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Evaluation of lattice sums for clean type-II superconductors*

Alexander L. Fetter

Institute of Theoretical Physics, Department of Physics, Stanford University, Stanford, California 94305

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A simplified treatment is presented for the lattice sums occurring in the theory of clean extreme type-II superconductors, rotating superfluid helium, and plasma oscillations in an array of filamentary conductors. Similar methods are applied to the mixed state of a thin superconducting film in a perpendicular magnetic field.

The mixed state of type-II superconductors[1] consists of quantized flux lines arranged in a triangular lattice with areal density $n=B/\phi_0$. Although the detailed theory of such materials is generally difficult, the analysis simplifies considerably for clean extreme type-II materials at low and intermediate flux densities ($H_{c1} \leq H \ll H_{c1}$). In this case, the core size ξ is much smaller than the penetration depth λ or the lattice spacing $\approx (n\pi)^{-1/2}$ (note that n^{-1} is the area per unit cell), and the London model applies. The physical properties of such superconductors are expressible in terms of lattice sums of the form $\sum_j' e^{i\vec{k}\cdot\vec{r}_j} F(\vec{r}_j)$, where the prime means that j runs over all lattice sites excluding the origin and $F(\vec{r}_j)$ is either a Bessel function of imaginary argument (for bulk materials[1-3]) or a combination of Struve and Neumann functions (for thin films[4,5]). The original calculations could evaluate these sums only to order k^2. Here we present a new general treatment that simplifies the previous analysis and extends it to all values of k^2.

For definiteness, first consider a bulk type-II material. Its Helmholtz free energy at low and intermediate flux density involves the quantity[1,6] $\sum_j' K_0(r_j/\lambda)$, where K_0 is the usual Bessel function that vanishes at infinity.[7] The free energy, in turn, fixes both the equilibrium lattice structure and the constitutive relation $B(H)$ in an applied magnetic field. Similarly, the general oscillation modes of the flux-line lattice[2,3] require sums of the form $\sum_j'(1-e^{i\vec{k}\cdot\vec{r}_j})K_0(qr_j)$ along with related but more complicated ones [see Eqs. (12a) and (12b) below]. Here $\vec{k}$ is a wave vector in the xy plane and $q\equiv(k_z^2+\lambda^{-2})^{1/2}$, with k_z the axial wave number associated with bending modes along the z axis. Finally, the sum $\sum_j' e^{i\vec{k}\cdot\vec{r}_j} K_0(k_z r_j)$ appears in the theory of plasma oscillations in an array of filamentary conducting strands.[8] These various lattice sums may be derived from the single quantity

$$S(\vec{k},q,\vec{r}) \equiv \sum_j e^{i\vec{k}\cdot\vec{r}_j} K_0(q\,|\vec{r}-\vec{r}_j|), \tag{1}$$

where j now runs over *all* lattice sites in the xy plane and $\vec{r}$ is an arbitrary two-dimensional vector ($\vec{r}\neq\vec{r}_j$).

If $qn^{-1/2}\gg 1$ (low-density limit), Eq. (1) converges rapidly and may be summed directly. For small $qn^{-1/2}$, however, an accurate evaluation requires many terms, and it is then convenient to use the two-dimensional form of the Poisson sum formula[9,10]

$$\sum_j e^{-i\vec{k}\cdot(\vec{r}-\vec{r}_j)} F(\vec{r}-\vec{r}_j) = n \sum_{\vec{g}} e^{i\vec{g}\cdot\vec{r}} \bar{F}(\vec{g}+\vec{k}), \tag{2}$$

where $\{\vec{g}\}$ is the set of two-dimensional reciprocal-lattice vectors and

$$\bar{F}(\vec{k}) = \int d^2r\, e^{-i\vec{k}\cdot\vec{r}} F(\vec{r}) \tag{3}$$

is the usual Fourier transform integrated over the whole xy plane. Equation (3) is easily evaluated for K_0,[7] and a slight rearrangement yields

$$S(\vec{k}, q, \vec{r}) = 2\pi n \sum_{\vec{g}} \frac{e^{i(\vec{g}+\vec{k})\cdot\vec{r}}}{(\vec{g}+\vec{k})^2 + q^2} . \tag{4}$$

