INTERNAL CURRENTS AND MAGNETIC FIELDS CLOSE TO THE SURFACE FOR A TYPE-II SUPERCONDUCTOR FOR APPLIED MAGNETIC FIELDS NEAR THE UPPER CRITICAL FIELD H_{c2}

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Based on the Ginzburg-Landau theory[1] of superconductivity, the shielding currents and the internal magnetic field were calculated as a function of distance from the surface for type-II superconductors when the applied magnetic field is near the upper critical field H_{c2}. There are two currents near the surface which flow in opposite directions, whose magnitudes are very large compared to the vortex currents[2] just below H_{c2}. Above H_{c2} the magnitudes of these currents are exactly equal, but below H_{c2} they are slightly different and give rise to a very small net surface current. The currents invert their direction within less than one coherence length from the surface. When the applied magnetic field is just below H_{c2} such that the condition $(H_{c2}-H_0)/H_{c2} \ll 1$ is satisfied, the smallest magnetic field close to the surface is considerably smaller than the smallest magnetic field in the bulk of the material. However, when the Ginzburg-Landau parameter $\kappa > 3$, the maximum deviation of the internal magnetic field near the surface from the external field is smaller than 2%.

Consider a semi-infinite superconducting half-space with the boundary surface at $x = 0$ and vacuum at $x < 0$. The z direction is assumed to be parallel to the applied magnetic field, and its magnitude is close to the upper critical field H_{c2}. Below H_{c2} our calculations are accurate within the Abrikosov approximation[2] $(H_{c2}-H_0)/H_{c2} \ll 1$. Between H_{c2} and H_{c3}[3] our general results are exact[4] solutions of the Ginzburg-Landau theory which is valid near the transition temperature T_c.

The normalized Ginzburg-Landau equations are

$$\left(\frac{i}{\kappa}\nabla + \vec{A}\right)^2 \Psi - \Psi + |\Psi|^2\Psi = 0, \tag{1}$$

$$-\mathrm{curl}\,\mathrm{curl}\vec{A} = \vec{A}|\Psi|^2 + i/2\kappa(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*), \tag{2}$$

where the order parameter Ψ is normalized with respect to the absolute value of the order parameter in zero field; the magnetic field with respect to $\sqrt{2}H_c$; the vector potential $\vec{A}$ with respect to $\sqrt{2}H_c\lambda$; the distances with respect to λ; H_c is the thermodynamic critical field; λ the penetration depth; $\kappa = \lambda/\xi$; and ξ is the coherence length. The normalized free energy of the superconductor at a constant value of the applied magnetic field H_0 is[1]

$$F_{SH} = b + c\int dV\left(\frac{1}{2}|\Psi|^4 - |\Psi|^2 + \left|\frac{i}{\kappa}\nabla\Psi + \vec{A}\Psi\right|^2 + H^2\right), \tag{3}$$

where b and c are constants and the integral is extended over the total volume of the superconductor.

We assume that near the surface of the metal the order parameter can be written as

$$\Psi = e^{ik_1 y}F(x), \tag{4}$$

where F is a function of x and k_1 is some as yet undetermined constant. We assume that for the above-stated approximation $\vec{A}(x)$ has the components $(0; H_0x + A_1(x) + C_1/\mu; 0)$, where $A_1(x)$ is a function of x. We have chosen the gauge such that at $x = 0$ the function $A_1(x) = 0$, and we assume that C_1/μ is the vector potential at $x = 0$. We introduce the parameter $\mu^2 = \kappa/H_0$ (≡ the upper critical field H_{c2} divided by the applied field in normalized units), and the new notation $\zeta = x\kappa/\mu$, $\zeta_1 = k_1\mu/\kappa$, and $n = (\kappa/\mu)^2$. In the new notation $A_1(x)$ becomes $A_1(\zeta) = a(\zeta)/\mu$ and the function $F(x)$ becomes $F(\zeta)$. We define the quantity $\zeta_1 - C_1 = \Gamma$. With the above-chosen vector potential and the definitions, Eqs. (1) to (3) are

$$d^2F/d\zeta^2 + [\mu^2(1-F^2) - (a-\Gamma+\zeta)^2]F = 0, \tag{1a}$$

$$n d^2a/d\zeta^2 = (a-\Gamma+\zeta)F^2, \tag{2a}$$

$$F_{SH} = B + C\int_0^\infty d\zeta\left[\left(\frac{dF}{d\zeta}\right)^2 + (a-\Gamma+\zeta)^2F^2 - \mu^2F^2(1-\tfrac{1}{2}F^2) + n\frac{da}{d\zeta}\left(2+\frac{da}{d\zeta}\right)\right], \tag{3a}$$

where the integral is proportional to the free energy of the superconductor per unit area in the yz plane at constant magnetic field, and B and C are constants.

