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LETTER TO THE EDITOR

Quasi-particle states of a linear chain of vortices in a mixed-state superconductor

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Abstract. We examine the low-lying quasi-particle states of a chain of vortices contained within a thin slab of superconductor and demonstrate that bound states of individual vortices hybridize to form bands of extended states. As a consequence of the phase gradient around a vortex, one such band is centred on zero energy and will therefore contribute to quasi-particle transport at energies far below the superconducting transition temperature.

Observations of the de Haas–van Alphen effect in the mixed state of strongly type II superconductors [1] and theoretical predictions of magnetic quantum oscillations near the upper critical field [2] have led to increasing interest in the quantum properties of dense vortex structures. If the contribution to quantum transport from quasi-particles is to be understood, it is necessary to ask how bound states in the cores of nearby vortices hybridize to form low-lying energy bands. Such bands, if they exist, will allow quasi-particle transport to occur at temperatures much less than the superconducting transition temperature. Of particular interest is the question of whether or not states exist at zero energy, since such states would allow a quasi-particle contribution to persist even to zero temperature.

The problem of computing quasi-particle states in the presence of a vortex lattice is complicated by the fact that although the magnitude of the order parameter is periodic, the phase is not. Consequently Bloch's theorem cannot be used to reduce the problem to that of a single unit cell. In this Letter, to gain insight into the nature of quasi-particle states, we consider the related problem of a linear chain of vortices, to which Bloch's theorem can be fruitfully applied.

Consider a linear chain of vortices aligned parallel to the z axis. Since the system is translationally invariant in the z direction, all quasi-particle states can be chosen to be proportional to a plane wave of the form $\exp \mathrm{i}k_z z$. The motion in the x, y plane is then described by the Bogoliubov–de Gennes equation

$$\begin{pmatrix} \mathbf{H}_0 & \mathbf{\Delta} \\ \mathbf{\Delta}^* & -\mathbf{H}_0^* \end{pmatrix} \begin{pmatrix} \psi(\boldsymbol{r}) \\ \phi(\boldsymbol{r}) \end{pmatrix} = E \begin{pmatrix} \psi(\boldsymbol{r}) \\ \phi(\boldsymbol{r}) \end{pmatrix} \tag{1}$$

where $\boldsymbol{r}$ is a position vector orthogonal to the z axis. In what follows we choose $k_z = 0$ and $\mathbf{H}_0$ to be a tight-binding model on a two-dimensional, triangular lattice of infinite length and width W sites. The matrix $\mathbf{H}_0$ has elements $(\mathbf{H}_0)_{ij} = \epsilon\delta_{ij} - v\delta_{jj_i}$, where j_i is the jth nearest neighbour of site i and after neglecting a small effect on the eigenvalue spectrum due to the presence of a vector potential [3], the nearest neighbour coupling strength v is chosen to be a constant of value unity. In what follows, except when stated otherwise, the diagonal element ϵ will be set to zero.

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The matrix $\boldsymbol{\Delta}$ has elements $\Delta_{ij} = \delta_{ij}\Delta(\boldsymbol{r}_i)$, where in the presence of a chain of vortices, the superconducting order parameter $\Delta(\boldsymbol{r})$ will be chosen to be periodic in the x direction, with period L. After taking advantage of translational invariance in the x direction, equation (1) can be reduced to a problem involving a single unit cell and then diagonalized numerically to yield the quasi-particle band structure at low energies. In what follows, with $\epsilon = 0$, since the eigenvalue spectrum is symmetric about $E = 0$ and $k_x = 0$, where k_x is the x component of the Bloch wavevector, only results for positive E and k_x are shown.