As expected from the logarithmic behavior of $K_0(x)$ for small x, the right-hand side of (4) diverges logarithmically as $r \to 0$. To isolate this behavior, we rewrite the sum

$$S(\vec{k}, q, \vec{r}) = 2\pi n \sum_{\vec{g}} \frac{e^{i(\vec{g}+\vec{k})\cdot\vec{r}}}{(\vec{g}+\vec{k})^2} - 2\pi n q^2 \sum_{\vec{g}} \frac{e^{i(\vec{g}+\vec{k})\cdot\vec{r}}}{(\vec{g}+\vec{k})^2[(\vec{g}+\vec{k})^2 + q^2]} , \tag{5}$$

where the second term converges absolutely and represents a small correction for $qn^{-1/2} \ll 1$. Although Eq. (5) is adequate for our purposes, the same process may obviously be used repeatedly to construct an expansion in powers of $q^2 n^{-1}$.

Equation (5) leads us to consider the slowly convergent lattice sums[11]

$$\Sigma_p(\vec{k}, \vec{r}) = \pi n \sum_{\vec{g}} \frac{e^{i(\vec{g}+\vec{k})\cdot\vec{r}}}{|\vec{g}+\vec{k}|^p} . \tag{6}$$

As in the more familiar three-dimensional case, the Ewald method[10] can recast Eq. (6) into a rapidly converging series. Note first the identity

$$\begin{aligned}\Gamma(\tfrac{1}{2}p)\,|\vec{g}+\vec{k}\,|^{-p} &= 2\int_0^\infty d\zeta\; \zeta^{p-1} \exp(-\zeta^2\,|\vec{g}+\vec{k}\,|^2) \\ &= 2\int_0^z d\zeta\; \zeta^{p-1}\exp(-\zeta^2\,|\vec{g}+\vec{k}\,|^2) + 2\int_z^\infty d\zeta\; \zeta^{p-1}\exp(-\zeta^2|\vec{g}+\vec{k}|^2),\end{aligned} \tag{7a}$$

which reduces Eq. (6) to an integral of phase-modulated Gaussian functions. Second, the particular case of the Poisson sum formula [Eq. (2)]

$$\sum_j e^{-i\vec{k}\cdot(\vec{r}-\vec{r}_j)} \exp[-(\vec{r}-\vec{r}_j)^2/4\zeta^2] = 4\pi n \zeta^2 \sum_{\vec{g}} e^{i\vec{g}\cdot\vec{r}} \exp[-\zeta^2(\vec{g}+\vec{k})^2] \tag{7b}$$

may be used to rewrite the portion of the integral from 0 to z. In this way, we obtain the desired expression

$$\Gamma(\tfrac{1}{2}p)\,\Sigma_p(\vec{k}, \vec{r}) = \pi n \sum_{\vec{g}} \frac{e^{i(\vec{g}+\vec{k})\cdot\vec{r}}}{|\vec{g}+\vec{k}\,|^p}\, \Gamma(\tfrac{1}{2}p,\; |\vec{g}+\vec{k}\,|^2 z^2) + \frac{1}{4}\sum_j e^{i\vec{k}\cdot\vec{r}_j}(\tfrac{1}{2}\,|\vec{r}-\vec{r}_j\,|)^{p-2}\,\Gamma(1-\tfrac{1}{2}p,\; |\vec{r}-\vec{r}_j\,|^2/4z^2), \tag{8}$$

where

$$\Gamma(a, x) = \int_x^\infty dt\, e^{-t}\, t^{a-1}$$

is the incomplete γ function[12] and $\Gamma(a) = \Gamma(a, 0)$ is the usual γ function. Equation (8) holds for arbitrary z, but the choice $z = (4\pi n)^{-1/2}$ maximizes the rate of convergence and will be used here consistently. If p is an even integer, the relevant integrals reduce to exponential integrals and exponentials[12]; for example, we find

$$\Sigma_2(\vec{k}, \vec{r}) = \pi n \sum_{\vec{g}} \frac{e^{i(\vec{g}+\vec{k})\cdot\vec{r}}}{(\vec{g}+\vec{k})^2} \exp\left[-\frac{(\vec{g}+\vec{k})^2}{4\pi n}\right] + \frac{1}{4}\sum_j e^{i\vec{k}\cdot\vec{r}_j} E_1[\pi n(\vec{r}-\vec{r}_j)^2] . \tag{9}$$