At the surface the Ginzburg-Landau boundary condition[1] must be satisfied, which in our case reduces to

$$dF/d\zeta = 0 \text{ at } \zeta = 0. \tag{5}$$

When the applied magnetic field is equal to or larger than the upper critical field H_{c2}, the additional boundary conditions $dF/d\zeta = 0$ and $F = 0$ at $\zeta = \infty$ must be satisfied because no superconductivity exists in the bulk of the material. When the external magnetic field H_0 is slightly smaller than the upper critical field H_{c2}, we may also assume that $dF/d\zeta \to 0$ and $F \to 0$ for $\zeta \to \infty$. This is justified if the order parameter in the bulk of the metal is very small compared to the order parameter near the surface. Below H_{c2} our calculation is valid within the approximation

$$F^2(0) \gg \langle |\Psi_B|^2 \rangle = \frac{\kappa - H_0}{\kappa\beta(1-1/2\kappa^2)}. \tag{6}$$

Ψ_B is the order parameter in the bulk of the metal for a vortex square lattice[2] and $\beta = 1.18$. It turns out that $F(0)$ is of the order of unity,[4] and therefore our calculations are correct within the Abrikosov approximation[2] $(\kappa - H_0)/\kappa \ll 1$, provided κ^2 is not too close to $\frac{1}{2}$.

The free energy, Eq. (3a), can be minimized with respect to Γ, from which one obtains

$$\int_0^\infty d\zeta [a - \Gamma + \zeta] F^2 = 0. \tag{7}$$

When Eq. (2a) is substituted into Eq. (7) and integrated, one obtains within our approximation an additional boundary condition $da/d\zeta = 0$ at $\zeta = \infty$, because the magnetic field at the surface is H_0, and hence $da/d\zeta = 0$ at $x = 0$. By substituting for $\zeta = \eta + \Gamma$ into Eq. (3a), one obtains

$$F_{SH} = B + C\int_{\eta_0(\Gamma)}^\infty d\eta \left[\left(\frac{\partial F}{\partial \eta}\right)^2 + (a+\eta)^2 F^2 - \mu^2 F^2 (1 - \tfrac{1}{2}F^2) + n\frac{da}{d\eta}\left(2 + \frac{da}{d\eta}\right)\right], \tag{3b}$$

where F is now $F(\eta;\Gamma)$. When Eq. (3b) is minimized with respect to the parameter Γ, and use is made of Eqs. (1a) and (2a), of the Ginzburg-Landau boundary condition $\partial F/\partial\eta = 0$ at $\eta = \eta_0(\Gamma)$, and of the condition that $\partial F/\partial\eta = 0$ at $\eta = \infty$, and also $F \to 0$ stronger than η^{-2} for $\eta \to \infty$, one obtains a more specific relation than Eq. (7):

$$\Gamma^2 = \mu^2[1 - \tfrac{1}{2}F^2(0)], \tag{8}$$

where $F(0)$ is the absolute value of the order parameter at the surface of the material. From Eqs. (1a) and (8), and also from Eqs. (2a) and (8), additional boundary conditions are obtained:

$$d^2F/d\zeta^2 = \tfrac{1}{2}\mu^2 F^3(0) \text{ at } \zeta = 0, \tag{9a}$$

$$-d^2a/d\zeta^2 = (\mu/n)F^2(0)[1 - \tfrac{1}{2}F^2(0)]^{1/2} \text{ at } \zeta = 0. \tag{9b}$$

From Eqs. (9a) and (5), it follows that $|\Psi|^2$ is always a minimum at the boundary surface for applied magnetic fields between H_{c2} and H_{c3}, and this is also correct within our approximation just below H_{c2}.

