Quantum motion of electrons in topologically distorted crystals

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Abstract. For the description of the long-wavelength quantum states of electrons in crystals with topological defects we establish a general framework on the basis of the continuum theory of defects. The resulting one-particle Schrödinger equation lives on a Riemann-Cartan manifold, representing the distorted crystal, and consists of two parts. All effects due to the topology of the defects are contained in the first part which has a covariant form and describes the purely geometric particle motion. The second part is non-covariant and derives from deformation-dependent tunneling rates of the particle which e.g. are responsible for the existence of bound states to edge dislocations.

Keywords: Topological defects; Quantum states of electrons

1 Introduction

The presence of dislocations or disclinations in a crystal destroys the symmetries of the ideal lattice and consequently leads to a breakdown of the Bloch theorem for electronic quantum states. Outside the core region of such topological defects the lattice locally looks perfect but globally is distorted at arbitrary distances from the core. One therefore expects that sufficiently dilute configurations of topological defects predominantly affect the long-wavelength quantum states of an electron.

In the deformation-potential approach \textsuperscript{[1]} the long-wavelength distortion of a lattice by topological defects essentially is treated as a perturbation of the ideal lattice. However, as pointed out by Kawamura \textsuperscript{[2]}, this is inadequate e.g. in the scattering process of electrons on a screw dislocation where, due to the global topological distortion, an incoming electron cannot be described by a simple plane wave. On the other hand the purely geometric approach by Kawamura misses such interesting effects as the appearance of bound states to edge dislocations, resulting from the deformation-potential approach \textsuperscript{[3]}.

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Both aspects of the problem are taken into account in two more recent treatments of the single-particle quantum motion in topologically distorted crystals. The first one has been worked out on a formal level [4] and is related to the gauge-field theory of topological defects [5]. The second one uses the differential-geometric language of the continuum theory of defects [6], and has been applied to the cases of edge and screw dislocations [7]. A more detailed foundation of the latter approach is given in the present paper.

Similar to previous approaches we first establish a tight-binding approximation for an electron moving on a topologically distorted lattice. The latter is mapped in the continuum limit to a Riemann-Cartan manifold where the torsion field represents the topological charge density, i.e. the density of Burgers vectors [6]. A purely geometric particle motion on the lattice can be described by constant transfer energies of the electron which in the continuum version lead to a covariant effective Hamiltonian.

As an additional ingredient we then allow the transfer energies to depend on the elastic deformations caused by the defects. In a microscopic picture the electrons spread out across the crystal essentially by tunneling which in fact is sensible to local lattice deformations. In the continuum description this effect gives rise to additional noncovariant terms in the Hamiltonian which resemble those of the deformation-potential approach.

The noncovariant terms even dominate the covariant ones in a crystal penetrated by edge dislocations. One then recovers the phenomenologically introduced model by Lifshitz and Pushkarov [3] who found an infinite number of bound states of a particle to an edge dislocation. In case of screw dislocations the covariant and noncovariant terms are of equal order. The former give rise to a kind of vector potential [2] whereas the latter essentially contribute a repulsive scalar potential, previously discussed on a phenomenological basis by Kosevich [8]. The impact of both contributions on the scattering of electrons on a screw dislocation will be discussed in a forthcoming paper [9].

2 Tight-binding model on a topologically distorted crystal

Consider an electron moving in an array of identical atomic potentials $V(x - n)$ attached to the sites $n$ of a d-dimensional topologically distorted lattice. Furthermore, assume that each potential offers a single orbit $\psi(x - m)$ to the electron, and that orbits at different sites have an overlap

$$G_{mn} = \int d^d x \psi^*(x - m) \psi(x - n).$$  \hspace{1cm} (1)

Then we can define orthonormalized wave functions

$$w_n(x) = \sum_m (G^{-1/2})_{nm} \psi(x - m)$$  \hspace{1cm} (2)

