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Gauge theory of sound propagation in crystals with dislocations

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Abstract
Within the framework of gauge field theory a general scheme for describing sound propagation in harmonic crystals with dislocations is worked out. As an application the theory confirms the appearance of local elastic vibrations in the strain field of edge dislocations and their absence in the case of screw dislocations. When the theory is applied to the scattering of sound waves on a screw dislocation, one recovers the appearance of Aharonov–Bohm interferences.

Elastic distortion fields, generated in harmonic crystals by frozen-in topological defects, can, in the continuum limit, be described by two different gauge theories. Both will be discussed here in a form exclusively designed to address the presence of dislocations.

The first version, proposed by one of us [1], relies on the Euclidean symmetry of the elastic energy density in the undistorted reference state. Accordingly, the gauge group consists of linear transformations of the Lagrange coordinates, representing the positions of material points in the reference state, at constant Euler coordinates which represent the displaced positions in the strained material.

In contrast, the second approach, presented by Kadic and Edelen [2], uses a gauge group consisting of linear transformations of the Euler coordinates at fixed values of the Lagrange coordinates. Accordingly, this type of gauge transformation operates as in the case of an internal symmetry. An apparent rationale of the procedure [2] is that, independently of the symmetry of the material parameters, the strain tensor of the reference system is already invariant under such transformations.

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The merit of the approach [1] is that it incorporates some important nonlinear couplings between dislocation-induced and externally generated distortions, including those due to sound waves with independently tunable amplitudes. Only if both kinds of distortion fields are treated as perturbations of equal magnitude does one recover in linear order the results of [2].

This observation applies to practically all subsequent papers, devoted to the description of topological defects using gauge fields, and, to our belief, represents an unnecessary limitation of the theories. Out of the large number of publications of that type we pick out the work by Osipov, since it also includes a discussion of vibrational states in topologically distorted media [3]. By comparing his results with ours for the case of a single screw dislocation, one can see what kinds of effects may be overlooked in such treatments.

We also mention a more recent paper by Lazar [4] which relies on the gauge theory of gravity, as formulated by Hehl *et al* [5]. Since this formulation uses the picture of an internal gauge symmetry, the Lazar procedure is, in this respect, also along the lines of the Kadic–Edelen approach.

In contrast to that, the theory of [1] follows the lines of the gauge theory of gravity given by Kibble [6] which starts from the group of external Poincaré transformations. In the context of dislocation theory the compensating field in [6] turns out to correspond directly to the distortion tensor in the differential-geometric approach to dislocation theory given by Kröner [7]. Due to this, we need not discuss the free part of the compensating field in the Lagrangian, but instead can adopt the results for the distortion tensor, following [7] for special defect configurations.

In order to describe the procedure in detail, we start from the expression for the elastic energy density of the reference system,

$$e(x) = \tfrac{1}{2}\,\epsilon_{ij}(x)\,c^{ijk\ell}\,\epsilon_{k\ell}(x), \tag{1}$$

where, in a Cartesian frame,

$$c^{ijk\ell} = \lambda\,\delta^{ij}\delta^{k\ell} + \mu\,(\delta^{ik}\delta^{j\ell} + \delta^{i\ell}\delta^{jk}) \tag{2}$$

are the elastic constants of an isotropic medium with Lamé coefficients λ, μ, and where, in terms of Lagrange and Euler coordinates x^i, and X^A,

$$\epsilon_{ij}(x) \equiv \tfrac{1}{2}\left\{\left[\partial_i X^A(x)\right]\delta_{AB}\left[\partial_j X^B(x)\right] - \delta_{ij}\right\} \tag{3}$$

defines the strain tensor. The components of the Euler position vectors have been labelled with capitals A, B, in order to indicate that they behave as scalars under linear transformations of the Lagrange coordinates.

According to Kibble [6], the symmetry of the distorted medium under local coordinate transformations can now be achieved by replacing the partial derivatives in the expression (3) by covariant derivatives $D_\alpha \equiv B^i_\alpha(x)\,\partial_i$ where in [1] the compensating fields $B^i_\alpha(x)$ have been identified with the defect-induced distortions, appearing in Kröner's theory of dislocations [7]. Factors $1/(\det B)$, converting local quantities into proper densities, will be suppressed in the following, since they turn out to cancel in all relevant equations.

