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Hall conductance of a pinned vortex lattice in a high magnetic field

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Abstract. We calculate the quasiparticle contribution to the zero-temperature Hall conductance of two-dimensional extreme type-II superconductors in a high magnetic field, using the Landau basis. As one enters the superconducting phase the Hall conductance is renormalized to smaller values, with respect to the normal-state result, until a quantum level-crossing transition is reached. At high values of the order parameter, where the quasiparticles are bound to the vortex cores, the Hall conductance is expected to tend to zero due to a theorem of Thouless.

1. Introduction

Numerous superconductors like high- T_c cuprates, A15 structure compounds, boro-carbides and many organics reveal the importance of Landau quantization at high magnetic fields and low temperatures, as evident, for instance, from the recent observation of the de Haas–van Alphen oscillations in the superconducting phase [1]. In these systems the cyclotron splitting (ω_c) between the Landau levels (LL) is the largest energy scale; in particular, $\omega_c > \Delta$ (where Δ is the superconductor order parameter). The effect of the Landau quantization has attracted theoretical attention and reveals itself in the appearance of gapless superconductivity [2, 3] and power-law dependence of the low- T thermodynamic properties. A good description of the de Haas–van Alphen oscillations has been obtained taking into account the Landau quantization [4]. The gapless nature of the spectrum also leads to an enhanced acoustic attenuation in contrast to the case for usual gapped superconductors [5] and it survives even in the presence of disorder [6].

Close to the upper critical field, and at small values of Δ , a diagonal approximation (DA), where the coupling between the LL is neglected, is appropriate [3, 5]. In this regime the quasiparticles propagate coherently throughout the vortex lattice. Associated with the zeros of the order parameter in real space are gapless points in the magnetic Brillouin zone. As Δ grows, the coupling between the LL has to be taken into account. A perturbation scheme in the off-diagonal couplings can then be followed, as long as there are no level-crossings [7], and it can be shown analytically to all orders in the perturbation theory that there is always a discrete set of gapless points. In general, a numerical solution of the Bogoliubov–de Gennes (BdG) equations has to be carried out. For large values of Δ a regime is reached where the quasiparticles are bound to the vortex cores with an energy spacing typical of an isolated single vortex [8]. In this regime one expects that a tight-binding approximation should yield good results, since in this low-field regime the vortex cores are sparse. Such a procedure has been carried out and a gapped regime is indeed found [8, 9] signalling a transition from the

high-field gapless regime to the low-field gapped regime. Between the small- Δ regime and this gapped regime several quantum level-crossings take place. This is a difficult numerical problem because the number of Landau levels increases considerably as the field lowers and it is not easy to determine the value of Δ for which the transition to the gapped regime takes place.

On the other hand, Thouless has shown that the Landau levels do not constitute a complete basis to be used in a tight-binding approximation scheme and therefore it is not possible to construct well localized representations of the magnetic translation group unless the Hall conductance, σ_{xy} , is zero [10]. Thouless showed that if Wannier functions are constructed, they decay with distance at most as $|\mathbf{r} - \mathbf{R}_i|^{-2}$ (if the Hall conductance is nonvanishing), but he also showed that well localized Wannier functions (decaying faster than any power) can be constructed if σ_{xy} vanishes. Using the Balian–Low theorem it has also been shown that in general [11] the Landau levels cannot be chosen sufficiently localized to make the Δx and Δy uncertainties finite. This is equivalent to the statement by Thouless on the slow decay rate of the Wannier functions with distance. The notable exception is a sub-band with zero Hall conductance. Since it is intuitive that in the limit in which the vortex concentration is low a tight-binding description should be appropriate, we expect, in the light of Thouless’s theorem, that σ_{xy} should be zero in this low-field regime. This is suggested by the localized nature evident from the numerical solution of the BdG equations. To determine whether the Wannier states are indeed a good basis is a delicate and difficult matter and in general a tight-binding description will have one conducting state at the band centre [12]. We expect however that in this low-field regime the functions will be well localized and we argue therefore that the Hall conductance could be used as an order parameter to signal the transition from the high-field gapless regime, where Landau quantization has been shown to occur (finite σ_{xy}), to the low-field gapped regime (zero σ_{xy}).