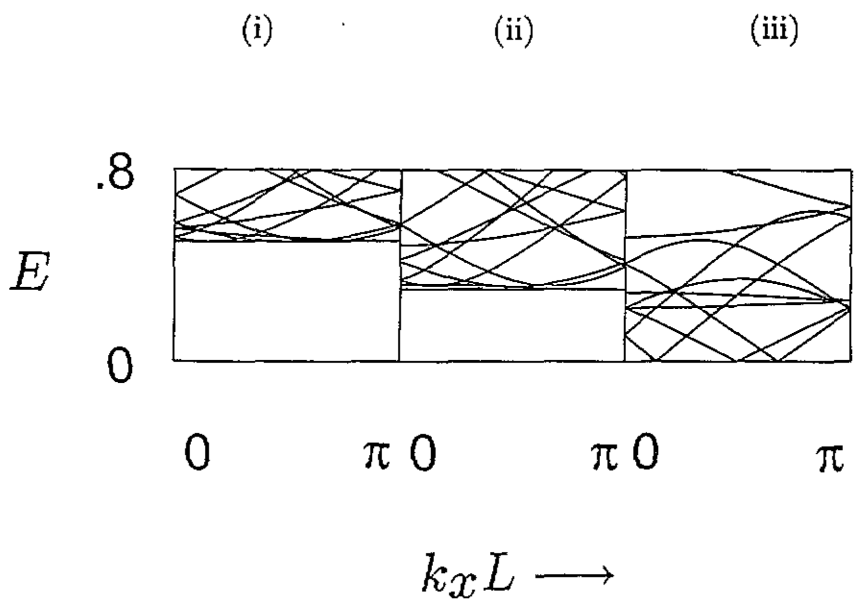

Figure 1. Quasi-particle dispersion curves for simple model order parameters on a slab of width $W = 5$ sites and unit cell of length $L = 11$ sites, obtained from equation (1) with $v = 1$, $\epsilon = 0$. Graph (i) shows results for a constant order parameter $\Delta(\boldsymbol{r}) = \Delta_0$, where $\Delta_0 = 1/2$. In graphs (ii) and (iii) the order parameter is defined by $\Delta(\boldsymbol{r}) = \Delta_0|\cos 2\pi x/L|$ and $\Delta(\boldsymbol{r}) = \Delta_0 \cos 2\pi x/L$ respectively.

One question of particular importance is whether or not there exists a band of quasi-particle states at $E = 0$, because in the absence of such states, an exponential decrease in the quasi-particle contribution to transport will occur at low enough temperatures. Before presenting results for a chain of vortices, it is illuminating to analyse some simple model order parameters. Figure 1(i) shows quasi-particle dispersion curves arising from a spatially independent order parameter $\Delta(\boldsymbol{r}) = \Delta_0$, where $\Delta_0 = 1/2$. For this calculation, the slab width is $W = 5$ sites and the unit cell is of length $L = 11$ sites. As expected, the resulting folded band structure exhibits an energy gap at $E = \Delta_0$. Figure 1(ii) shows results for the same values of W and L, but with a one-dimensional order parameter variation of the form $\Delta(\boldsymbol{r}) = \Delta_0|\cos 2\pi x/L|$. This demonstrates that the presence of nodes in the order parameter does indeed lead to bound states below the bulk energy gap, which hybridize to form bands. Figure 1(iii) shows results arising from a variation of the form $\Delta(\boldsymbol{r}) = \Delta_0 \cos 2\pi x/L$. In this case, the magnitude of $\Delta(\boldsymbol{r})$ is the same as in figure 1(ii), but in addition, the order parameter can change sign. Figure 1(iii) illustrates that the effect of such a sign change is to generate a band of states centred on $E = 0$.

Before proceeding, it is also of interest to examine the lowest bound state energy E_0 obtained from the discrete model (1) for a single isolated vortex, and to compare the result with the value $\tilde{E}_0$ predicted by de Gennes [3]. For an order parameter variation of the form $\Delta(r) = |\Delta(r)|\exp(i\theta)$, where $|\Delta(r)| = \Delta_0 r/R$ for $r \leqslant R$ and $|\Delta(r)| = \Delta_0$ for $r > R$, the latter predicts

$$\tilde{E}_0 = g\Delta_0(2k_F R)^{-1} \tag{2}$$

where E_F is the Fermi energy, k_F the Fermi momentum and g a dimensionless parameter of order unity. Equation (1) defines a discrete model with a non-spherical Fermi surface, while the analysis of reference [3] applies to a continuum model with a spherical Fermi surface. Nevertheless such a comparison should demonstrate whether or not the lowest bound state energy is sensitive to lattice structure.

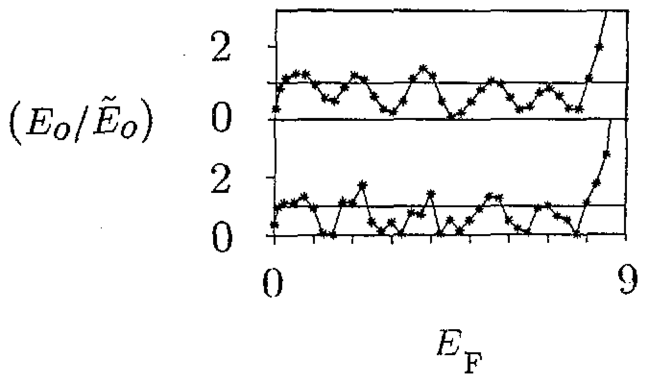

Figure 2. Graphs showing the ratio of the numerical result E_0 and the continuum prediction $\tilde{E}_0$ for the lowest energy of an isolated vortex as a function of the Fermi energy E_F. Numerical results are for a system of width $W = 13$ sites and of length $L = 13$ sites. The top graph shows results for a core radius of $R = 3$ sites, and a maximum order parameter of $\Delta_0 = 2/3$, while the values for the bottom graph are $R = 4$ sites and $\Delta_0 = 1/2$. In each case the position of the Fermi energy is measured from the bottom of the band and is in units of the hopping strength v.

