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Gauge properties of $\mathbf{k}\cdot\mathbf{p}$ Hamiltonians for crystals with linear topological defects

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A general expression for the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian in crystals with linear topological defects such as dislocations, disclinations, and dispirations has been found. It has been shown to contain gauge potential terms corresponding to a non-Abelian gauge group, $E(3)$, which is the proper Euclidean group. The gauge field is confined within the cores of topological defects and influences the carriers in the bulk of the crystal through the gauge potential which extends beyond it. A general expression for the gauge potential $\mathbf{A}(\mathbf{r})$ is presented. For a crystal that contains only dislocations the gauge group $E(3)$ degenerates into $T(3)$, the Abelian subgroup of translations. The corresponding gauge potential becomes $\hat{\mathbf{A}}(\mathbf{r})=i\beta^T(\mathbf{r})(\hat{\mathbf{p}}/\hbar-\mathbf{k}_\alpha)$, where $\mathbf{k}_\alpha$ is the electron wave vector related to the point in the Brillouin zone for which the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian is written, $\hat{\mathbf{p}}$ is the momentum-operator matrix in the basis of Bloch functions corresponding to $\mathbf{k}_\alpha$, and $\beta(\mathbf{r})$ is the distortion tensor.

I. INTRODUCTION

The method of the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian has proved to be very helpful when a precise description of electron energy band structure of crystal solids in the vicinity of symmetry points of the Brillouin zone is required. This approach is a valuable tool for finding expressions for effective-mass Hamiltonians in terms of energy gaps and matrix elements of momentum operator when it is combined with the $\mathbf{k}\cdot\mathbf{p}$ perturbation theory.[1-5]

A generalization of this approach for strained crystals is also possible. In this case the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian contains additional terms, so-called deformation potential terms,[6-9] whose general form can be found by a method of invariants from an analysis of the local symmetry of the crystal lattice.[10,11]

The method of obtaining the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian for strained crystals is based on a continuous transformation of the system of coordinates that allows the atomic coordinates in strained lattices to be put into their original places, thus restoring the initial symmetry of the crystal lattice.

It can be seen, however, that this approach fails when it is applied to crystals containing topological defects because in this case no continuous transformation of the defected lattice into the perfect one is possible.

It was first observed by Kawamura[12] that the effective Hamiltonian for a crystal with a screw dislocation contains additional terms that can produce an Aharonov-Bohm-type scattering of carriers by dislocations.

Several more detailed theoretical investigations have been made to find a general form of the effective-mass Hamiltonian for a crystal with dislocations.[13-16] The most advanced theory[15,16] suggests that in the presence of a distortion of the crystal lattice $\beta(\mathbf{r})$ the momentum operator $\mathbf{p}$ changes into a gauge-invariant momentum operator $\mathbf{p}+\mathbf{a}$ and, correspondingly, the band-structure energy operator changes from $E(\mathbf{p})$ into $E(\mathbf{p}+\mathbf{a})$, where $\mathbf{a}=\beta^T\mathbf{p}$.

However, such a form of the Hamiltonian leads to confusion because it gives a nonzero gauge potential when applied to an electron embedded in a topologically imperfect lattice with zero crystal potential, i.e., the free-electron case.

An investigation into this problem in this paper has shown that there are two different factors contributing to the gauge potential. One is related to a nonuniform distortion of the crystal lattice around a topological defect and the other is related to the many-valued character of the mapping of the Bloch-type electron wave function onto a topologically imperfect crystal lattice. Both factors should be taken into consideration in order to obtain a correct expression for the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian.

Having done this, a general form of the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian for crystals with dislocations, disclinations, and dispirations was found. The resulting $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian is gauge invariant and the corresponding gauge group is a non-Abelian group $E(3)$, of proper Euclidean transformations of three-dimensional space. It has been shown that the gauge field is confined within the cores of the topological defects and influences the carriers in the bulk of the crystal only through the gauge potential that extends beyond it.

II. THE $\mathbf{k}\cdot\mathbf{p}$ HAMILTONIAN FOR CRYSTALS WITH DISTORTED LATTICE

We will start our consideration with the usual $\mathbf{k}\cdot\mathbf{p}$ Hamiltonians for strained crystals with the topologically perfect lattices. Although this Hamiltonian is well known, we would like to calculate it using a mathematical way of derivation, which is more compact than the traditional one (see, for example, Ref. 11) and allows the gauge properties of the Hamiltonian to be clarified.

Let us start with the following general form of the wave function for an electron in the perfect crystal:

$$\Psi(\mathbf{r})=\sum_{\alpha,n,i} f^{(i)}_{\alpha,n}(\mathbf{r})\Psi^{(i)}_{\mathbf{k}_\alpha,n}(\mathbf{r})\ , \qquad (1)$$

where $f^{(i)}_{\alpha,n}(\mathbf{r})$ are the overlapping wave functions and

$\Psi^{(i)}_{\mathbf{k}_\alpha,n}(\mathbf{r})$ is the Bloch wave function for an electron with wave vector $\mathbf{k}_\alpha$ which transforms according to irreducible representation Γ_i of the crystal space group G. The sum in Eq. (1) is over $\mathbf{k}_\alpha$ from a star of wave vectors, $\{\mathbf{k}_\alpha\}$, irreducible representations Γ_i, associated with the star $\{\mathbf{k}_\alpha\}$, and the degeneracy index n, numerating the basic functions of the irreducible representation of a small group related to $\mathbf{k}_\alpha$.