A combination of Eqs. (5) and (9) leads to a convenient expression for the original series $S(\vec{k}, q, \vec{r})$ in Eq. (1).

The required lattice sums now follow as limits of $S(\vec{k}, q, \vec{r})$. In particular,

$$\begin{aligned}\sum_j{}' e^{i\vec{k}\cdot\vec{r}_j} K_0(qr_j) &= \lim_{\vec{r}\to 0}[S(\vec{k}, q, \vec{r}) - K_0(qr)] \\ &= \lim_{\vec{r}\to 0}[S(\vec{k}, q, \vec{r}) - \ln(2/qr) + \gamma] ,\end{aligned} \tag{10}$$

where $\gamma \approx 0.5772$ is Euler's constant. On the right-hand side of Eq. (5), the second term converges for $r = 0$; moreover, the logarithmic divergence in (9) occurs only in the term $j = 0$. A straightforward calculation gives the exact expression

$$\begin{aligned}\sum_j{}' e^{i\vec{k}\cdot\vec{r}_j} K_0(qr_j) &= \frac{2\pi n}{k^2+q^2} - \tfrac{1}{2}\ln\left(\frac{4\pi n}{q^2}\right) + \tfrac{1}{2}\gamma - \frac{2\pi n}{k^2}\left[1 - \exp\left(-\frac{k^2}{4\pi n}\right)\right] \\ &+ \frac{1}{2}\sum_j{}' e^{i\vec{k}\cdot\vec{r}_j} E_1(\pi n r_j^2) + 2\pi n \sum_{\vec{g}}{}' \frac{\exp[-(\vec{g}+\vec{k})^2/4\pi n]}{(\vec{g}+\vec{k})^2} - 2\pi n q^2 \sum_{\vec{g}}{}' \frac{1}{(\vec{g}+\vec{k})^2[(\vec{g}+\vec{k})^2 + q^2]} ,\end{aligned} \tag{11}$$

where the primed sum on $\vec{g}$ omits the term $\vec{g}=0$. The first two terms on the right-hand side of (11) are independent of the detailed lattice structure; they agree with those obtained in the continuum approximation, where the primed sum over j is replaced by an integral, excluding a small circle of radius $(\pi n)^{-1/2}$ about the origin. Thus the discrete lattice affects only the constant term (independent of q) and terms of order q^2 and higher in Eq. (11). The sum needed for the free energy of the lattice is obtainable directly from (11) merely by letting $k\to 0$, and those required for the vibration frequencies involve the combination $S(0, q, \vec{r}) - S(\vec{k}, q, \vec{r})$, which is finite at $r=0$. In particular, recursion relations for Bessel functions show that

$$\lim_{\vec{r}\to 0}\left\{\frac{\partial^2}{\partial x\,\partial y}[S(0,q,\vec{r})-S(\vec{k},q,\vec{r})]\right\}=q^2\sum_j{}'(1-e^{i\vec{k}\cdot\vec{r}_j})\frac{x_j y_j}{r_j^2}K_2(qr_j), \tag{12a}$$

$$\lim_{\vec{r}\to 0}\left\{\left(\frac{\partial^2}{\partial y^2}-\frac{\partial^2}{\partial x^2}\right)[S(0,q,\vec{r})-S(\vec{k},q,\vec{r})]\right\}=q^2\sum_j{}'(1-e^{i\vec{k}\cdot\vec{r}_j})\frac{y_j^2-x_j^2}{r_j^2}K_2(qr_j). \tag{12b}$$