With all these boundary conditions Eqs. (1a) and (2a) have been solved simultaneously on an analog computer.[4] The values of $F(\zeta)$ ($\propto$ order parameter), $d^2a/d\zeta^2$ ($\propto$ current density), $da/d\zeta$ ($\propto$ internal magnetic field), and a ($\propto$ vector potential) have been calculated for various values of $1/\mu^2$ and n. For $0.8 \leq 1/\mu^2 \leq 1.1$ and $n > 1$, the functions $F(\zeta)$ are quite similar to the $D(\zeta)$ which were calculated previously[5] (although not the same) with $a(\zeta)$ and C_1 neglected in Eq. (1a). In the present scheme only the quantity $\Gamma = \zeta_1 - C_1$ is of significance and not ζ_1 and C_1 individually. The Γ value [Eq. (8)] is closely related to the ζ_0 value of reference 5 [Eq. (10)]. In the present work we make use of the approximate values[5] for $F(\zeta)$, and we shall estimate the approximate current and magnetic-field distribution for the above restricted values of μ and n. The exact numerical solution[4] will be published elsewhere.

The current $(4\pi/c)\vec{j} = \text{curl}\vec{H} = \text{curl curl}\vec{A}$, and therefore it follows from Eq. (2a) that

$$\frac{d^2a}{d\zeta^2} = -\frac{4\pi}{c}\frac{\mu}{n} j(\zeta), \tag{10}$$

where $j(\zeta)$ is the current density normalized with respect to $\sqrt{2}H_c/\lambda$. At $\zeta = 0$, the current density is [Eqs. (9b) and (10)]

$$(4\pi/c)j(0) = F^2(0)[1 - \tfrac{1}{2}F^2(0)]^{1/2}. \tag{11}$$

At $\zeta = \zeta_c$, the current density reverses its sign. The reversal point is determined by the relation $\Gamma = a(\zeta_c) + \zeta_c$, which can be seen readily from Eqs. (2a) and (10). For magnetic fields larger than or equal to H_{c2}, Eq. (7) is exactly satisfied, which means that near the surface two currents of equal magnitude are flowing in opposite directions. Equation (7) will also hold approximately for magnetic fields just below H_{c2} if the order parameter in the bulk of the material is small compared to the order parameter near the surface as shown by Eq. (6).

This relation is satisfied for magnetic fields near the upper critical field[5] where $F^2(0) \gtrsim \frac{1}{2}$.

One can see now that the currents have to be distributed as shown schematically in Figs. 1(a) and 1(b) when the applied magnetic field is just slightly smaller than the upper critical field. J_{s1} and J_{s2} are the currents (per unit length