(similar to those introduced in [10]), and from the microscopic Hamiltonian project out the tight -- binding form

$$H = -\frac{1}{2} \sum_{m,n} q^\dagger(m) \left[ t(m,n) + t^*(n,m) \right] q(n)$$  \hspace{1cm} (3)
where

\[ \varphi(n) = \int d^d x \, w_n^*(x) \, \Phi(x), \]

and

\[ t(m, n) = -\frac{\hbar^2}{2M} \Delta + \int_v V(x - I) \, w_n(x). \]

Here \( \Phi(x) \) and \( \Phi^\dagger(y) \) are annihilation and creation operators, obeying the anti-commutation relations

\[ \{ \Phi(x), \Phi^\dagger(y) \} = \delta(x - y), \]

and \( M \) is the bare mass of the electron.

If the electron transfer is taken into account only between nearest-neighbour sites \( n \) and \( n + a(n) \), the transfer energies have the form

\[ t(m, n) = \sum_{a(n)} t(a(n)) \delta_{m, n + a(n)}, \]

and (3) reduces to the Hamiltonian

\[ H = -\frac{1}{2} \sum_n \sum_{a(n)} t(a(n)) (\varphi^\dagger(n + a(n)) \varphi(n) + \varphi^\dagger(n) \varphi(n + a(n))), \]

used in [7] (up to a different trivial normalization of \( \varphi \) and \( \varphi^\dagger \)).

For a simple-cubic crystal the set of the bond vectors \( a(n) \) can be written in the form

\[ \{ a(n) \} = \{ a_\alpha^+(n), a_\alpha^-(n) \}, \quad \alpha = 1 \ldots d, \]

where \( a_\alpha^- \) essentially is opposite to \( a_\alpha^+ \). The latter statement has to be made more precise, since the \( a_\alpha^\pm \) in general are not tangential to the lattice lines connecting neighbouring sites along a path of minimum potential energy. However, if \( a \) is a parameter along such a line, the derivatives

\[ \frac{d}{da} a_\alpha^\pm(n) = \pm B_\alpha(n + a_\alpha^\pm(n)) \]

are tangential to this line at the sites \( n + a_\alpha^\pm(n) \). The value \( a \), corresponding to nearest-neighbour sites, measures the lattice constant of the undistorted lattice where by definition the components of the \( B_\alpha(n) \) in some laboratory frame reduce to \( B_\alpha^0(n) = \delta_{\alpha}^\alpha \). In the distorted lattice \( B_\alpha^0(n) = B_\alpha^0 \delta_{\alpha}^\alpha(n) - \delta_{\alpha}^\sigma \) is the distortion tensor at \( n \), caused by the defects. Here a summation convention is used over repeated indices, and \( B_\alpha^0 \) means the inverse of \( B_\alpha^0 \) in the sense \( B_\alpha^0 B_\beta^0 = \delta_{\alpha}^\delta, B_\alpha^0 B_\beta^0 = \delta_{\alpha}^\beta \).

Given the set of the \( B_\alpha^0(n) \), equation (10) represents a set of differential equations which allow to eliminate the \( a(n) \) in (8) in favour of the \( B_\alpha(n) \). With regard to the continuum limit of (8) the solutions

\[ a_\alpha^\pm(n) = \pm a B_\alpha(n) + \frac{a^2}{2} \left( B_\alpha(n) \cdot \frac{\partial}{\partial n} \right) B_\alpha(n) + O(a^3) \]
of (10) are sufficient (replacing the nonsymmetric but equivalent expressions used in [7]). In $O(a^2)$ equation (11) implies the expansion

$$\varphi(n + a_\alpha^\dagger(n)) = \varphi(n) \pm a \left( B_\alpha(n) \cdot \frac{\partial}{\partial n} \right) \varphi(n) + \frac{a^2}{2} \left( B_\alpha(n) \cdot \frac{\partial}{\partial n} \right)^2 \varphi(n)$$ (12)

where, as in (11), differential operators on a lattice have provisionally been defined. For the transfer energies in (8) we assume in leading order the form

$$t(a_\alpha(n)) = \frac{\hbar^2}{2m(a_\alpha(n))^2} = \frac{\hbar^2}{2ma^2} \frac{1}{(\mathbf{B}_\alpha(n))^2} + O(1)$$ (13)

which defines the effective electron mass $m$, and ensures that the $O(a^2)$-terms in (12) lead to finite contributions in the limit $a \to 0$.