The calculation of the Hall conductance in the superconducting phase is also interesting in itself. Several authors have given attention to the Hall conductance of the vortex lattice. In general, there are two contributions: one is due to the vortex motion and the other to the quasiparticle contribution (usually associated with modes localized in the normal region inside the vortex cores). One of the reasons for this interest is that in the superconducting phase σ_{xy} has a different sign with respect to the one of the normal phase [13]. This has been shown to be due to the vortex motion part since the localized modes are predicted to give a contribution with the same sign as the normal-phase value.

In this paper we focus solely on the quasiparticle contribution which is the only remaining contribution if the vortex lattice is pinned to some imperfection (in this case the vortex motion is frozen). We do not address here the sign change, but study the influence of the coherent propagation of the quasiparticles. Also, we take into consideration the Landau quantization in a regime where a quasiclassical approximation is not valid [14].

2. Calculation of the Hall conductance

We calculate the Hall conductance using the Kubo formula

$$\sigma_{xy}(\mathbf{r}, \mathbf{r}') = -i\hbar L^2 \sum_{\beta \neq 0} \{ \langle 0 | J_x(\mathbf{r}) | \beta \rangle \langle \beta | J_y(\mathbf{r}') | 0 \rangle - \langle 0 | J_y(\mathbf{r}') | \beta \rangle \langle \beta | J_x(\mathbf{r}) | 0 \rangle \} \frac{1}{(\epsilon_\beta - \epsilon_0)^2} \quad (1)$$

where the currents are given by

$$J_i(\mathbf{r}) = \frac{e\hbar}{2imc} \sum_{\sigma} \left\{ \psi_{\sigma}^{\dagger}(\mathbf{r}) \left(\frac{\partial}{\partial x_i} \psi_{\sigma}(\mathbf{r}) \right) - \left(\frac{\partial}{\partial x_i} \psi_{\sigma}^{\dagger}(\mathbf{r}) \right) \psi_{\sigma}(\mathbf{r}) \right\} - \frac{e^2}{mc^2} A_i \sum_{\sigma} \psi_{\sigma}^{\dagger}(\mathbf{r}) \psi_{\sigma}(\mathbf{r}). \quad (2)$$

Here σ is the spin projection, $i = x, y, z$, \mathbf{A} is the vector potential, $\psi_{\sigma}(\mathbf{r})$ is the electron field operator, the energies ϵ_{β} are the full solution of the many-body problem and $\beta = 0$ is the ground state. We consider a square lattice of side L .

We calculate the Hall conductance, obtaining the energies from the solution of the BdG equations [2, 3]. The field operators are written as

$$\begin{aligned} \psi_{\uparrow}(\mathbf{r}) &= \sum_{v,q} (u_q^v(\mathbf{r}) \gamma_{v,q,\uparrow} - v_q^{*v}(\mathbf{r}) \gamma_{v,q,\downarrow}^{\dagger}) \\ \psi_{\downarrow}(\mathbf{r}) &= \sum_{v,q} (u_q^v(\mathbf{r}) \gamma_{v,q,\downarrow} + v_q^{*v}(\mathbf{r}) \gamma_{v,q,\uparrow}^{\dagger}) \end{aligned} \quad (3)$$

and

$$\epsilon_{\beta} = \sum_{\sigma,v,q} \epsilon_q^v \gamma_{v,q,\sigma}^{\dagger} \gamma_{v,q,\sigma}. \quad (4)$$

Here $\gamma_{v,q,\sigma}^{\dagger}$ creates a quasiparticle in the level v , with momentum \mathbf{q} and spin σ . The problem is diagonal in \mathbf{q} (vectors of the magnetic Brillouin zone) due to the periodicity of the Abrikosov vortex lattice. The amplitudes u and v are expanded in the Landau basis (n is the Landau level) as

$$u_q^v(\mathbf{r}) = \sum_n u_{qn}^v \phi_{qn}(\mathbf{r}) \quad (5)$$

and

$$v_q^{*v}(\mathbf{r}) = \sum_n v_{qn}^{*v} \phi_{-qn}(\mathbf{r}). \quad (6)$$

Here $\phi_{qn}(\mathbf{r})$ are the eigenfunctions of the magnetic translation group in the Landau gauge ($A_x = -Hy$, $A_y = 0$, $A_z = 0$) belonging to the n th Landau level. The amplitudes u_{qn}^v and v_{qn}^v are the solutions of the BdG equations and ϵ_q^v are the energy eigenvalues. The BdG equations to be solved are