The result for the local elastic energy in the presence of the defects reads

$$E(x) = \tfrac{1}{2}\,\varepsilon_{\alpha\beta}(x)\,c^{\alpha\beta\gamma\delta}\,\varepsilon_{\gamma\delta}(x) \tag{4}$$

where $c^{\alpha\beta\gamma\delta}$ is numerically identical to $c^{ijk\ell}$, and where

$$\varepsilon_{\alpha\beta}(x) \equiv \tfrac{1}{2}\left\{\left[D_\alpha X^A(x)\right]\delta_{AB}\left[D_\beta X^B(x)\right] - \delta_{\alpha\beta}\right\}. \tag{5}$$

In order to describe sound propagation in the distorted medium, we now allow in (5) a time dependence of the Euler coordinate $X^A(x,t)$ and introduce a displacement field $u_i(x,t)$ by writing $X^A(x,t) = \delta^A_i\,x^i + \delta^{iA}\,u_i(x,t)$. Then, in terms of the frozen-in strain field,

$$E_{\alpha\beta}(x) \equiv \tfrac{1}{2}\left[B^i_\alpha(x)\,\delta_{ij}\,B^j_\beta(x) - \delta_{\alpha\beta}\right], \tag{6}$$

the total strain is given by

$$\varepsilon_{\alpha\beta}(x,t) = E_{\alpha\beta}(x) + \tfrac{1}{2}\left[B^i_\alpha(x)D_\beta + B^i_\beta(x)D_\alpha\right]u_i(x,t) + \tfrac{1}{2}\left[D_\alpha\, u_i(x,t)\right]\delta^{ij}\left[D_\beta\, u_j(x,t)\right]. \tag{7}$$

By an expansion of (7) to linear order in the quantities $\partial_j u_i$ and $\beta^i_\alpha \equiv B^i_\alpha - \delta^i_\alpha$ one recovers the strain tensor, appearing in the Kadic–Edelen approach. The neglected higher order terms, however, turn out to contribute in an essential way to the process of sound propagation.

Insertion of the full expression (7) into (4) implies $E(x,t) = U(x) + W(x,t)$ where

$$U(x) \equiv \tfrac{1}{2}\, E_{\alpha\beta}(x)\, c^{\alpha\beta\gamma\delta}\, E_{\gamma\delta}(x) \tag{8}$$

is the local energy of the dislocation-distorted background system, and, in the harmonic approximation,

$$W(x,t) \equiv \tfrac{1}{2}\left[D_\alpha\, u_i(x,t)\right] C^{\alpha i\beta j}(x)\left[D_\beta u_j(x,t)\right] \tag{9}$$

with effective elastic coefficients

$$C^{\alpha i\beta j}(x) \equiv B^i_\gamma(x)\, c^{\alpha\gamma\beta\delta}\, B^j_\delta(x) + S^{\alpha\beta}(x)\,\delta^{ij}. \tag{10}$$

Here $S^{\alpha\beta} \equiv c^{\alpha\beta\gamma\delta}E_{\gamma\delta}$ is the stress tensor due to the frozen-in defects which also enters the equilibrium condition $D_\alpha\, \partial U/\partial B^i_\alpha = D_\alpha\, S^{\alpha\beta}\delta_{ij}B^j_\beta = 0$. The latter statement has, in fact, been used in order to exclude in W linear terms in u_i.

Since $D_\alpha\, \partial W/\partial D_\alpha u_i$ measures the force exerted on a material point at x^i, the wave equation, following from (9), reads

$$\rho\,\delta^{ij}\,\partial_t^2 u_j(x,t) = D_\alpha\, C^{\alpha i\beta j}(x)\, D_\beta\, u_j(x,t) \tag{11}$$

where ρ is a constant mass parameter.

The result (11) is valid for arbitrary arrangements and kinds of dislocations in isotropic materials. Whereas the topological nature of the defects is essentially hidden in the covariant derivatives, the defect-induced changes of the elastic properties are contained in the coefficients (10). It should be noted that in practical applications the core regions of the defects in general require separate consideration [8].

