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# Berry's phase and acoustic modes in the presence of an edge dislocation

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Abstract. Acoustic phonon modes in the presence of an edge dislocation in a simple cubic lattice are computed by means of the covering space technique. Berry's phase and the associated topological interaction for the phonon propagating on this background give rise to a rather unconventional normal mode consisting of the standing wave (if any) and a necessary vibrating tail located on a glide plane  $\mathscr{G}$  of the defect.

### 1. Introduction

The aim of this paper is two-fold.

Firstly we show that a non-trivial topological background in the form of a linear defect contributes to the phonon defect interaction which is additional to the conventional one (Lifshits and Kosevitch 1966, Maradudin 1970, Ninomiya 1970). We call it 'topological' as the topological or Berry's phase (Berry 1984) is responsible for the effect. Thus, we enlarge the family of problems where topology effects the behaviour of elementary excitations (see Avron *et al* 1988).

The other aim of this article is to demonstrate the covering space technique which is particularly useful when solving this type of problem. The typical structure involved is what may be called a singular  $\mathfrak{S}$ -bundle  $\mathcal{N} \xrightarrow{P} \mathfrak{B}$  over the two-dimensional base  $\mathfrak{B}$ isomorphic to a plane  $\mathbb{R}^2$  with r points removed:  $\mathfrak{B} \approx \mathbb{R}^2 \setminus \bigcup_i \mathfrak{P}_i$  (i=1,2...r). The bundle curvature is the distribution located at points  $\mathfrak{P}_i$ . It manifests itself in the external part of the space due to the non-trivial holonomy group  $\mathfrak{G}$ . For evident reasons we call this space an r-polycone and denote it by  $\mathscr{C}(\mathfrak{S}, r)$ . The particular type of such spaces with cone-like singularities were discussed in Scott (1983) as orbifolds. A complete three-dimensional space  $\mathcal{M}$  may be obtained as the product  $\mathcal{M} \approx \mathbb{R}^1 \times \mathfrak{B}$ . Then the points  $\mathfrak{P}_i$  transform into parallel straight lines, called flux tubes for  $\mathfrak{S} = U(1)$ and line defects for some other groups. When r=1 we use the simplified notation  $\mathscr{C}(\mathfrak{S})$  for the cone. The parallel transport of the field  $\Psi$  along the closed path encircling the defect induces the discrete holonomy group transformation

$$\hat{h}\Psi = \exp\left(i\oint \omega^{(i)}\hat{\tau}_i\right)\Psi \qquad \hat{h}\in\mathfrak{H}, i=1,2,3.$$
(1)

Here  $\omega^{(i)}$  are the closed connection one-forms and  $\hat{\tau}_i$  are generators of the relevant representation. As is well known, a non-trivial holonomy group may lead to the diffraction of the  $\Psi$ -wave by the defect.

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The idea is to continue the initial equation from the space  $\mathcal{V} \approx \mathbb{R}^1 \times \mathscr{C}(\mathfrak{S}, r)$  onto the covering space  $\tilde{\mathcal{V}} \xrightarrow{P} \mathcal{V}$  which has the monodromy group  $\mathfrak{M}$  isomorphic to a holonomy group  $\mathfrak{H}$  of  $\mathcal{M}$ . As is well known from Riemann, this is achieved by taking points of  $\tilde{\mathcal{V}}$  to be pair: point of  $\mathcal{V}$  and the holonomy transformations corresponding to closed paths starting at this point. Thus, encircling the cone apex on  $\mathcal{V}$  one transfers to another sheet of the branched Riemann surface  $\tilde{\mathcal{V}}$ . On  $\tilde{\mathcal{V}}$  the topological interaction (T1) term in the phonon wave equation may be gauged by means of the unitary transformation

$$\tilde{\Psi} \mapsto \exp\left(-\mathrm{i}\int^{x}\omega^{(i)}\hat{\tau}_{i}\right)\tilde{\Psi}.$$