Below, the expansion in $a$ will be complimented by an additional one in $\beta^\dagger$. The lowest-order term of the resulting double expansion merely corresponds to a constant energy shift of the electron which in the following will be ignored. Furthermore, the $O(a)$-terms in (12) cancel in (8), which demonstrates that the inversion symmetry of the ideal lattice survives in the distorted lattice in this order. The remaining terms of the Hamiltonian can be converted into the contributions

$$H_c = -\frac{1}{4m} \sum_n \sum_\alpha \left\{ \left( B_\alpha(n) \cdot \frac{\partial}{\partial n} \right)^2 \varphi(n) \right\} \varphi(n) + \varphi(n) \left( B_\alpha(n) \cdot \frac{\partial}{\partial n} \right)^2 \varphi(n) \right\},$$ (14)

describing the purely geometric travel of the electron, and

$$H_d = -\frac{\hbar^2}{2ma^2} \sum_n \sum_\alpha \left( \frac{1}{\mathbf{B}_\alpha^2} - 1 \right)$$

$$\times \left\{ \varphi(n) \varphi(n) + \frac{a^2}{2} \left[ \left( \frac{\partial^2}{\partial n^2} \varphi(n) \right) \varphi(n) + \varphi(n) \frac{\partial^2}{\partial n^2} \varphi(n) \right] \right\}$$ (15)

which accounts for dynamic effects due to deformation-dependent transfer energies (13). Compared to (14), the differential operators in (15) have been replaced by their leading terms, since the prefactor, generated by the transfer energies, is already of order $\beta^\dagger$.

### 3 The continuum limit

The matrix field $B^\dagger_\alpha(x)$, arising in the limit $a \to 0$, locally maps the line elements $dx^i$ in the laboratory frame to line elements $d\xi^\alpha(x)$ in an internal frame, attached to the local crystallographic axes [6]. Except at the cores of the defects, the internal frames are assumed to be Euclidean, i.e. to have the trivial metric tensor $g_{\alpha\beta} = \delta_{\alpha\beta}$ and affine connection $\Gamma_{\alpha\beta}^\gamma = 0$. The latter are mapped by the relations

$$g_{ij} = B^\alpha_i B^\beta_j \delta_{\alpha\beta} , \quad \Gamma_{ij}^k = B^k_\alpha \partial_i B^\alpha_j ,$$ (16)
onto the manifold supporting the field $B_i^\alpha(x)$. We point out again that the quantities (16), as well as the inverse $g^{ij}$ of $g_{ij}$ are undefined at the core site of a defect, where even the coordination number differs from that of the regular lattice. These singular points, however, have no weight in the continuum limit of the lattice.

The covariant derivative $\nabla_i$ implied by the affine connection in (16) commutes with the metric since $\nabla_k g_{ij} \equiv \partial_k g_{ij} - \Gamma^l_{ki} g_{jl} - \Gamma^l_{ji} g_{kl} = 0$. Whereas the gradient of some scalar $\Phi$ is given by $\nabla_i \Phi = \partial_i \Phi$ the divergence of a vector $V^i$ turns out to be $\nabla^T_i V^i$ where

$$\nabla^T_i \equiv \nabla_i + 2T^i_{ij}$$

(17)

with the torsion tensor

$$T^i_{ij} \equiv \frac{1}{2} (\Gamma^k_{ij} - \Gamma^k_{ji})$$

(18)

which measures the defect density [6]. For practical calculations it is convenient to use the form $(1/\sqrt{g}) \partial_i \sqrt{g}$ for the operator (17) where $g$ is the Jacobian of the metric tensor (16). The distortion tensor and consequently the quantities (16)–(18) are explicitly known for the most familiar topological defects [6].