$$\begin{aligned} \epsilon_n u_{qn}^v + \sum_m \Delta_{nm}(\mathbf{q}) v_{qm}^v &= \epsilon_q^v u_{qn}^v \\ -\epsilon_n v_{qn}^v + \sum_m \Delta_{nm}^*(\mathbf{q}) u_{qm}^v &= \epsilon_q^v v_{qn}^v \end{aligned} \quad (7)$$

where $\epsilon_n = (n + 1/2) - \mu/\hbar\omega_c$ (μ is the chemical potential), $\Delta_{nm}(\mathbf{q})$ is the matrix element of the order parameter $\Delta(\mathbf{r})$ connecting electronic states (\mathbf{q}, n) and $(-\mathbf{q}, m)$ [4]. In general, the order parameter is expanded in the LL for a charge $2e$, which leads to a complicated structure for the BdG equations which have to be solved self-consistently, since the order parameter satisfies $\Delta(\mathbf{r}) = V \langle \psi_{\uparrow}(\mathbf{r}) \psi_{\downarrow}(\mathbf{r}) \rangle$, where V is the electron–electron interaction. In the DA these equations are easily solved:

$$\begin{aligned} \epsilon_q^v &= \pm \sqrt{\epsilon_n^2 + |\Delta_{nm}(\mathbf{q})|^2} \equiv \epsilon_q^n \\ u_{qn} &= \frac{1}{\sqrt{2}} \left(1 + \frac{\epsilon_n}{\epsilon_q^v} \right)^{1/2} \\ v_{qn} &= \frac{1}{\sqrt{2}} \left(1 - \frac{\epsilon_n}{\epsilon_q^v} \right)^{1/2} \end{aligned} \quad (8)$$

(and, therefore, $v \equiv n$). In this case

$$u_{qn}^v v_{-qn}^{*v} = \frac{\Delta_{nn}(\mathbf{q})}{2\epsilon_q^n}. \quad (9)$$

As Δ grows, the off-diagonal terms become increasingly important. Recently, the leading corrections to the normal and pairing self-energies have been found by delaying the Nambu rotation to the last step and it was obtained [7] that the renormalized quasiparticle energies can be written as in the DA like

$$\epsilon_{nq}^v = \pm \sqrt{\bar{\epsilon}_n(\mathbf{q}) + |\bar{\Delta}_{nn}(\mathbf{q})|^2} \quad (10)$$

but with renormalized normal and pairing terms which to leading order are given by

$$\begin{aligned} \bar{\epsilon}_n(\mathbf{q}) &= \epsilon_n + \sum_{p \neq 0} \frac{|\Delta_{n,n+p}(\mathbf{q})|^2}{p} \\ \bar{\Delta}_{nn}(\mathbf{q}) &= \Delta_{nn}(\mathbf{q}) - \sum_{p \neq 0, p' \neq 0} \frac{\Delta_{n,n+p}(\mathbf{q}) \Delta_{n+p,n+p'}^*(-\mathbf{q}) \Delta_{n+p',n}(\mathbf{q})}{pp'}. \end{aligned} \quad (11)$$

The effect of the off-diagonal couplings is taken into account by renormalizing the diagonal (in the Landau index) terms keeping a diagonal problem to be Nambu rotated (v is still $v \equiv n$).

In figure 1(a) we show the energy of the lowest band above the Fermi level, obtained from equation (8), as a function of \mathbf{q} (we only show one quadrant of the magnetic Brillouin zone due to the square lattice symmetry) for $\Delta = 0.1$ and $n_c = 10$ (we fix μ at this LL energy). In figures 1(b) and 1(c) we show the same band taking into account the off-diagonal terms in equation (7) considering $\Delta = 0.1$ and $\Delta = 0.5$, respectively. Results similar to these were previously presented in other forms (see e.g. [3, 8]) but we present them here as well to stress the role of the off-diagonal terms. The energy of the lowest band above the Fermi level is given by the gap function $|\Delta_{nn}(\mathbf{q})|$ in the DA. This is given by [3]