Of course, it may turn out that to compute modes  $\tilde{\Psi}$  on  $\tilde{\mathcal{V}}$  is not more simpler than those for  $\mathcal{V}$ . Indeed, problems are just shifted from one place to another for the holonomy of  $\mathcal{V}$  is recoded into the monodromy of  $\tilde{\mathcal{V}}$ . The point is that groups  $\mathfrak{H}$  which have different geometrical origin may be isomorphic to the same substitution group  $\mathfrak{M}$  of  $\tilde{\mathcal{V}}$ . So the covering space technique allows one to analyse various problems in an elegant and systematic way. Having the solution  $\tilde{\Psi}$  on  $\tilde{\mathcal{V}}$  we obtain the solution  $\Psi$ on  $\mathcal{V}$  as the automorphic projection

$$\Psi(\mathbf{x}) = \sum_{i} \hat{m}_{i} \tilde{\Psi}(\mathbf{y}) \qquad \hat{m}_{i} \in \mathfrak{M} \approx \mathfrak{H} \qquad \mathbf{x} \in \mathscr{V} \qquad \mathbf{y} \in \tilde{\mathscr{V}}.$$
(2)

All this is quite familiar to mathematicians. The study of various applications was undertaken by Dowker and collaborators (Banach and Dowker 1979, Dowker 1990, and references therein; see also Hart 1983).

There are a number of cone-like structures pertinent to physics. The 'textbook' example is the  $\mathscr{C}(U(1))$  cone in the celebrated Aharonov-Bohm effect (for a review see Olariu and Popescu 1985). Later,  $R^1 \times \mathscr{C}(SO(2))$  appeared as the model for geometry of the external part of the space around the cosmic string (Israel 1977, Vilenkin 1985). In condensed matter physics the  $\mathscr{C}(\mathfrak{S})$  cone ( $\mathfrak{S}$  is the subgroup of the semisimple product  $SO(3) \triangleright T(3)$ ) describes the geometrical structure of the deformed elastic continuum in the presence of a linear defect (Bilby *et al* 1955, Kadič and Edelen, 1983).

During the last decade a great deal of attention was paid to the study of the problem with elementary excitations propagating on a topologically non-trivial background, including that of a cone. The existence of the TI between the free electrons propagating through the crystal and the screw dislocation was recognized quite a long time ago (see references in Bird and Preston (1988)). Its importance for the correct description of metal conductivity was conjectured by Kawamura. He computed the scattering amplitude by the screw dislocation for the conductivity electrons both in a continuum (Kawamura 1978a) and on a lattice (Kawamura 1978b). The diffraction pattern for the free electrons scattered by the screw dislocation in graphite was obtained recently (Bird and Preston 1988). This also gives indirect support for Kawamura's conjecture.

It is evident that if electrons moving in  $\mathbb{R}^3$  feel the non-trivial geometry of the dislocated lattice ( $\approx \mathcal{V}$ ) then one has to account for this when describing phonons moving just in  $\mathcal{V}$ . The physical consequences of this fact were discussed by the present author (Serebrjany 1990). In that article the spectral density of the energy loss due to the sound radiation by the homogeneously moving source in the presence of the screw dislocation or disclination was computed. The wave equation for this background may be solved directly due to the high symmetry of the problem. This is not the case for the edge dislocation where the holonomy transformation is the translation normal to a defect line. The corresponding Schrödinger equation for the electrons was characterized in Kawamura (1978a) as 'intractable'. However, it is tractable by means of the

covering space technique mentioned above. Now we show how all this works for the dislocation.

#### 2. Phonon modes: general formulae

We solve the equation

$$-\omega^2 u = V_{\rm T}^2 [\nabla \nabla u + \nabla \nabla u] + (V_{\rm L}^2 - 2V_{\rm T}^2) \nabla \nabla u$$
(3)

for the continuous version of the simple cubic lattice. Here linked vectors are contracted,  $V_{\rm T}$  and  $V_{\rm L}$  are transverse and longitudinal sound velocities correspondingly, u(x) is the phonon field. Components of the gradient operator  $\nabla$  are duals of the form  $\omega^{(i)}$ , which in local Cartesian coordinates  $x^{j}$  may be written as follows:

$$\omega^{(i)} = (\delta_j^i + \partial u_{st}^i / \partial x^j) \, \mathrm{d} x^j \qquad (i, j = 1, 2, 3).$$
(4)