Since in the continuum limit we only want to keep track of the leading terms in (14) and (15), it is sufficient in both expressions, to replace the sum over $n$, after multiplication with $a^d$, by an integral over the invariant volume element $d^d x \sqrt{g}$. This conforms to the transition from $\varphi(n)/a^{d/2}$ to field operators $\varphi(x)$, obeying the anti-commutation relations

$$\{\varphi(x), \varphi^\dagger(y)\} = \frac{1}{\sqrt{g(x)}} \delta(x - y).$$

(19)

Then, due to (16) and the definition of covariant derivatives, the lattice Hamiltonian (14) transforms into

$$H_c = -\frac{\hbar^2}{4m} \int d^d x \sqrt{g} \ g^{ij} \{ (\nabla_i \nabla_j \varphi^\dagger) \varphi + \varphi^\dagger \nabla_i \nabla_j \varphi \}.$$  

(20)

The identity $\partial_i \sqrt{g} = \Gamma^k_{ik} \sqrt{g}$ implies that, with respect to the measure $d^d x \sqrt{g}$, the adjoint of the operator $\nabla_i$ is $-\nabla^T_i$. Therefore, two partial integrations convert (20) into

$$H_c = -\frac{\hbar^2}{4m} \int dS^i \sqrt{g} \ \nabla^T_i \{ g^{ij} [ (\nabla_i \varphi^\dagger) \varphi - \varphi^\dagger \nabla_i \varphi ] \}$$

$$-\frac{\hbar^2}{4m} \int d^d x \sqrt{g} \ g^{ij} \varphi \{ \nabla^T_i \nabla^T_j + \nabla_i \nabla_j \} \varphi,$$

(21)

where the boundary of the surface integral, with the surface element $dS^i$, can be shifted to infinity. If this region is free of defects and defect distortions, the integrand of the surface integral becomes proportional to the particle current density. The integral then yields vanishing contributions in any stationary bound or scattering state. In any case, the surface integral in (21) will be ignored in the following discussions. The remaining bulk term is just the hermitian part of the Hamiltonian, proposed by Kleinert [17], which therefore heals a serious drawback of the latter aproach.
According to the definitions (17) and (18) the bulk integral in (22) can be re-written in the form

\[ H_c = -\frac{\hbar^2}{2m} \int d^4x \sqrt{g} \varphi^\dagger \left[ g^{ij} \nabla_i \nabla_j + (g^{ij} T^j_{\ k}) \right] \varphi \]  

(22)

(used in [7]). Obviously, \( H_c \) is manifestly covariant, i.e. it has the same universal form for arbitrary types and configurations of topological defects. The expression \( g^{ij} \nabla_i \nabla_j \) in the kinetic part of (22) is identical to the Laplace-Beltrami operator \( \frac{1}{\sqrt{g}} \partial_i \sqrt{g} g^{ij} \partial_j \) and in general differs from the operator \( g^{ij} \nabla_i \nabla_j \), entering the diffusion equation on a manifold [13]. The potential energy in (22) is proportional to the divergence of the torsion vector \( T^i \equiv g^{ij} T^j_{\ k} \) which is the only nontrivial scalar of the manifold in addition to the scalar curvature \( R \).

In a phenomenological approach the imposition of covariance also would lead to the sum of the Laplace-Beltrami kinetic part and a potential energy, consisting of the divergence of the torsion vector and an additional scalar-curvature term. Then, however, each one of these terms would carry its own phenomenological coupling constant.

Explicit calculations show that \( \nabla^j T^i = 0 \) for screw dislocations and \( \nabla^j T^i \neq 0 \) for edge dislocations, whereas \( R = 0 \) for both types of dislocations [6]. As an example of a defect with \( R \neq 0 \) we mention a kind of disclination defined by a distortion field \( B^a_i(x) \) which describes local rotations of the lattice [17] and implies \( \nabla^j T^i = R/4 \).