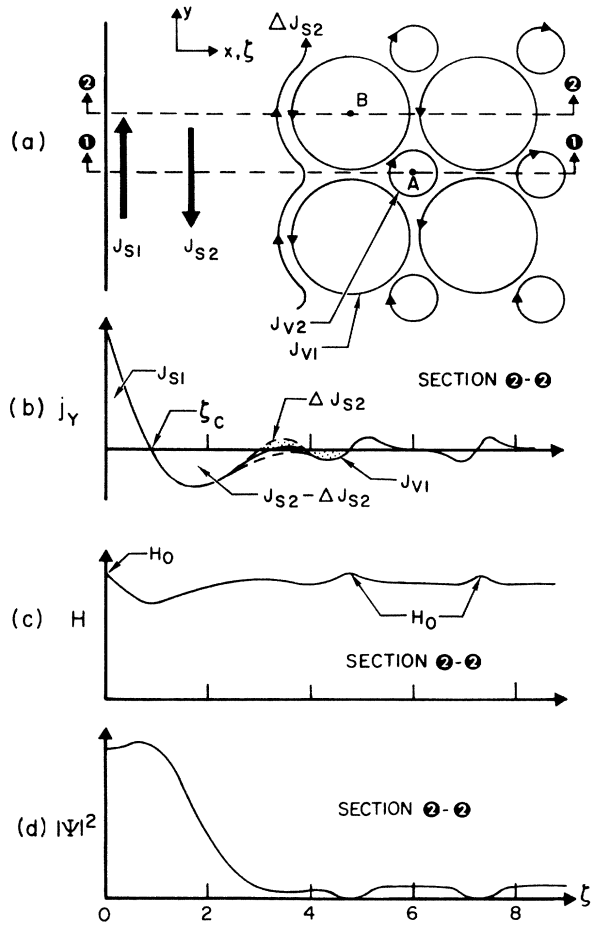

Fig. (a) The schematic distribution of the internal currents for a type-II superconductor in the xy plane near the boundary between vacuum and metal which is located at $\zeta = 0$. (b) The schematic distribution of the current density j_y perpendicular to section ②-② of (a). The applied magnetic field is parallel to the z direction, and it is smaller than the upper critical field H_{c2} such that $(H_{c2}-H_0)/H_{c2} \ll 1$ is satisfied. The currents J_{s1} and J_{s2} and also ΔJ_{s2} and J_{v1} are of equal magnitudes, respectively, but $J_{s1} \gg J_{v1}$. The approximate distance from the surface is normalized in units of $\zeta = (x/\xi)(H_0/H_{c2})^{1/2}$, where ξ is the coherence length. (c) The schematic variation of the internal magnetic field H for section ②-② in (a). (d) The schematic variation of the square of the absolute value of the order parameter $|\Psi|^2$ for section ②-② in (a).

in the z direction) obtained from Eq. (7), and superimposed on them is the current distribution of a vortex square lattice.[2] The bulk solution will presumably establish itself at a distance from the surface at which the square of the order parameter of the sheath solution[5] is approximately the same as the average of the square of the order parameter in the bulk; which is about 3 to 4 or more coherence lengths from the surface. Between the vortex current J_{v1} and J_{v2} and the surface there must be an additional surface current ΔJ_{s2}. This can be seen readily from the following argument. The line integral around a closed loop is

$$\oint \vec{H} \cdot d\vec{s} = \frac{4\pi}{c} I, \tag{12}$$

where $I = Jl$ is the total current enclosed by a loop and l the projection of the path of the loop onto the z direction. Let us imagine a loop through B in Fig. 1(a), parallel to the section ②-② and closed outside the metal (where the field is H_0). At point B the order parameter $|\Psi_B|^2 = 0$, and therefore $H_B = H_0$, and Eq. (12) becomes

$$|J_{s1}| - |J_{s2}| + |\Delta J_{s2}| - |J_{v1}| = 0. \tag{13}$$

From Eq. (7) it follows that $|J_{s1}| - |J_{s2}| = 0$, and therefore

$$|J_{v1}| = |\Delta J_{s2}|. \tag{14}$$

If the loop through B is rotated slightly around B, it is clear that ΔJ_{s2} has to follow a path similar to that shown in Fig. 1(a). Consider now A in Fig. 1(a) where the order parameter is a maximum, and therefore the internal field in the bulk of the metal is a minimum ($H_A = H_{\min}$). If we put a loop through A parallel to section ①-① and close the loop outside the material, Eq. (12) reduces to

$$H_0 - H_{\min} = (4\pi/c)(|J_{s1}| - |J_{s2}| + |\Delta J_{s2}| + |J_{v2}|), \tag{15}$$

where from Eq. (7) $|J_{s1}| - |J_{s2}| = 0$, and from Eq. (14) $|\Delta J_{s2}| = |J_{v1}|$. $|J_{v1}|$ and $|J_{v2}|$ can be calculated from Abrikosov's theory.[2] They are $(4\pi/c)|J_{v1}| = (1/2\kappa)C_0^2\alpha$ and $(4\pi/c)|J_{v2}| = (1/2\kappa)C_0^2(\beta-\alpha)$, where $C_0^2 = 2\sqrt{2}\kappa(\kappa-H_0)/(2\kappa^2-1)\beta$ and $\alpha = 0.8345$. From Eq. (15) it follows that $H_{\min} = H_0 - \sqrt{2}(\kappa-H_0)/(2\kappa^2-1)$, which checks with Abrikosov's expression[2] for $H_{\min}$.