They are induced by the static displacement field

$$\boldsymbol{u}_{st}(\boldsymbol{x}) = \boldsymbol{b}\boldsymbol{\phi}/2\pi + \delta\boldsymbol{u}_{st}(\boldsymbol{x}). \tag{5}$$

Thus equation (3) is obtained from the 'flat' one by the coordinate transformation

$$x \mapsto x + u_{\rm st}(x). \tag{6}$$

The angle  $\phi$  in equation (5) changes by  $2\pi$  when one traces the closed contour encircling the defect. The second term is zero for the screw dislocation, and for the edge dislocation placed along the z-axis of the cylindrical coordinate frame  $(z, \rho, \phi)$  it reads (Landau and Lifshitz 1988)

$$\delta \boldsymbol{u}_{st}(\boldsymbol{x}) = \delta \boldsymbol{u}^{(x)} \boldsymbol{e}_{\boldsymbol{x}} + \delta \boldsymbol{u}^{(y)} \boldsymbol{e}_{\boldsymbol{y}}$$

$$\delta \boldsymbol{u}^{(x)} = \frac{b}{4\pi(1-\sigma)} \sin \phi \cos \phi \qquad (7)$$

$$\delta \boldsymbol{u}^{(y)} = -\frac{b}{4\pi(1-\sigma)} [(1-2\sigma) \ln \rho + \cos^2 \phi].$$

The Burgers vector  $\mathbf{b} = b\mathbf{e}_x$  is supposed to be directed along the x-axis. The first term in equation (5) is universal in that it is independent (in contrast to the second one) on the particular elastic properties of the media. (Poisson ratio  $\sigma$ ). This term is responsible for the TI in question. Indeed, the shift  $\phi \mapsto \phi + 2\pi$  results in the translation

$$u_{\rm st} \mapsto u_{\rm st} + b. \tag{8}$$

This leads to the holonomy representation transformation (discrete subgroup of T(1)) for any physical field  $\Psi$  on such a background. Thus the map (6) from the homogeneous to a dislocated state has to be viewed as the map from  $R^2$  to the  $\mathscr{C}(T(1))$  cone and so it carries the standard 'flat' acoustic wave equation to  $R^1 \times \mathscr{C}(T(1))$ . In its turn this means that the solution to equation (3) could not be obtained merely by the coordinate transformation of the 'flat' solution. The obstacle is the curvature of the T(3) bundle located on the defect line.

From equations (4), (5) and (7) it is clear that the wave operator in equation (3) may be naturally continued as *periodic* onto the  $\mathcal{V} = R^1 \times \mathfrak{U}$  where  $\mathfrak{U}$  is the branched Riemannian surface of the complex logarithm with monodromy isomorphic to the additive group of pure numbers:  $\mathfrak{M} \approx \mathbb{Z}$ . On  $\tilde{\mathcal{V}}$  there is no periodicity condition on

solutions to equation (3). Now if  $\tilde{\chi}(x)$  is the solution on  $\tilde{\mathcal{V}}$  and one places the defect along the branch line it is possible to obtain the solution  $\tilde{\Psi}(x)$  for the dislocated space by the coordinate transformation

$$\tilde{\Psi}(\mathbf{x}) = \tilde{\chi}(\mathbf{x} + \mathbf{u}_{st}(\mathbf{x})). \tag{9}$$

Following Serebrjany (1991) we separate variables on  $\tilde{\mathcal{V}}$  (before transformation (9) is fulfilled) on the complex basis  $e_{\pm} = e_{\rho} \pm i e_{\phi}$ . All the components of the vector modes have the same dependence on the  $\phi$ - and z-coordinates which we take in the form exp i( $\mu\phi + kz + \mu/2$ ). The orbital momentum  $\mu$  is arbitrary real, and the constant phase shift is chosen for convenience. The radial mode we present in a matrix form:

$$\boldsymbol{u}_{\mu}(\boldsymbol{\rho}) = \mathfrak{Z}_{\mu}(\boldsymbol{\rho}) \cdot \boldsymbol{A} \tag{10}$$