These latter sums determine the dispersion relation for oscillations of a dense $(n\xi^2 \ll 1 \ll n\lambda^2)$ flux-line lattice in an extreme type-II material. For example, a triangular lattice can be shown to have the spectrum

$$\omega^2 \approx \left(\frac{eB}{mc}\right)^2\left(\frac{k_z^4\lambda^4+k_z^2k^2\lambda^4}{(1+k^2\lambda^2+k_z^2\lambda^2)^2}+\frac{k^4\lambda^2}{16\pi n(1+k^2\lambda^2+k_z^2\lambda^2)}\right), \tag{13a}$$

where the wave numbers satisfy the condition $k^2+k_z^2 \ll n$, but with $(k^2+k_z^2)\lambda^2$ arbitrary. This expression agrees with that found in the continuum approximation,[3] confirming earlier conjectures.[2,5] In the limit $\lambda\to\infty$ and with the factor eB/mc replaced by $n\kappa$, Eq. (13a) reduces to

$$\omega^2=(n\kappa)^2[k_z^2+(k^4/16\pi n)](k_z^2+k^2)^{-1}, \tag{13b}$$

applicable to a neutral superfluid rotating at an angular velocity $\Omega=\frac{1}{2}n\kappa$, where κ is the quantum of circulation.[13]

We shall briefly consider the similar but more intricate case of a thin superconducting film in a perpendicular magnetic field. The magnetic flux again penetrates the sample in quantized bundles surrounded by circulating supercurrents, but the associated magnetic fields have an algebraic tail owing to their extension into the surrounding vacuum. This long-range behavior introduces a dependence on the shape and size of the sample, so that the free-energy density diverges in the thermodynamic limit. The vibration frequencies remain well-defined, however, and may be derived from the series

$$s(\vec{k},\vec{r}) \equiv \sum_j e^{i\vec{k}\cdot\vec{r}_j}\,\psi(|\vec{r}-\vec{r}_j|/\Lambda), \tag{14}$$

where Λ is the effective penetration depth[4,5] and

$$\psi(x)=x^{-1}-\tfrac{1}{2}\pi[\mathbf{H}_0(x)-\mathbf{Y}_0(x)], \tag{15}$$

with $\mathbf{H}_0$ and $\mathbf{Y}_0$ the Struve and Neumann functions of order zero.[4,5,14] If the lattice constant $(n\pi)^{-1/2}$ exceeds Λ, then (14) may be evaluated by expanding ψ in powers of $\Lambda/|\vec{r}-\vec{r}_j|$ and using (8).[5] On the other hand, if $(\pi n)^{1/2}\Lambda$ is large, the Poisson sum formula (2) provides a more convenient expression

$$s(\vec{k},\vec{r})=2\pi n\Lambda^2\sum_{\vec{g}}\frac{e^{i(\vec{g}+\vec{k})\cdot\vec{r}}}{1+\Lambda|\vec{g}+\vec{k}|}, \tag{16}$$

where the Fourier transform of ψ follows from a standard integral representation.[14] Equation (15) indicates that $\psi(x)$ diverges like x^{-1} as $x\to 0$. Thus it is preferable to rewrite (16) as

$$s(\vec{k},\vec{r})=2\Lambda\,\Sigma_1(\vec{k},\vec{r})-2\pi n\Lambda\sum_{\vec{g}}\frac{e^{i(\vec{g}+\vec{k})\cdot\vec{r}}}{|\vec{g}+\vec{k}|(1+\Lambda|\vec{g}+\vec{k}|)}, \tag{17}$$

where the first term dominates for large $n\Lambda^2$. Moreover, $\Sigma_1(\vec{k},\vec{r})$ contains the leading behavior for small $r(\propto r^{-1})$, and the remaining part of (17) is only logarithmically singular as $r\to 0$. As in the similar case of Eq. (5) for a bulk sample, Eq. (17) may be manipulated to yield an exact expansion in inverse powers of $n^{1/2}\Lambda$, but the present form suffices for our purposes.