$$\Delta_{nn}(\mathbf{q}) = \frac{\Delta}{\sqrt{2}} \frac{(-1)^n}{2^{2n} n!} \sum_k e^{2ikq_y a - (q_x + \pi k/a)^2 l^2} H_{2n} \left[\sqrt{2} \left(q_x + \pi \frac{k}{a} \right) l \right] \quad (12)$$

where a is the lattice constant of the square vortex lattice and l is the magnetic length:

$$l = \sqrt{\frac{\hbar c}{eH}} = \frac{a}{\sqrt{\pi}}.$$

The gap $|\Delta_{nn}(\mathbf{q})|$ has zeros in the magnetic Brillouin zone at momentum points (q_j) which are in direct correspondence with the positions of the vortices in real space (z_i) such that $q_j l = z_i/l$ [3]. These gapless points are due to the centre-of-mass motion of the Cooper pairs in the presence of a high magnetic field and not due to the internal structure of the gap function as in d-wave superconductors. The gapless points grow considerably in number as n_c grows [3]. However, they preserve in the magnetic cell the vorticity per unit cell of the order parameter in real space. Away from the gapless points the gap expands to a scale of the order of Δ giving rise to a complicated structure that oscillates ever more strongly as n grows. Increasing Δ only rescales the energy. The energy has a linear dispersion around most of the zeros (-1 vorticity). Other sets of zeros have a quadratic dispersion for the square (triangular) lattice corresponding to a -2 (-3) vorticity, respectively. This dispersion leads to power-law behaviour at low temperatures, as mentioned above. On including off-diagonal terms, small gaps open in the spectrum [7] which are due to the normal (pairing) part of the self-energy and which are of order Δ^2 (Δ^3). However, throughout the Brillouin zone the numerical prefactors are very small and the spectrum is similar almost everywhere to the one obtained in the DA. The notable exceptions are the Eilenberger points (EP) (e.g. $\mathbf{q} = (-0.5, 0.5)$) where the gap

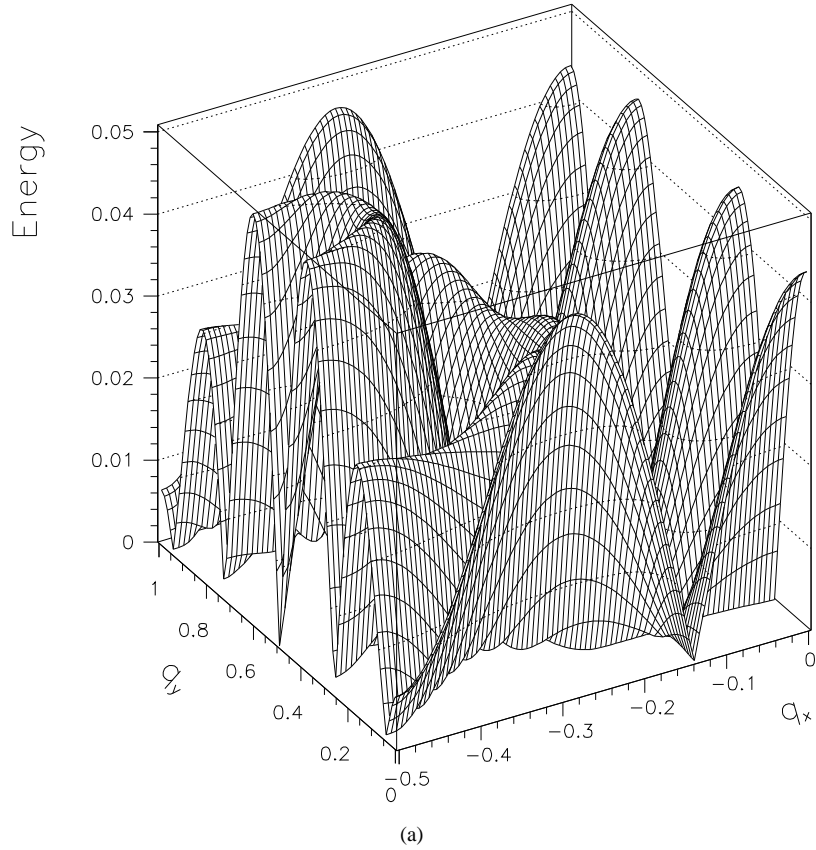


Figure 1. The lowest energy band as a function of \mathbf{q} for (a) $\Delta = 0.1$ in the DA and including off-diagonal terms for (b) $\Delta = 0.1$ and (c) $\Delta = 0.5$, respectively. Only one quadrant of the Brillouin zone is shown.

increases significantly as Δ grows [7]. The off-diagonal matrix elements $\Delta_{nm}(\mathbf{q})$ have in general a different structure of zeros. If $n + m$ is even, the Eilenberger points remain, but otherwise they are absent.