where A is the constant vector amplitude and

$$\mathfrak{Z}_{\mu}(\rho) = \begin{vmatrix} (P_{\mathrm{L}}V_{\mathrm{L}}/2i\omega)J_{\mu-1}(L) & (1/2)J_{\mu-1}(T) & (kV_{\mathrm{T}}/2i\omega)J_{\mu-1}(T) \\ (iP_{\mathrm{L}}V_{\mathrm{L}}/2\omega)J_{\mu+1}(L) & (1/2)J_{\mu+1}(T) & (ikV_{\mathrm{T}}/2\omega)J_{\mu+1}(T) \\ (kV_{\mathrm{L}}/\omega)J_{\mu}(L) & 0 & (-P_{\mathrm{T}}V_{\mathrm{T}}/\omega)J_{\mu}(T) \end{vmatrix}$$
(11)

for  $\mu > 0$ . For negative  $\mu$  one has to reverse the sign of all the indices in the Bessel functions  $J_{\sigma}(x)$ . Arguments L and T denote  $\rho P_{\rm L}$  and  $\rho P_{\rm T}$  correspondingly. The following dispersion relations are fulfilled:

$$P_{\rm L}^2 + k^2 = \omega^2 / V_{\rm L}^2 \qquad P_{\rm T}^2 + k^2 = \omega^2 / V_{\rm T}^2. \tag{12}$$

The first column in equation (11) is the longitudinal wave and other two are the transverse ones. The polarization space  $\mathfrak{P}$  is the linear shell of vectors

$$e_{\rm L} = e_{\rm p} = p/|p| \qquad e_{\rm T1} = [e_p \times e_z]/\sin \theta \qquad e_{\rm T2} = [e_p \times [e_p \times e_z]]/\sin \theta \cos \theta = e_p e_z \qquad e_{\rm L} = [e_{\rm T1} \times e_{\rm T2}].$$
(13)

Now we briefly discuss the boundary condition on the defect line  $\rho = 0$ . Normally when dealing with the string model of a defect a physically natural regularity condition is imposed. In Serebrjany (1991) it was shown that generally this is not possible. For the screw dislocation there are at least two singular phonon vector modes (i.e. modes possessing if only one singular component) with quantized orbital momentum. These modes give an important contribution to the scattering matrix leading to polarization transmutations for the phonon scattered by the defect. Referring to that paper for details we note that in order not to destroy the longitudinal or transverse nature of the solution one is forced to keep in the present problem the whole family of singular modes. All of them are parametrized by the orbital momentum  $\mu$  taking on values such that  $|\mu| < 1$ .

As is evident from equation (11) the building block for the free modes on  $\tilde{\mathcal{V}}$  is

$$\tilde{\Xi}_{\mu}(\rho, \phi) = \exp(i\mu\phi)J_{\mu+s}(\rho P)$$

$$s = 0 \pm 1 \qquad \mu > 0 \qquad P = P_{\rm L} \text{ or } P_{\rm T}.$$
(14)

To perform the map (9) we have to use the local Cartesian coordinates (x, y) which cover just one leaf of  $\tilde{\mathcal{V}}$ . We then use

$$\exp i(\mu\phi + \pi\mu) = \exp[i\pi\mu \operatorname{sgn}(y)] \left(\frac{x + i|y|}{x - i|y|}\right)^{\mu/2} \qquad 0 < \tan^{-1}(|y|/x) < \pi.$$
(15)

This formula allows one to perform computations for positive y. The corresponding result for y < 0 may be obtained by the phase shift in accordance with equation (15). Applying equation (9) to equation (14) one has to transform appropriately each vector mode. The new reference frame  $\partial_{x'}$  and the old one  $\partial_x$  are related by the position-dependent matrix  $\partial x/\partial x'$  which is single valued just in  $\tilde{\mathcal{V}}/\mathfrak{M}$  due to the linearity of x' in  $\phi$ . So the essential information is stored in the scalar-transformed expression (14). It reads for y > 0

$$\tilde{\Xi}_{\mu}(\xi,\eta) = \left(\frac{\xi + i\eta}{\xi - i\eta}\right)^{\mu/2} J_{\mu+s}[P(\xi^2 + \eta^2)^{1/2}]$$

$$\xi = x + b\phi/2\pi + \delta u^{(x)}(x,y) \qquad \eta = y + \delta u^{(y)}(x,y) > 0.$$
(16)