We now estimate the current J_{s1} from Eqs. (2a), (8), (10), and (11) [area of the "triangle" in Fig. 1(b)]:

$$\frac{4\pi}{c}J_{s1} = -\frac{1}{\mu}\int_0^{\zeta_c} d\zeta(a-\Gamma+\zeta)F^2 \approx \frac{\mu}{2}F^2(0)[1-\tfrac{1}{2}F^2(0)]. \quad (16)$$

On the right-hand side of Eq. (16) we have neglected $a(\zeta_c)$ with respect to $\Gamma[\zeta_c = \Gamma - a(\zeta_c)]$. This is justified[4] to the first approximation for $n > 1$.

The surface currents J_{s1} and J_{s2} are independent of κ and a direct consequence of the Ginzburg-Landau boundary condition. They depend only on the magnitude of the order parameter at the surface of the material. The ratio of the vortex current J_{v1} to the sheath current J_{s1} is

$$\left|\frac{J_{v1}}{J_{s1}}\right| = \frac{2\sqrt{2}\alpha(\kappa-H_0)}{\mu\beta(2\kappa^2-1)F^2(0)[1-\frac{1}{2}F^2(0)]}. \quad (17)$$

For $\kappa > 1$, $|J_{v1}/J_{s1}| \ll 1$ provided $(\kappa-H_0)/\kappa \ll 1$, and for $\kappa \gg 1$, $|J_{v1}/J_{s1}| \to 0$ as $(\kappa-H_0)/\kappa^2$, which shows that the surface currents J_{s1} and J_{s2} are always much larger than the surface current ΔJ_{s2} and the vortex currents J_{v1} and J_{v2}. In Fig. 1(b), the area between the ζ axis and the current density j_y, which corresponds to the currents J_{s1} and J_{s2}, is much larger than the areas which correspond to the currents ΔJ_{s2} and J_{v1}. The area ΔJ_{s2} is equal to the area J_{v1} and it is subtracted from J_{s2}.

Let us now estimate the minimum internal magnetic field near the surface. The internal magnetic field is

$$H = H_0 + H_1(\zeta) = H_0(1 + da/d\zeta), \quad (18)$$

where $H_0 da/d\zeta$ is the deviation of the internal field near the surface from the external field. The minimum field occurs at $\zeta = \zeta_0$. To the first approximation,[4] $a(\zeta_c) \ll \zeta_c$, and therefore $\Gamma \approx \zeta_c$. Hence it follows from Eqs. (2a), (10), and (16) that

$$\left(\frac{da}{d\zeta}\right)_{\min} = \int_0^{\zeta_c}\frac{d^2a}{d\zeta^2}d\zeta = -\frac{4\pi}{c}\frac{\mu}{n}\int_0^{\zeta_c} j(\zeta)d\zeta \approx -\frac{\mu^2}{2n}F^2(0)[1-\tfrac{1}{2}F^2(0)]. \quad (19)$$

For $\mu \sim 1$, $F^2(0) \sim \frac{1}{2}$, and $\kappa \sim 1$, $(H_1/H_0)_{\min} \sim -0.2$; and for $\mu \sim 1$ and $\kappa \sim 3$, $(H_1/H_0)_{\min} \sim 0.02$. $|(H_1/H_0)|_{\min}$ is appreciably smaller for κ values larger than 3. From Eq. (19) and Abrikosov's theory,[2] we are able to estimate the approximate ratio of maximum deviation of the internal magnetic field from the applied field in the bulk of the material and near the surface. We obtain

$$\frac{|H_{1B}|_{\max}}{|H_{1S}|_{\max}} \approx \frac{\sqrt{2}}{\mu^2F^2(0)[1-\frac{1}{2}F^2(0)]}\left(\frac{2\kappa^2}{2\kappa^2-1}\right)\left(\frac{\kappa-H_0}{\kappa}\right). \quad (20)$$

From Eq. (20), it follows that the smallest magnetic field near the surface is smaller than the smallest magnetic field in the bulk of the material, provided the applied field is just below the upper critical field such that the condition $(\kappa-H_0)/\kappa \ll 1$ is satisfied and κ^2 is not too close to $\frac{1}{2}$. The internal magnetic field is shown schematically in Fig. 1(c) for $(\kappa-H_0)/\kappa \ll 1$. In Fig. 1(d), the order parameter corresponding to section ②-② in Fig. 1(a) is shown schematically for completeness' sake.