The basic functions $\Psi^{(i)}_{\mathbf{k}_\alpha,n}(\mathbf{r})$ for a given star $\{\mathbf{k}_\alpha\}$ are general solutions of the Schrödinger equation with Hamiltonian $H[\mathbf{p},V_0(\mathbf{r})]$ for an electron in crystal field,

$$H[\mathbf{p},V_0(\mathbf{r})]=\frac{\mathbf{p}^2}{2m}+V_0(\mathbf{r})+\frac{i}{4m^2c^2}\sum_{s,l,q}e_{slq}\sigma_s\mathbf{p}_l V_0(\mathbf{r})\mathbf{p}_q\ , \tag{2}$$

where $\mathbf{p}=-i\hbar\nabla$, σ_S are Pauli matrices, and the third term in Eq. (2) is the spin-orbit interaction written in terms of $\mathbf{p}$, σ, and $V_0(\mathbf{r})$ operators, and e_{slq} are the components of the Levi-Civitá tensor.

To find the matrix **k·p** Hamiltonian $\hat{H}(\nabla,\mathbf{r})$ for an overlapping wave function $f^{(i)}_{\alpha,n}(\mathbf{r})$, which can be considered as a vector function with respect to α, n, and i indexes, we can just substitute the matrix expressions $\hat{\mathbf{p}}-i\hbar\nabla$ and $\hat{V}_0$ into Eq. (2) instead of operators $\mathbf{p}$ and $V_0(\mathbf{r})$

$$\hat{H}(\nabla,\mathbf{r})=H[\hat{\mathbf{p}}-i\hbar\nabla,\hat{V}_0]\ , \tag{3}$$

where $\hat{\mathbf{p}}$ and $\hat{V}_0$ are coordinate-independent matrices given by

$$\begin{aligned}(\hat{V}_0)_{\alpha,n,i;\alpha',n',i'}&=\delta_{\alpha,\alpha'}\int_\Omega d\mathbf{r}\,\Psi^{(i)*}_{\mathbf{k}_\alpha,n}(\mathbf{r})V_0(\mathbf{r})\Psi^{(i')}_{\mathbf{k}_\alpha,n'}(\mathbf{r})\ ,\\(\hat{\mathbf{p}})_{\alpha,n,i;\alpha',n',i'}&=\delta_{\alpha,\alpha'}\int_\Omega d\mathbf{r}\,\Psi^{(i)*}_{\mathbf{k}_\alpha,n}(\mathbf{r})\mathbf{p}\Psi^{(i')}_{\mathbf{k}_\alpha,n'}(\mathbf{r})\ .\end{aligned} \tag{4}$$

It is worth noting that the **k·p** Hamiltonian $\hat{H}(\nabla,\mathbf{r})$ given in Eq. (3), is an exact matrix Hamiltonian for the overlapping function $f^{(i)}_{\alpha,n}(\mathbf{r})$. An approximate effective-mass Hamiltonian can be obtained from Eq. (3) by applying the so-called **k·p** perturbation theory, i.e., treating the ∇-linear and ∇-square terms in $\hat{H}(\nabla,\mathbf{r})$ as perturbations (see, for example, Ref. 11).

For a strained crystal, the **k·p** Hamiltonian may be found in a similar way if the following form of the electron wave function is used instead of that given in Eq. (1):

$$\Psi(\mathbf{r})=\sum_{\alpha,n,i}f^{(i)}_{\alpha,n}(\mathbf{r})\Psi^{(i)}_{\mathbf{k}_\alpha,n}(\mathbf{r}')\ . \tag{5}$$

Here all the notations are the same as in Eq. (1) except that $\Psi^{(i)}_{\mathbf{k}_\alpha,n}(\mathbf{r}')$ now depends on the coordinate position $\mathbf{r}'$ of a point in an imaginary unstrained crystal instead of $\mathbf{r}$, the position of the point in the real crystal.

The corresponding coordinate transformation is

$$\mathbf{r}'=\mathbf{r}+\mathbf{s}(\mathbf{r})\ , \tag{6}$$

where $\mathbf{s}(\mathbf{r})$ is the displacement vector.

The electron wave function given in Eq. (5) can also be written in the form

$$\Psi(\mathbf{r})=\sum_{\alpha,n,n',i}f^{(i)}_{\alpha,n}(\mathbf{r})\Psi^{(i)}_{\mathbf{k}_\alpha,n'}(\mathbf{r})[\exp\{i\mathbf{s}(\mathbf{r})\hat{\mathbf{p}}/\hbar\}]_{n'n}\ , \tag{7}$$

where the operator $\exp\{i\mathbf{s}(\mathbf{r})\hat{\mathbf{p}}/\hbar\}$ provides the necessary transformation $\Psi(\mathbf{r})\rightarrow\Psi(\mathbf{r}')$.