As a first application we now consider the problem of localized vibrations in the strain field of a single straight edge dislocation. For this special case the distortion field is that of a two-dimensional defect in a plane, normal to the dislocation line. In a frame where this line is chosen as the x^3-axis, this means $\beta^3_\alpha = \beta^i_3 = \partial_3\beta^i_\alpha = 0$. Due to translational symmetry in the x^3-direction the sound-wave displacement field, furthermore, consists of plane waves $u_i(x,t) = v_i(x^1,x^2)\exp[\mathrm{i}(kx^3 - \omega t)]$ where k is a free wavenumber.

Next, we note that β^b_a with $a,b = 1,2$ is of order b/r where b is the magnitude of the Burgers vector, and $r \equiv \sqrt{(x^1)^2 + (x^2)^2}$. If localized states of lateral size $1/\kappa$ exist, then, for sufficiently large k, the ratio κ/k may, as in [8], serve as a second small parameter.

To leading order in an expansion in b/r and κ/k, equation (11) decouples into a longitudinal part and a transverse part. In terms of the related sound velocities $c_\parallel \equiv \sqrt{(\lambda+2\mu)/\rho}$, $c_\perp \equiv \sqrt{\mu/\rho}$, the corresponding wave equations read $(\omega^2 - c_\parallel^2 k^2)v_3 = 0$, and $(\omega^2 - c_\perp^2 k^2)v_a = 0$, so the components $v_3 = 1$, $v_a = 0$ form one of the eigenvectors of the system.

In order to determine corrections to this eigenvector, we evaluate the wave equation for v_a to first order. If the resulting expression $v_a = (-\mathrm{i}/k)\partial_a v_3 = \mathrm{O}(\kappa/k)\, v_3$ is inserted into the wave equation for v_3, one finds, up to second order, the closed equation

$$\left[\partial^2 + (\omega/c_\parallel)^2 - k^2 - V(\mathbf{r})\right] v_3(\mathbf{r}) = 0 \tag{12}$$

where $\mathbf{r} \equiv (x^1, x^2)$, $\partial^2 \equiv \partial_1^2 + \partial_2^2$, and, with the notation $\mathrm{Tr}\ E \equiv \delta^{ab} E_{ab}$,

$$V(\mathbf{r}) \equiv (\lambda k^2/\rho\, c_\parallel^2)\,\mathrm{Tr}\, E(\mathbf{r}). \tag{13}$$

The result (12) resembles a Schrödinger equation with an attractive potential of strength b/r in the dilatation region around the defect, analysed for a related topic by Lifshitz and Pushkarov [9]. Using the explicit form $\mathrm{Tr}\, E = (b/2\pi)[2\mu/(\lambda+2\mu)]\, x^2/[(x^1)^2+(x^2)^2]$, valid for the choice $\mathbf{b} = (b, 0, 0)$ of the Burgers vector, they found a discrete set of phonon bound states.

It should be mentioned that a second mechanism for the possible appearance of localized vibrations close to dislocation lines has been discussed [10]. This mechanism is due to changes of elastic coefficients in the core region of dislocations which, however, is beyond the scope of the present analysis.

We also point out that our derivation of the result (12) avoids using a scalar model where the tensor of bare elastic constants as well as the displacement vector are replaced by scalar quantities [8]. In particular, the ansatz $v_a = 0$, $v_3 = v$, used e.g. in [3], fails to be a consistent solution of the wave equation (11) for edge as well as for screw dislocations.

In the derivation of (12) we have effectively replaced the covariant derivatives by ordinary derivatives, since, within our perturbation scheme, the differences $D_\alpha - \partial_\alpha$ only affect higher order terms, not included in (12). This means that for localized vibrations close to an edge dislocation the topological nature of the defect is of minor importance as compared to the elastic deformations, described by the potential (13).