Encircling the defect line anticlockwise we find that equation (16) acquires the phase multiple  $\exp(2\pi i\mu)$  and the argument  $\xi$  will be shifted by the Burgers vector b. This new function also gives a solution to the wave equation (3) on  $\tilde{\mathcal{V}}$  for the wave operator was continued on  $\tilde{\mathcal{V}}$  periodically. It follows that one may build up a new solution  $\Xi(\xi, \eta)$  periodic on the quotient space  $\tilde{\mathcal{V}}/\mathfrak{M}$ :

$$\Xi_{\mu}(\xi,\eta) = \sum_{n} \exp(2\pi i \mu n) \tilde{\Xi}_{\mu}(\xi + bn,\eta).$$
<sup>(17)</sup>

This is the automorphic projection from equation (2). Using the Poisson summation formula we arrive at the final expression

$$\Xi_{\mu}(\xi,\eta) = \frac{1}{Pb} \sum_{n} \exp[-2\pi i(n+\mu)\xi/b] I_{s}[2\pi(\mu+n)/bP,\mu,\eta P]$$
(18)

where

$$I_{s}(\alpha, \mu, u) = \int_{-\infty}^{\infty} dt \exp(i\alpha t) \left(\frac{t + iu}{t - iu}\right)^{\mu/2} J_{\mu+s}[(t^{2} + u^{2})^{1/2}].$$
 (19)

#### 3. Explicit results and discussion

The integral (19) is the key quantity we have to compute. Its most important property is the threshold behaviour in the parameter  $\alpha$ . The asymptotic expression when  $|u| \mapsto \infty$  depends crucially on whether  $\alpha$  exceeds 1 or not. The asymptotic form of expression (19) when  $u \mapsto \infty$  is as follows:

$$-\frac{1}{2}\exp(-i\pi\mu/2)I_{s}(\alpha,\mu,u)$$

$$=\sin \pi(\mu+s/2)\exp(-\mu\theta-u\sinh\theta)/\sinh\theta$$

$$(for \alpha < -1: |\alpha| \equiv \cosh\theta, 0 < \theta < \infty)$$

$$=\sin(\pi s/2)\exp(\mu\theta-u\sinh\theta)/\sinh\theta$$

$$(for \alpha > 1: \alpha \equiv \cosh\theta, 0 < \theta < \infty)$$

$$= -\cos(u\sin\theta-\mu\theta-\pi s/2)/\sin\theta$$

$$(20b)$$

So that for  $\alpha > 1$  the asymptotic falls off exponentially, otherwise it shows oscillating behaviour. Accounting for the explicit form  $\alpha = 2\pi (n + \mu)/Pb$  where (for the acoustic

phonons)  $Pb \ll 1$  one finds that in the sum (18) the oscillating contributions survive if  $-\mu$  lies near some pure number  $n: n - \varepsilon < -\mu < n + \varepsilon$ ,  $\varepsilon \leq Pb \ll 1$ . So just one term in equation (17) may be oscillating when  $\mu$  is 'almost' quantized. The oscillating term (if any) is accompanied by the vibrating one located on the glide plane  $\mathscr{G}$  stretched on a pair  $(e_z, b)$ . The vibrating tail is represented by the infinite sum with terms decreasing exponentially both as functions of variable u and number n.

It is interesting to note that for s=0 the formulae above are *exact*. This can be shown by means of the Lambe generalization of the Shläfli integral representation for the Bessel functions (Bateman and Erdelyi 1953). The expression (20a) is evidently the vibration contribution mentioned above and (20b) gives rise to the standing wave. From equation (18) one may infer that it is composed of two plane waves propagating in the x-y plane and crossing the glide plane  $\mathscr{G}(y=0)$  at the angle  $\pm \cos^{-1} \alpha$  in the Burgers vector direction. In accordance with equation (15) both waves undergo the phaseshift  $\exp(2\pi i\mu)$  when crossing  $\mathscr{G}$ . They also have the relative phaseshift  $\exp(2i\mu \cos^{-1} \alpha)$ .