Near H_{c2} and between H_{c2} and H_{c3}, the currents of the surface sheath for large-κ materials are not effective to make the internal field appreciably different from that of the applied field. For a long solid cylinder of macroscopic dimensions parallel with its symmetry axis to the applied magnetic field, two surface currents of equal magnitude flow around the cylinder in opposite directions. The flux is effectively uniformly distributed across the sample for $H_{c2} \leq H_0 \leq H_{c3}$. The inside of the cylinder is in the normal state and has a finite resistance and the surface sheath is multiply connected and has zero resistance. Such a sample will therefore behave like a perfectly conducting tube ($R = 0, B = H_0$). The flux and the magnetization will change irreversibly when the applied magnetic field is changed.

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SURFACE THERMAL DIFFUSE SCATTERING FROM TUNGSTEN*

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We have observed an anisotropic diffuse background superimposed on the expected low-energy electron diffraction pattern from the clean (110) surface of a tungsten single crystal, using a Varian system, with 230- to 700-eV electrons over the temperature range from 300 to 1600°K. No such structured background appears in the x-ray diffraction patterns from tungsten.[1]

We attribute this anisotropic background to thermal diffuse scattering from a region near the surface of the tungsten crystal.

It has been found by Wallis and others[2-6] that the introduction of a surface to an infinite elastic continuum and to a one-dimensional chain crystal introduces surface normal modes in addition to the bulk modes. The solution for a three-dimensional crystal with surface does not exist. These modes must be considered in the interpretation of the diffraction pattern because the low penetration of low-energy electrons requires the major part of the scattering to take place near the surface, where these modes are important. Surface modes are described by amplitudes (u_{nqj}) which decay exponentially with increasing distance from the surface into the crystal.

It is assumed that the deviation of the ionic position from equilibrium ($\vec{u}_n$) can be described by a superposition of the normal modes of vibration of the crystal[7-10]:

$$\vec{u}_n = \sum_{qj} u_{nqj} \vec{e}_{qj} \exp(i\omega_{qj} t + 2\pi i \vec{q}\cdot\vec{r}_n),$$

where $\vec{e}_{qj}$ is the polarization vector of the phonon of wave vector $\vec{q}$ and polarization j; ω_{qj} is the angular frequency of the phonon; and $\vec{r}_n$ is the vector position of the nth atom in the undisplaced crystal.

As a first approximation, the exponential decay of the surface mode amplitudes will be neglected, and we will use instead a model in which the amplitude is represented by a step function. The scattered intensity from the vibrating crystal is then due to the entire phonon spectrum, including the surface modes. We assume that the electron scattering takes place in this region where the surface modes have nonzero amplitude, which we define as the surface layer.

The intensity function can therefore be written as[10,8]

$$I(\vec{S}/\lambda) = |f_0|^2 e^{-2M} \sum_N I_N$$

$$= |f_0|^2 e^{-2M} (I_0 + I_1 + \cdots I_N),$$

where

$$I_0(\vec{S}/\lambda) = \sum_{nn'} \alpha_n \alpha_{n'} \exp[2\pi i (\vec{S}/\lambda)\cdot(\vec{r}_n - \vec{r}_{n'})]$$

is the Bragg scattering function of the undisplaced lattice,

$$I_1(\vec{S}/\lambda) = \tfrac{1}{2} \sum_{qj} G_{qj} [I_0(\vec{S}/\lambda + \vec{q}) + I_0(\vec{S}/\lambda - \vec{q})]$$

is the thermal diffuse scattering intensity function due to single-phonon processes, and $I_N(\vec{S}/\lambda)$ is the Nth-order phonon-process intensity function.

$$G_{qj} = [\hbar/(2mn)][(k\vec{S}\cdot\vec{e}_{qj})^2/\omega_{qj}] \coth(\hbar\omega_{qj}/2kT)$$

is the amplitude of the intensity I_1 of the scattering due to the single phonon qj, and $\vec{S}/\lambda = \vec{k} - \vec{k}'$ is the scattering vector of the electron (see Fig. 1). Here α_n is an attenuation factor describing the decrease in scattering as the electron beam penetrates the crystal.[11] $\exp(-2M)$ is the Debye-Waller factor.

Since I_0 has appreciable values only when its argument is a vector in the reciprocal lattice, we see that the value of I_1 at $\vec{S}/\lambda$ is due to the contribution of the single phonon q which satis-