For screw dislocations it is essential, however, to keep the full covariant derivatives. This follows from the fact that in the case of a straight dislocation line with Burgers vector $\mathbf{b} = (0, 0, b)$, the distortion field β_i^α has as the only nonzero components $\beta_1^3(x) = -(b/4\pi)\partial_2 \ln[(x^1)^2 + (x^2)^2]$, and $\beta_2^3(x) = (b/4\pi)\partial_1 \ln[(x^1)^2 + (x^2)^2]$. Using again translational symmetry in the x^3-direction, this leads, after replacing $D_3 = \partial_3$ by ik, to the expressions

$$\begin{aligned} D_a &= \partial_a + \mathrm{i}\,\partial_a \Phi(x^1, x^2), \\ \Phi(x^1, x^2) &\equiv (kb/2\pi)\arctan(x^2/x^1). \end{aligned} \tag{14}$$

Since (14) effectively uses a Debye approximation in the x^3-direction, kb can be of order 1, in which case the two contributions in D_a have equal weight and thus should be retained for both localized and scattering states. It should also be noted that (14) looks like a standard covariant derivative in a fixed gauge.

The existence of localized vibrations in the strain field of a screw dislocation is not obvious, since this type of defect apparently does not generate a region of lattice dilatation. In order to clarify this problem within our approach, we copy the procedure used above for the case of an edge dislocation.

To lowest order in b/r and κ/k one recovers the same eigenvector $v_3 = 1$, $v_a = 0$ as before. The first-order result for v_a now reads $v_a = (-\mathrm{i}/k)D_a v_3 + [\mu/(\lambda+\mu)]\beta_a^3 u_3$ which again leads to a closed equation for v_3.

A reduction to the form of a Schrödinger equation can in this case be achieved by employing polar coordinates $x^1 = r\cos\phi$, $x^2 = r\sin\phi$. In the frame $\mathbf{e}_r = (\cos\phi, \sin\phi)$, $\mathbf{e}_\phi = (-\sin\phi, \cos\phi)$ the components of the covariant derivative read $D_r = \partial_r$, and

$$D_\phi = \frac{1}{r}\left(\partial_\phi + \mathrm{i}\frac{kb}{2\pi}\right). \tag{15}$$

Returning from $\mathrm{i}k$ to ∂_3, one observes that (15) reflects the spiral-staircase symmetry of the screw dislocation. As pointed out by Kosevich [11], this symmetry implies a separation ansatz of the form

$$v_3(r,\phi) = \chi(r)\exp\{\mathrm{i}[m - kb/(2\pi)]\phi\} \tag{16}$$

with integer m.

For the radial part we find the differential equation

$$\left[\partial_r^2 + \frac{1}{r}\,\partial_r + \left(\frac{\omega}{c_\parallel}\right)^2 - k^2 - V(r)\right]\chi(r) = 0 \tag{17}$$

where, following from the relations Tr $E = (b/2\pi r)^2$, and $D_\phi v_3 = \mathrm{i}(m/r)v_3$, the potential reads

$$V(r) \equiv \left[\frac{c_\perp^4}{(c_\parallel^2 - c_\perp^2)c_\parallel^2}\left(\frac{kb}{2\pi}\right)^2 + 2\,\frac{c_\parallel^2 + c_\perp^2}{c_\parallel^2}\left(\frac{kb}{2\pi}\right)m + m^2\right]\frac{1}{r^2}. \tag{18}$$

Since this potential is repulsive for all known materials, we conclude that in our model localized vibrational states do not exist in the strain field of a screw dislocation.

Results with the general structure (17) and (18) have previously been found by Kosevich [11] within a scalar model which includes anharmonic elastic constants. These replace the coefficients of order k^2 and k in (18), and in some range allow localized states with $m = 0$.

The last topic to be discussed is the scattering of a sound wave on a straight screw dislocation. In this case the ratio κ/k can no longer serve as a small expansion parameter. Our arguments, however, for keeping the full covariant derivatives still apply, in accordance with the fact that the defect-generated topology of space is felt at arbitrary distances from the dislocation line.

A perturbation scheme for the scattering process can now be organized by splitting the elastic coefficients (10) into those of the reference system (2) and the rest which then is considered as a perturbation. Such a procedure, incidentally mentioned by Brown [12], is different from all previous approaches which, disregarding topological aspects, simply expand around the wave equation of the bare reference system, as exemplified in [13].