One may also be interested in the exact value of the integral (19) for arbitrary s. Using formulae from Prudnikov et al (1983) it is possible to express it through the Whittaker functions  $W_{\alpha,\beta}(z)$  and  $M_{\alpha,\beta}(z)$ . The vibrational component when  $|\alpha| > 1$ reads (for u > 0)

$$-\frac{1}{2}\exp(-i\mu\pi/2)I_{s}(\alpha,\mu,u) = \sin(\pi s/2)\Gamma\begin{bmatrix} s/2\\ \mu+s \end{bmatrix} u\left(\frac{d}{du} - \frac{\mu+s-1}{u}\right)u^{-1}$$

$$\times W_{\mu/2,(\mu+s-1)/2}(u_{+})M_{\mu/2,(\mu+s-1)/2}(u_{-}) \qquad \alpha > 1$$

$$= \sin[\pi(2\mu+s)/2]\Gamma\begin{bmatrix} (2\mu+s)/2\\ \mu+s \end{bmatrix} u\left(\frac{d}{du} - \frac{\mu+s-1}{u}\right)u^{-1}$$

$$\times W_{-\mu/2,(\mu+s-1)/2}(u_{+})M_{-\mu/2,(\mu+s-1)/2}(u_{-}) \qquad \alpha < -1$$

$$u_{\pm} \equiv u[\alpha \pm (\alpha^{2}-1)^{1/2}] \qquad \Gamma\begin{bmatrix} x\\ y \end{bmatrix} = \Gamma(x)/\Gamma(y).$$

One has to substitute equation (21) into equation (18) to obtain the quantity  $\Xi_{\mu}(\xi, \eta)$ . In contrast to vibrating modes encountered in Lifshits and Kosevitch (1966), Maradudin (1970) and Ninomiya (1970) which are located both in the lattice near the defect line and in the momentum space these new vibrating modes are located near the plane  $\mathscr{G}$  and their spectrum fits the Brillouin zone well (see equation (11)).

The  $\mu$  dependence of the physical modes is quite complicated and has nothing to do with the orbital momentum. For single-valued derivatives of the map (6) it follows that  $\mu$  is an eigenvalue of the image of the momentum operator  $(-i\partial/\partial\phi)$  on  $\tilde{\mathcal{V}}$  under map (6). Being the superposition of rotations and dilatations on  $\mathcal{B}$  the momentum operator has position-dependent coefficients which are not possible to express even in elementary functions. So in the base of the bundle  $\mathscr{C}(T(1))\mu$  is also the integral of motion; however, its geometrical meaning in terms of  $\mathcal{B}$  is not transparent.

In Serebrjany (1990) we speculated (using the Born approximation) that the edge dislocation may produce more effective sound scattering in contrast to a screw one. The present result shows that there is no scattering at all in this case. Indeed, due to a threshold behaviour of equation (19) the scattering problem for the phonon mode is effectively one dimensional (along the y-axis). Each plane wave in equation (18) does not diminish its amplitude, but just acquiring the phaseshift when crossing the

line y = 0. In contrast to the two-dimensional case such a phase multiple for a partial wave does not lead to scattering.

From the considerations above it is clear that our modes show all the features pertinent to waves propagating in a periodic potential. The background periodic structure is the system of glide planes introduced on the covering apace  $\mathfrak{L}$  by the map (9) and periodicity entered the wavefunctions through the automorphic projection (17). One has the band structure for  $\mu$ : the 'allowed' values when a phonon propagates freely are thin strips centred on pure numbers. For all other 'forbidden' values of  $\mu$  phonons turns out to be located on  $\mathscr{G}$ . Modes are not scattered by the glide plane and acquire only a phaseshift when crossing it in accordance to a Bloch theorem. A priori one may expect that interference effects like this are negligible for elementary excitations in condensed media. Our calculations show that the effect may be well strong.

Summarizing one may say that the  $\tau_1$  gives rise to quite complex modes exhibiting rather unconventional behaviour both as functions of momenta and space variables. As is evident the above analysis may be applied to the Schrödinger equation for electrons in the tight binding model (à la Kawamura) showing that there will be no scattering, in contrast to a screw dislocation. However, the edge dislocation exerts an electric field upon an orbiting charged particle. So the  $\tau_1$  effect (or its absence) will be spoiled. Still, one may hope to observe anisotropy in the metal conductivity along and across the glide planes in a sample containing parallel dislocation lines.

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