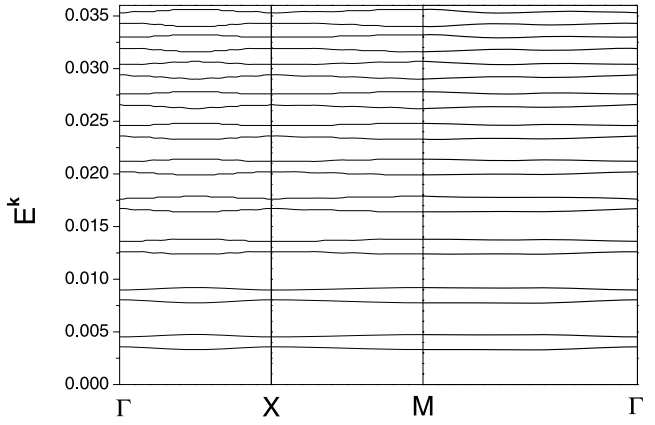

Figure 2. The quasiparticle spectrum in the magnetic Brillouin zone. See the text for details.

In figure 1 we show the spatial variation of the self-consistent pair potential within one 80 × 160-sized magnetic unit cell, in which two superconducting vortices are situated. The s-wave pairing potential vanishes at the center of each of the two 80 × 80 squares and increases with the distance from the core center, recovering its bulk value approximately with a length scale ξ_0. The variation of the pairing potential around the vortex core exhibits almost circular symmetry, as shown in the figure. The reasons are twofold. Firstly, the Fermi level is far away from the van Hove singularity and accordingly the Fermi surface is approximately circular. Secondly, the impact from neighboring vortices which are arranged squarely is weak because the distance between the adjacent vortices is about one order of magnitude larger compared to the characteristic coherence length.

Figure 2 displays the quasiparticle spectra along three high-symmetry lines in the magnetic Brillouin zone, where ΓX, XM and $M\Gamma$ connect two of the three points: $\Gamma = (0, 0)$, $X = (\frac{\pi}{N_x a}, 0)$ and $M = (\frac{\pi}{N_x a}, \frac{\pi}{N_y a})$. As shown in the figure, the vortex bound states, which are localized in a isolated vortex line, as revealed in [16, 17], are broadened into energy bands in the superconducting vortex lattice owing to the interference effect. However, due to the localized nature of the vortex states, the overlapping of the quasiparticle wavefunctions belonging to different vortices is weak, especially for the low-lying states. Consequently, the bands with lower energies are flatter, and the level spacing between pairs of the first few lowest-lying bands is of the order of $\Delta_0^2/E_{\mathrm{F}}$. These results are consistent with previous works [4, 5, 18].

In figure 3 we plot the local density of states (LDOS) as a function of energy at the vortex core center and the inter-vortex site. At the center of the vortex core, the LDOS is greatly enhanced at the energy approximately equal to $\Delta_0^2/E_{\mathrm{F}}$ due to the strongly localized vortex bound states, while depressed around $E = \pm\Delta_0$ as compared with the LDOS at the inter-vortex site. The model calculation shows the feasibility of our methods in studying the vortex lattice with a large unit cell.

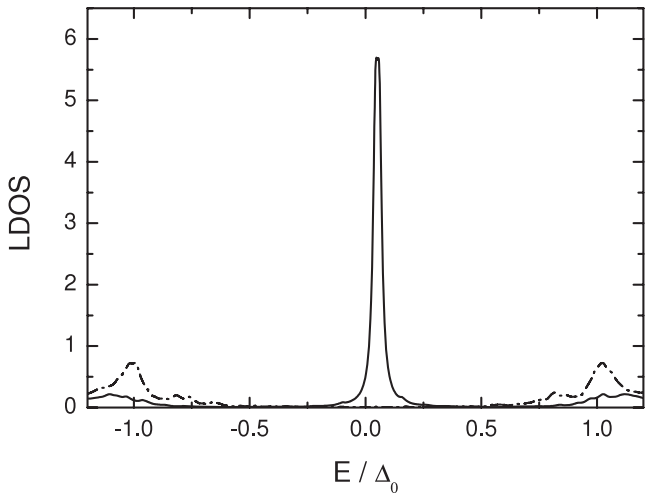

Figure 3. LDOS as a function of energy at the vortex core center (solid line) and the inter-vortex site (dash–dotted line).

5. Conclusion

The discrete BdG equations developed in the 2D tight-binding lattice have been used to study the magnetic-field-induced superconducting vortex lattice state in the literature. The size of the system studied in previous works was limited due to directly performing the full diagonalization of the BdG Hamiltonian. In this paper, we have extended this method by constructing a truncated eigenspace for the normal-state electrons moving on a 2D square lattice in the presence of a uniform magnetic field. The motion of the electrons is governed by the vector potential, which imposes a (quasi-)periodic boundary condition along the x and y directions of the magnetic unit cell. We have presented two consecutive unitary transformations to reduce the Hermitian matrix for the 2D electrons exactly into a tridiagonal matrix. By doing so, we have successfully related the desired eigenbasis with that of the celebrated Harper equation, which is the eigenequation for a periodic tridiagonal matrix. Then a second transformation is applied to further reduce the periodic tridiagonal matrix to a tridiagonal one. This greatly reduces the cost of CPU time and helps us to treat systems with a much larger size. To test our method and elucidate it more specifically, we have applied our results to study the vortex lattice states of an s-wave superconductor. The extension of our method to a more sophisticated band structure, as well as to 2D triangular or honeycomb lattices, will be performed in future works.

It will also be quite interesting to investigate the effect of superconductivity on the nested band structure of the normal-state electronic spectrum, i.e. the so-called Hofstadter butterfly [12]. In fact, the pairing potential term in equation (1) combines two initially decoupled Hofstadter Hamiltonians, and the modulation of the pairing potential caused by the superconducting vortex lattice will certainly deform the original Hofstadter spectrum. With the help of our numerical method, such an effect can be studied for a wide range of magnetic fields with the vortex lattice calculated self-consistently. However, we emphasize that the method developed in this work is suitable for vortex lattices whose periodicity is commensurate with that of the underlying lattice, and accordingly the magnetic flux per plaquette is rational (more precisely $\alpha = 1/N_x N_y$). A significant challenge exists to investigate the incommensurability effect by the extension of our method.

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