These results are best summarized by considering the density of states (DOS). In figure 2 we plot the DOS as a function of energy for different values of Δ . For small Δ the DOS is broadened from the Landau level locations by an amount of the order of Δ . The DOS is high at low energies. As Δ grows the energy interval grows and eventually at Δ of the order of the cyclotron energy the lowest band and the next band approach each other and a quantum level-crossing transition occurs. Note that as Δ grows and the DOS spreads over to higher energies, there remains a high DOS at low energies due to the low gap states that retain the characteristic spectrum of the DA. Therefore, it is expected that the DA will be appropriate at low Δ [3, 5] (see however reference [8] for a thorough discussion).

To calculate the Hall conductance we insert equations (2), (3) in the expression for σ_{xy} , equation (1), and obtain for the average Hall conductance

$$\sigma = \frac{1}{L^4} \int dx \int dx' \int dy \int dy' \sigma_{xy}(x, y; x', y') \quad (13)$$

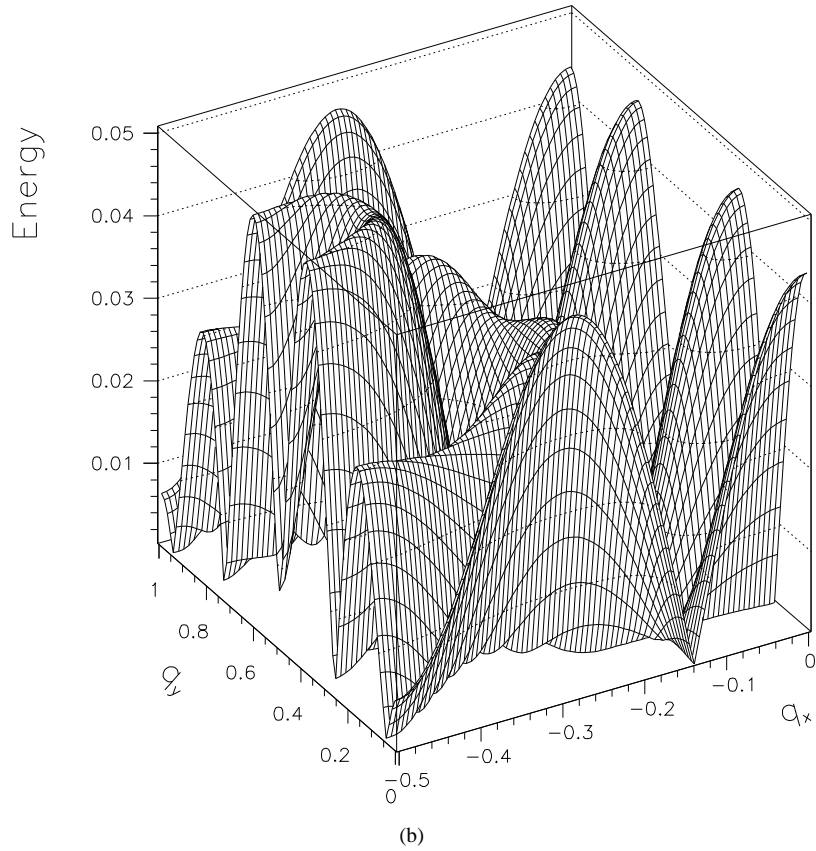


Figure 1. (Continued)