Figure 2 shows the ratio of the numerical result E_0 to the continuum results $\tilde{E}_0$ as a function of E_F. Physically R is expected to be of the order of a coherence length $\sim k_F^{-1}E_F/\Delta_0$ and therefore both k_F and R vary with E_F. For the purpose of comparing E_0 with $\tilde{E}_0$, we fix R and allow only k_F to vary. For the model of equation (1), with a lattice constant a, typically $k_F^{-1} \sim a$ and $E_F \sim v$ and therefore for the purpose of comparing with equation (2) we choose $R = 2a/(\Delta_0/v)$. With this choice, equation (2) becomes $\tilde{E}_0 = g(\Delta_0^2/v)(4k_F a)^{-1}$. For a triangular lattice with $E_F \ll v$, where the Fermi surface is almost circular, $ak_F = (E_F/2v)^{1/2}$ and therefore the continuum prediction reduces to

$$\tilde{E}_0 = g(\Delta_0^2/4v)(E_F/2v)^{-1/2}. \tag{3}$$

For the model of equation (1), with $v = 1$, since $E_F = -\epsilon + 6$, the Fermi energy is most conveniently changed by varying the diagonal elements ϵ. The top graph of figure 2 shows results for the ratio $\tilde{E}_0/E_0$ as a function of E_F, for a vortex of size $R = 3a$ embedded in a system of size 13×13 sites, with $\Delta_0 = 2/3$. The bottom graph of figure 2 shows results for the same system, except with $R = 4a$, $\Delta_0 = 1/2$. In both case the dimensionless parameter g has been set to unity. Although the numerical results exhibit some structure associated with the periodicity of the underlying lattice, provided that E_F does not approach the top of the tight-binding band and $E_F/\Delta_0 < 1$, the discrete model yields values that are of the same order as those obtained from a continuum model [3].

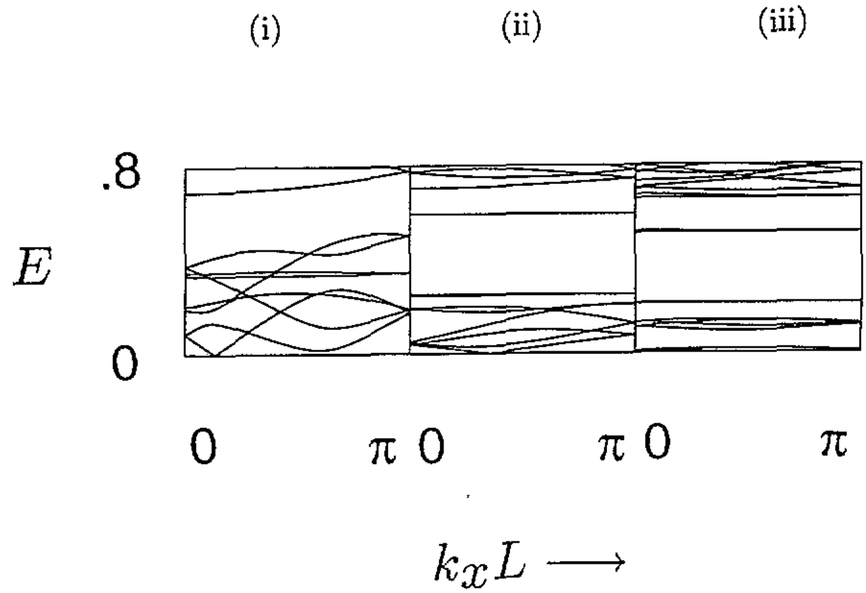

Figure 3. Quasi-particle dispersion curves for an order parameter of the type defined in equation (4) for a slab width of $W = 5$ sites. Graphs (i), (ii) and (iii) show results for the cases $L = 11$, $L = 19$ and $L = 25$ respectively.