Since, in our approach, topological effects are expected to emerge even in the lowest order of our expansion, the discussion will be restricted here to this case. In terms of the covariant operator $\mathbf{D} \equiv [D_1, D_2, \mathrm{i}k]$ the related wave equation for $\mathbf{v} \equiv (v_1, v_2, v_3)$ then reads

$$-\rho\,\omega^2\mathbf{v} = (\lambda + \mu)\mathbf{D}(\mathbf{D}\cdot\mathbf{v}) + \mu\,\mathrm{D}^2\mathbf{v}. \tag{19}$$

Like in the standard procedure of solving equations of the type (19), we decompose $\mathbf{v}$ via the identity

$$\mathbf{v} = \mathbf{D}\left(\mathbf{D}\cdot\mathrm{D}^{-2}\mathbf{v}\right) - \mathbf{D}\times\left(\mathbf{D}\times\mathrm{D}^{-2}\mathbf{v}\right) \equiv \mathbf{v}_\parallel + \mathbf{v}_\perp \tag{20}$$

into longitudinal and transverse components where (20) follows from the representation (14) in the form

$$\mathbf{D} = \exp(-\mathrm{i}\Phi)\,[\partial_1, \partial_2, \mathrm{i}k]\exp(\mathrm{i}\Phi). \tag{21}$$

Here, D^{-2} means the inverse of the operator D^2, and is explicitly given by an integral operator with the kernel $\exp[-\mathrm{i}\Phi(\mathbf{r})](-1/2\pi)K_0(k|\mathbf{r}-\mathbf{r}'|)\exp[\mathrm{i}\Phi(\mathbf{r}')]$, involving the modified Bessel function $K_0(kr)$.

Whereas, due to (21), all components of $\mathbf{D}$ commute with each other, commutation of $\mathbf{D}$ with D^{-2} requires partial integrations which generate surface contributions. These, however, vanish, if, following [11], the dislocation core is enclosed by a tube which is impenetrable to phonons. Using this, the decomposition (20) leads to the independent wave equations

$$-\omega^2\mathbf{v}_a = c_a^2\,\mathrm{D}^2\mathbf{v}_a, \qquad a = \ \parallel, \perp\,. \tag{22}$$

In a scattering event an incoming wave with wavevector $[-q_a, 0, k]$ has the form

$$\mathbf{v}_a^{\text{in}} = \mathbf{s}_a \exp(-\mathrm{i}\, q_a x^1) \exp[-\mathrm{i}\Phi(x^1, 0)] \tag{23}$$

where $\mathbf{s}_a$ means a polarization vector. The constraints $\mathbf{D} \times \mathbf{v}_\parallel = \mathbf{D} \cdot \mathbf{v}_\perp = 0$ imply the two possibilities $\mathbf{s}_\perp^1 \propto [k, 0, q_\perp]$ and $\mathbf{s}_\perp^2 \propto [0, 1, 0]$, and $\mathbf{s}_\parallel \propto [-q_\parallel, 0, k]$.

Since, in the present approximation, polarizations are unaffected by the scattering process, the problem gains some similarity with the famous phenomenon of electron scattering on a magnetic flux line, discussed by Aharonov and Bohm [14]. Adopting their procedure, we obtain for the scattered sound wave, far from the defect,

$$\mathbf{v}_a^{\text{sc}} = \mathbf{s}_a \frac{\mathrm{e}^{\mathrm{i}q_a r}}{(2\pi q_a r)^{1/2}} \sin(kb/2) \frac{\mathrm{e}^{\mathrm{i}\phi/2}}{\cos(\phi/2)}. \tag{24}$$

The result (24) has been derived, without any further approximation, from the wave equation (19) which has previously been established in a different way by Serebryanyi [15]. A behaviour similar to (24) has also been obtained by Kawamura for the scattering of an electron on a screw dislocation [16]. In the case of electron scattering on a magnetic flux line the wavenumber k is essentially replaced by the total magnetic flux Φ [14]. Whereas k is restricted by the Debye cut-off, Φ can be tuned over a wide range which allows one to observe the oscillatory behaviour of the scattering cross section due to the sine function in (24).

The common feature of all these seemingly unrelated physical objects is the non-trivial topology of space. As mentioned in [17] and worked out in [18] for the case of electron scattering, material deformations due to the defect may also markedly affect the scattering behaviour. The discussion of similar effects in the present case due to the effective coefficients (10) will be presented elsewhere.

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