and, after several straightforward but lengthy steps ($q = 2e$),

$$\begin{aligned}
 \frac{\sigma}{q^2/h} = & - \sum_{\beta \neq 0} \frac{1}{(\epsilon_\beta - \epsilon_0)^2} \sum_{v, v'} \frac{1}{N_\phi} \sum_{nm} [n_{vq\uparrow} n_{v'q\downarrow} + n_{vq\downarrow} n_{v'q\uparrow}]' \\
 & \times \Re \left\{ \left[v_{-qn}^v u_{qm}^{*v'} \left(u_{qn+1}^{v'} \sqrt{\frac{n+1}{2}} + u_{q, n-1}^{v'} \sqrt{\frac{n}{2}} \right) \right. \right. \\
 & \times \left. \left(v_{-qm+1}^{*v'} \sqrt{\frac{m+1}{2}} - v_{-q, m-1}^{*v'} \sqrt{\frac{m}{2}} \right) \right] \\
 & + \left[v_{-qn}^v u_{qm}^{*v'} \left(u_{qn+1}^{v'} \sqrt{\frac{n+1}{2}} + u_{q, n-1}^{v'} \sqrt{\frac{n}{2}} \right) \right. \\
 & \times \left. \left. \left. \left(v_{-qm+1}^{*v} \sqrt{\frac{m+1}{2}} - v_{-q, m-1}^{*v} \sqrt{\frac{m}{2}} \right) \right] \right\}. \quad (14)
 \end{aligned}$$

The sum is extended over the excited states. Since the current operator is a two-particle operator, the excited states only differ from the ground state by the occupation of two quasiparticle (fermionic) states (this is the reason for the prime in the number occupation term). Here N_ϕ is the number of momenta appearing in the sum, which equals the number of vortices in the system. The energies have been rescaled by $\hbar\omega_c$.

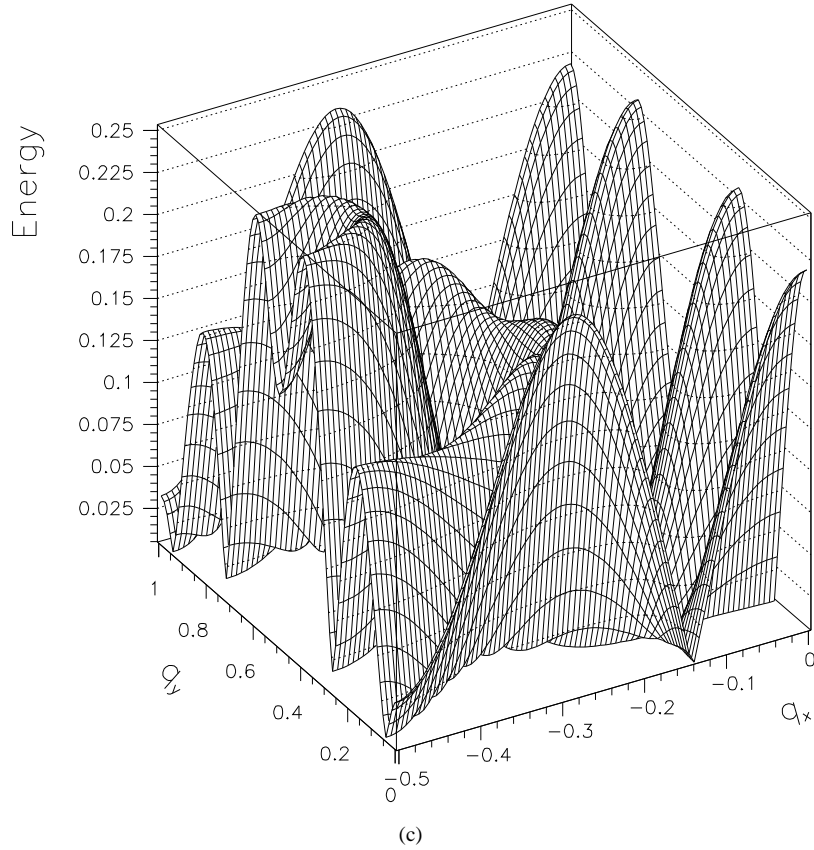


Figure 1. (Continued)