The continuum limit of (15) reads

\[ H_d = -\frac{\hbar^2}{2ma^2} \int d^4x \sqrt{g} \sum_a \left( \frac{1}{\partial_i B^a_i B^a_i} - 1 \right) \left[ 2\varphi^\dagger \varphi + a^2 \varphi^\dagger \Delta \varphi \right], \]  

(23)

where \( \Delta \) means the usual Euclidean Laplacian. Due to its appearance and, more importantly, due to the Kronecker delta in (23), \( H_d \) is not covariant. Below, it will turn out that \( H_d \) essentially represents the deformation potential of previous approaches [1].

### 4 Application to edge and screw dislocations

In a three-dimensional reference crystal with isotropic elastic constants \( C_{ijkl} = \lambda \delta_{ij}\delta_{kl} + \mu (\delta_{jk}\delta_{il} + \delta_{ik}\delta_{jl}) \) we now consider the case of a single straight edge-dislocation line along the \( x^3 \)-axis, i.e. with a Burgers vector \( b \) in the \( x^1, x^2 \)-plane. The distortion tensor, caused by this defect, has the non-zero components [6]

\[ \beta_{ij} = \frac{b^k}{2\pi} \left[ (\delta_{ij}\epsilon_{kl} + \epsilon_{ij}\delta_{kl}) \partial_l - \frac{1}{2(1-\nu)} (\partial_i\partial_j)^2 \epsilon_{kl}x^l \right] \ln \sqrt{(x^1)^2 + (x^2)^2}, \]  

(24)

where \( i, j = 1, 2, \epsilon_{ij} = -\epsilon_{ji}, \epsilon_{12} = 1, \) and \( \nu = \lambda/[2(\lambda + \mu)] \) is the Poisson ratio. The position of indices is irrelevant in (24), since to lowest order in \( \beta_{ij} \) one can use \( g_{ij} = \delta_{ij} \).
From (24) and (16) one can calculate the explicite form of the Hamiltonian (22) for the present case, which eventually leads to the Schrödinger equation
\[
\frac{i\hbar}{2m} \left( \Delta - \frac{b}{2\pi(1 - \nu)} \right) \left[ (1 - 2\nu) \left( \sin \phi \right) \left( \Delta - \partial_{\phi}^2 \right) - \frac{1}{r} \right] \times \left( \partial_{\phi} \cos \phi + r \partial_r \frac{1}{r} \cos \phi \partial_{\phi} \right) + \frac{1}{2} \left( \mathbf{b} \times \nabla \delta(r), \right) \psi(x, t).
\]
(25)

Here, cylinder coordinates \( x^1 = r \cos \phi, \ x^2 = r \sin \phi, \ x^3 = z \) have been used, \( \nabla \) means the Euclidean nabla operator, and \( r \equiv (x^1, x^2) \). Elastic stability requires \(-1 < \nu < 1/2\) and consequently rules out the singular cases \( \nu = 1/2, 1 \) in (25).

The core potential in (25) is unable to bind the electron, since in dimension \( d = 2 \) an attractive \( \delta \)-potential as well as its derivative are known to have no bound states [19]. This also rules out the possibility of bound states for the above-mentioned disclination-like defects for which one finds \( \nabla_i^T T^i = (\Omega/2) \delta(r) \) with a Frank angle \( \Omega \) [17]. It is interesting to note that the potential for a dipole of such defects in the limit of infinite Frank angle and vanishing dipole length resembles that of an edge dislocation which is known to be equivalent to a dipole of true disclinations [20].