The evaluation of (17) requires the identity

$$\Sigma_1(\vec{k},\vec{r})=\pi n\sum_{\vec{g}}\frac{e^{i(\vec{g}+\vec{k})\cdot\vec{r}}}{|\vec{g}+\vec{k}|}\operatorname{erfc}\left(\frac{|\vec{g}+\vec{k}|}{2(\pi n)^{1/2}}\right)+\frac{1}{2}\sum_j\frac{e^{i\vec{k}\cdot\vec{r}_j}}{|\vec{r}-\vec{r}_j|}\operatorname{erfc}[(\pi n)^{1/2}|\vec{r}-\vec{r}_j|], \tag{18}$$

which follows from Eq. (8) with $\operatorname{erfc} x=\pi^{-1/2}\Gamma(\frac{1}{2},x^2)$ the complementary error function. An elementary analysis gives the expansion

$$\sum_j{}'(1-e^{i\vec{k}\cdot\vec{r}_j})\,\psi(r_j/\Lambda)=2\pi n\Lambda^2\,\Lambda k(1+\Lambda k)^{-1}-2n^{1/2}\Lambda\{1-(\pi n^{1/2}/k)\operatorname{erf}[k/2(\pi n)^{1/2}]\}+\Lambda\sum_j{}'(1-e^{i\vec{k}\cdot\vec{r}_j})\,r_j^{-1}\operatorname{erfc}[(\pi n)^{1/2}r_j]$$

$$+2\pi n\Lambda\sum_{\vec{g}}{}'\{g^{-1}\,\mathrm{erfc}[g/2(\pi n)^{1/2}]-|\vec{g}+\vec{k}|^{-1}\,\mathrm{erfc}[|\vec{g}+\vec{k}|/2(\pi n)^{1/2}]\}-2\pi n\sum_{\vec{g}}{}'\{[g(g+\Lambda^{-1})]^{-1}$$
$$-[|\vec{g}+\vec{k}|(|\vec{g}+\vec{k}|+\Lambda^{-1})]^{-1}\}, \qquad (19)$$

where the logarithmic singularity in (17) has disappeared, and the last term remains finite as $n^{1/2}\Lambda \to \infty$. Equation (19) and related but more complicated sums [compare Eq. (12)] arise in calculating the normal modes of the mixed state in a thin superconducting film. In this way, it is possible to confirm the earlier conjecture[5] that a moderately dense triangular lattice ($n\Lambda^2 \gg 1$) in such a film has the same oscillation spectrum as the continuum model:

$$\omega^2 = \left(\frac{eB}{mc}\right)^2 \frac{k^2}{16\pi n}\,\frac{k\Lambda}{1+k\Lambda}, \qquad (20)$$

assuming $kn^{-1/2} \ll 1$ but $k\Lambda$ arbitrary. It is interesting that (20) differs from the spectrum of the nonbending modes in a bulk triangular lattice [Eq. (13a) with $k_z = 0$] only in the substitution of the nonanalytic function $k\Lambda(1+k\Lambda)^{-1}$ of k^2 for the analytic one $k^2\lambda^2(1+k^2\lambda^2)^{-1}$. This alteration reflects the long-range interaction between flux lines in a thin film. At long wavelengths ($k\Lambda \ll 1$), it affects certain elastic properties of the corresponding lattice, in particular the compressibility[15,16] and the limiting form of the vibration spectrum.[5] For shorter wavelengths ($k\Lambda \gg 1$ in thin films or $k\lambda \gg 1$, $k_z = 0$ in bulk samples), however, the anomalous behavior disappears, and Eqs. (13a) and (20) become identical.

This note has presented a new and simplified treatment of two-dimensional lattice sums occurring in the theory of clean type-II superconductors, rotating He II, and plasma oscillations in filamentary conductors. The resulting expressions extend to shorter wavelengths the previous calculations of vibration frequencies in a triangular array of flux lines. They confirm that the spectrum is identical with that evaluated in the continuum approximation, both for bulk type-II materials and for thin films.

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