To model a linear chain of vortices in a thin slab of superconductor, in view of the Ginzburg–Landau solution for $\Delta(\boldsymbol{r})$ near H_{c2} [4], we choose a spatial variation of the form

$$\Delta(\boldsymbol{r}) = \Delta_0[f_1(y)\exp(\mathrm{i}qx) + f_2(y)\exp(-\mathrm{i}qx)]. \tag{4}$$

In this equation, $f_j(y) = \exp[-(y - y_j)^2\Delta_0^2/2]$, $y_1 = d_c/2$ and $y_2 = W - d_c/2$, where $d_c = 1.84/\Delta_0$ is the film thickness above which the nucleation site for superconductivity is no longer located at the mid-point of the film [4]. Figures 3(i), 3(ii) and 3(iii) show results for ($W = 5$, $L = 11$), ($W = 5$, $L = 19$) and ($W = 5$, $L = 25$) respectively. As expected, the degree of hybridization decreases as the vortex spacing $L/2$ increases. Similarly, figures 4(i), 4(ii) and 4(iii) illustrate results for the cases ($W = 7$, $L = 11$), ($W = 7$, $L = 19$) and ($W = 7$, $L = 25$). Since the nucleation centres y_1 and y_2 are a fixed distance from the edges of the slab, equation (4) yields an order parameter that is now more strongly suppressed at the slab centre than that used in figure 3. Consequently for an isolated vortex, the low-lying-level separation is decreased. For a chain of widely separated vortices typified by the $W = 7$, $L = 25$ results, this leads to a more densely packed spectrum of energy bands.

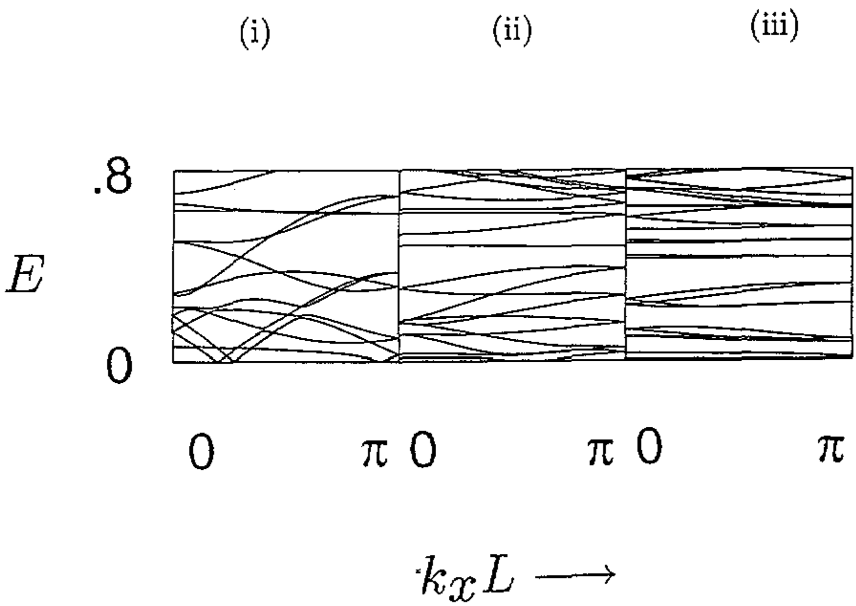

Figure 4. Quasi-particle dispersion curves for an order parameter of the type defined in equation (4) for a slab width of $W = 7$ sites. Graphs (i), (ii) and (iii) show results for the cases $L = 11$, $L = 19$ and $L = 25$ respectively.

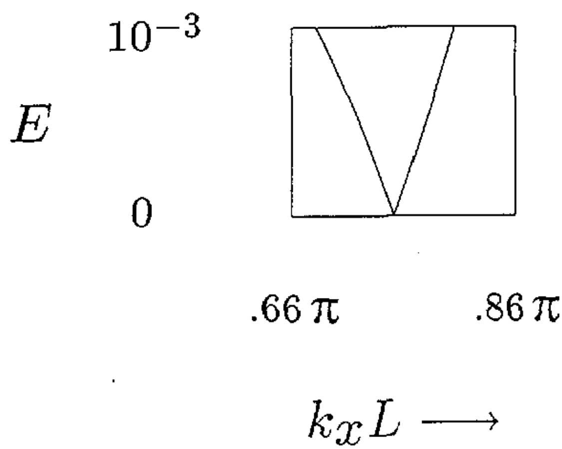

Figure 5. A magnified portion of the graph of figure 3(iii) where $W = 5$ and $L = 25$, which indicates that the lowest energy band does indeed pass through $E = 0$ in the case of more widely spaced vortices.

In this work, we have presented results for the low-lying quasi-particle bands associated with a linear chain of vortices. In all cases, figures 3 and 4 show that there exists a band of states centred on $E = 0$, resulting from the phase change of π at a vortex centre. In the case of the more widely spaced vortices, this is not immediately obvious and so figure 5 shows a magnification of part of the lowest band on the graph of figure 3(iii), for which

($W = 5$, $L = 25$). The higher resolution on this scale indicates that this energy band does indeed pass through $E = 0$, and therefore, for an ordered chain of vortices, we do not expect a low-temperature cut-off in the quasi-particle contribution to transport properties.

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