A selection rule in the DA implies that $\nu \neq \nu'$. We can therefore sum over the spin variables. The expression for σ then takes the form

$$\begin{aligned} \frac{\sigma}{q^2/h} = & -\frac{1}{4} \sum_{\beta \neq 0} \frac{1}{(\epsilon_\beta - \epsilon_0)^2} \frac{1}{N_\phi} \\ & \times \sum_q \sum_n \Re \left\{ (n_{nq} n_{n+1,q})' (n+1) \left[\frac{\Delta_{nn}^* \Delta_{n+1,n+1}}{\epsilon_q^n \epsilon_q^{n+1}} - \frac{\epsilon_q^n - \epsilon_n \epsilon_q^{n+1} + \epsilon_{n+1}}{\epsilon_q^n \epsilon_q^{n+1}} \right] \right. \\ & \left. - (n_{nq} n_{n-1,q})' (n) \left[\frac{\Delta_{nn}^* \Delta_{n-1,n-1}}{\epsilon_q^n \epsilon_q^{n-1}} - \frac{\epsilon_q^n - \epsilon_n \epsilon_q^{n-1} + \epsilon_{n-1}}{\epsilon_q^n \epsilon_q^{n-1}} \right] \right\}. \end{aligned} \quad (15)$$

Here $\epsilon_\beta = \epsilon_q^n + \epsilon_q^{n+1}$ in the first term and $\epsilon_\beta = \epsilon_q^n + \epsilon_q^{n-1}$ in the second term. Fixing the chemical potential at the level n_c ($n_c + 1$ occupied levels) and taking $\Delta = 0$ (normal phase) we get that $\bar{\sigma} = \sigma h/q^2 = n_c + 1$, as expected. The only contribution comes from the first term with $n = n_c$. Taking now a small value of Δ , the two dominant contributions come from the previous term and from the first term with $n = n_c - 1$. This leads to a discontinuity in σ : at $\Delta = 0$ the Hall conductance $\bar{\sigma} = (n_c + 1)$, while at small, but nonzero Δ , $\bar{\sigma} \sim (n_c + 1) - 1/2$. As Δ grows, $\bar{\sigma}$ decreases continuously.

In figure 3 we show $\bar{\sigma}$ as a function of Δ for the DA and for the leading-order perturbation theory (PT) for the range of values of Δ up to the order of the first level-crossing. We consider

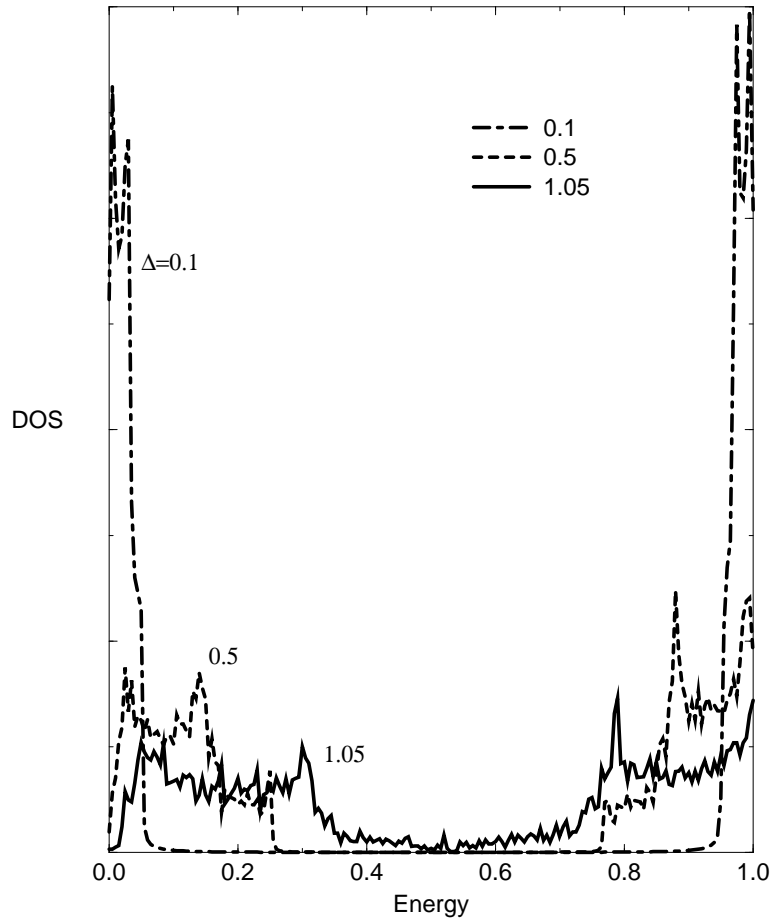


Figure 2. The density of states (DOS) in arbitrary units as a function of energy for $n_c = 10$. The first two bands are shown.