When the contribution (23) is taken into account, another more important potential arises in the Schrödinger equation. Ignoring the kinetic part in (23), equation (24) yields to lowest order in \( \beta_{ij} \)
\[
V(r, \phi) = -\frac{\hbar^2}{2ma^2} \frac{4}{\text{Tr}(\beta)} = \frac{\hbar^2}{2ma^2} \frac{1 - 2\nu}{1 - \nu} \frac{2b \sin \phi}{\pi r}.
\]
(26)

If this is balanced with the leading kinetic term in (25), and if \( b \) is assumed to be of order \( a \), then the wave numbers \( q^1, q^2, q^3 \equiv k \) have typical values of order \( 1/\sqrt{ar} \). As a result all other terms in (25) and (23) can be neglected, so that the Hamiltonian of the system reduces to
\[
H(k, p, r) = \frac{(\hbar k)^2}{2m} + \frac{p^2}{2m} + V(r),
\]
(27)

where \( p \) means the operator \( \hbar i \partial / \partial r \), and \( V(r) \) is given by (26).

Up to a phenomenological coupling constant in the potential, (27) is just the Hamiltonian, considered by Lifshitz and Pushkarov [3]. They pointed out that the potential (26) has a long-ranged attractive section in the plane transverse to the dislocation line, generating an infinite number of bound states which accumulate at \( V(r = \infty) = 0 \). Close to the accumulation point the number of states \( N \) below some energy \( E \) can be calculated in a quasiclassical approximation [21], i.e., in terms of the classical Hamiltonian,
\[
N = \hbar^{-2} \int d^2p \int d^2r \Theta(E - H(k, p, r)).
\]
(28)

Solved for the energy, this yields the level spectrum
\[
E_N(k) = \frac{(\hbar k)^2}{2m} - \left( \frac{b}{2\pi a} \frac{1 - 2\nu}{1 - \nu} \right)^2 \frac{\hbar^2}{2ma^2} \frac{1}{N},
\]
(29)
where corrections to the quasiclassical approximation give rise to higher-order terms in \(1/N\).

In a three-dimensional elastically isotropic crystal we next consider a single screw-dislocation line along the \(z\)-axis with Burgers vector \(b = be_z\). In this case the only non-zero components of the distortion tensor turn out to be [6]

\[
\beta_{ij} = \frac{\varepsilon_{ij3}}{2\pi} \ln \sqrt{(x^1)^2 + (x^2)^2}.
\]

(30)

Via (16) and (22) this leads in terms of cylinder coordinates to the Schrödinger equation

\[
i\hbar \partial_t \psi(x, t) = -\frac{\hbar^2}{2m} \left[ A + \frac{b}{\pi r^2} \left( \partial_{\phi} \partial_{\phi} + \frac{b}{4\pi} \partial_z^2 \right) \right] \psi(x, t).
\]

(31)

As observed by Kawamura [2] the separation \(\psi(r, z) = \chi(r) \exp(ikz)\) converts (31) into the Aharonov-Bohm-like equation

\[
i\hbar \partial_t \chi(r, t) = -\frac{\hbar^2}{2m} \left[ \partial_r^2 + \frac{1}{r} \partial_r + \frac{1}{r^2} \left( \partial_{\phi} + i \frac{kb}{2\pi r} \right)^2 - k^2 \right] \chi(r, t).
\]

(32)

In (32) it is consistent to allow \(k\) to be of order \(1/b \propto 1/a\). Then, (23) gives rise to the deformation potential

\[
V(r) = \frac{\hbar^2}{2ma^2} \text{Tr} (\beta \beta^T) \left[ 2 - (ak)^2 \right] = \frac{\hbar^2 b^2}{4\pi^2 r^2} \left[ 2 - (ak)^2 \right].
\]

(33)

A potential of this form has previously been found in a phenomenological approach by Kosevich [8], who argued that in some semiconductors this potential might carry a negative prefactor and then again imply the existence of bound states. In our model, however, the potential is definitely repulsive and therefore does not allow the formation of bound states to screw dislocations.

A Hamiltonian similar to that in (32) and (33) has been used by Stehle and Seeger [22] to discuss the scattering of electrons on a screw dislocation. However, their analysis pays no attention to the topological nature of (32) which, according to Kawamura [2], gives rise to an Aharonov-Bohm-like effect. Kawamura’s approach, on the other hand, ignores the deformation potential (33). Both aspects of the scattering problem will be taken into account in a forthcoming publication [9].

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