the cases $n_c = 4, 10$. As Δ grows, the off-diagonal terms renormalize the Hall conductance downwards with respect to the DA value. In the normal phase ($\Delta = 0$), the Fermi level (for a completely filled level) is in the gap between two Landau levels. As Δ is turned on, μ is kept fixed at $\mu = n_c + 1/2 + \eta$ ($\eta \rightarrow 0$) and the levels spread to higher energies, which leads to a decrease of the Hall conductance since the fraction of low-energy states that may conduct decreases. The presence of the off-diagonal terms increases the rate of decrease for larger values of Δ , for the same reason. At very low Δ the two methods agree, as expected. Close to the level-crossing the study is very difficult because a fully self-consistent calculation is needed to properly cover the crossover to the gapped regime. Going beyond the DA, several eigenfunctions of the BdG equations have components in the various Landau indices, which due to the gapless (or almost gapless) nature of the spectrum causes difficult numerical problems due to the energy denominator in equation (13). Also, strong mixing of the LL destroys the LL structure beyond the level-crossing transition(s). There is a discontinuity in the Fermi level due to this level-crossing (by $\pm 2\omega_c$ because of the doubling due to the particle and hole bands, u and v , respectively). After the transition, $\bar{\sigma}$ is expected to decrease again and to tend to zero as Δ grows even further (eventually after several level-crossings).

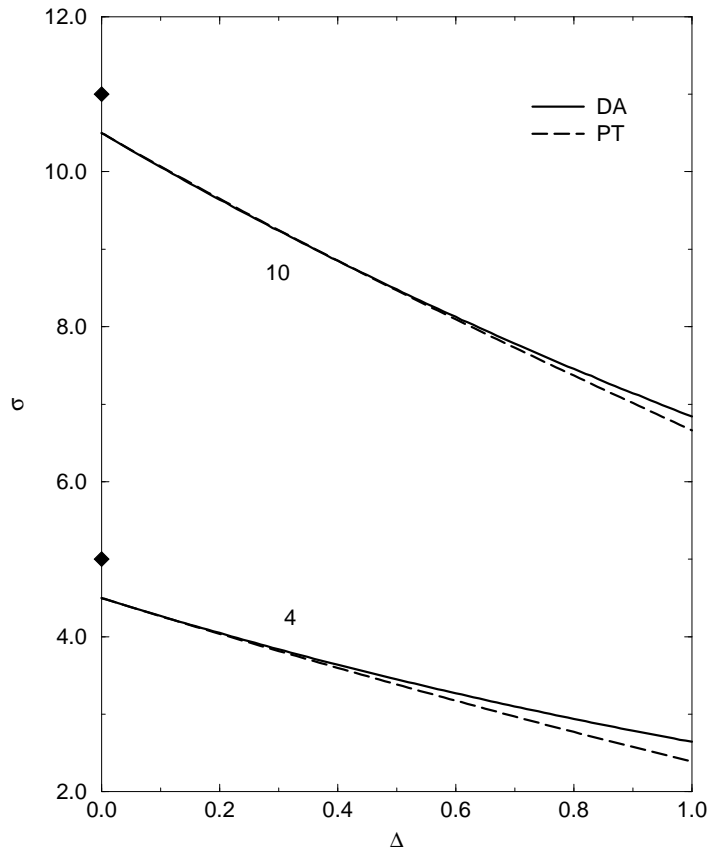


Figure 3. The Hall conductance for $n_c = 4, 10$ as a function of Δ for the two methods considered: the diagonal approximation (DA) and leading-order perturbation theory (PT). The two points at $n_c + 1$ are the $\Delta = 0$ result (normal phase).

3. Conclusions

In summary, we have calculated the Hall conductance of a pinned vortex lattice in a high magnetic field using the Kubo formula and the solution of the Bogoliubov–de Gennes equations for the wave-function amplitudes expanded in the Landau basis. We compared the diagonal approximation with the leading-order perturbation theory recently introduced [7]. The Hall conductance decreases from the normal-state value due to the presence of the low-lying states immediately above the Fermi energy. As Δ grows, the spread in energy increases and σ decreases. We limited the study to the region of validity of the PT. We suggest that σ may be used as an order parameter to detect the transition from the gapless regime (finite σ) to the gapped region (zero σ) where a tight-binding description should be appropriate.

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