Generally, the one-electron Hamiltonian $\tilde{H}(\mathbf{p},\mathbf{r})$ for a crystal with a strained lattice can be written in the same form as the Hamiltonian for the perfect crystal which is given in Eq. (2) using a substitution $V_0(\mathbf{r})=V_0(\mathbf{r}')+\delta V[\mathbf{r}',\beta(\mathbf{r})]$, which accounts for the corresponding changes in the crystal potential:

$$\tilde{H}(\mathbf{p},\mathbf{r})=H\{\mathbf{p},V_0(\mathbf{r}')+\delta V[\mathbf{r}',\beta(\mathbf{r})]\}\ . \tag{8}$$

Here $\delta V[\mathbf{r}',\beta(\mathbf{r})]$ is the perturbation of the crystal potential by the lattice distortion. This can be considered as a periodic function of $\mathbf{r}'$ and a functional of the distortion field $\beta(\mathbf{r})$, $\beta_{ij}(\mathbf{r})=-\partial s_i(\mathbf{r})/\partial r_j$.

The matrix **k·p** Hamiltonian $\hat{H}(\nabla,\mathbf{r})$ for the electron overlapping wave function $f^{(i)}_{\alpha,n}(\mathbf{r})$ in the crystal with distorted lattice can be found from Eqs. (5)–(8):

$$\hat{H}(\nabla,\mathbf{r})=H\{\hat{\mathbf{p}}-i\hbar(\nabla+\hat{\mathbf{A}}_1),\hat{V}_0+\delta\hat{V}[\beta(\mathbf{r})]\}\ , \tag{9}$$

where $\hat{A}_1=i\beta^T\hat{\mathbf{p}}/\hbar$ is the gauge potential originating from the factor $\exp\{i\mathbf{s}(\mathbf{r})\cdot\hat{\mathbf{p}}/\hbar\}$ in the expression for electron wave function given in Eq. (7), which leads to the following transformation of the gradient operator:

$$\begin{aligned}\nabla&\rightarrow\exp\{-\exp[i\mathbf{s}(\mathbf{r})\cdot\hat{\mathbf{p}}/\hbar]\}\nabla\exp\{\exp[i\mathbf{s}(\mathbf{r})\cdot\hat{\mathbf{p}}/\hbar]\}\\&=\nabla+i\beta^T\hat{\mathbf{p}}/\hbar\ .\end{aligned} \tag{10}$$

The explicit general expression for $H[\mathbf{p},V(\mathbf{r})]$ is the same as for a crystal with a perfect lattice given in Eqs. (1) and (2). The corresponding operators $\hat{\mathbf{p}}$ and $\hat{V}_0$ are given in Eq. (4) and the matrix function $\delta\hat{V}[\beta(\mathbf{r})]$ is

$$\begin{aligned}&\{\delta\hat{V}[\beta(\mathbf{r})]\}_{\alpha,n,i;\alpha',n',i'}\\&\quad=\delta_{\alpha,\alpha'}\int_\Omega d\mathbf{r}'\Psi^{(i)*}_{\mathbf{k}_{\alpha'},n,i}(\mathbf{r}')\delta V[\mathbf{r}',\beta(\mathbf{r})]\Psi^{(i')}_{\mathbf{k}_{\alpha'},n'}(\mathbf{r}')\ ;\end{aligned} \tag{11}$$

here $\mathbf{r}$ and $\mathbf{r}'$ are considered as independent variables in this integral. In the deformation potential approach [6–11] the functional $\delta\hat{V}[\beta(\mathbf{r})]$ is usually approximated in the following way:

$$\delta\hat{V}[\beta(\mathbf{r})]=\sum_{i,j}\hat{V}^{ij}\varepsilon_{ij}(\mathbf{r})\ , \tag{12}$$

where $\hat{V}^{ij}$ are some constants and $\varepsilon_{ij}(\mathbf{r})=[\beta_{ij}(\mathbf{r})+\beta_{ji}(\mathbf{r})]/2$ is the strain tensor. The Hamiltonian given in Eq. (9) is gauge invariant with respect to the following gauge transformation:

$$\begin{aligned}&f(\mathbf{r})\rightarrow\exp\{i\mathbf{t}(\mathbf{r})\cdot\hat{\mathbf{p}}/\hbar\}f(\mathbf{r})\ ,\\&\hat{\mathbf{A}}_1(\mathbf{r})\rightarrow\hat{\mathbf{A}}_1(\mathbf{r})-i\nabla\mathbf{t}(\mathbf{r})\cdot\hat{\mathbf{p}}/\hbar\ ,\\&\hat{V}_0\rightarrow\exp\{i\mathbf{t}(\mathbf{r})\cdot\hat{\mathbf{p}}/\hbar\}\hat{V}_0\exp\{-i\mathbf{t}(\mathbf{r})\cdot\hat{\mathbf{p}}/\hbar\}\ ,\\&\delta\hat{V}[\beta(\mathbf{r})]\rightarrow\exp\{i\mathbf{t}(\mathbf{r})\cdot\hat{\mathbf{p}}/\hbar\}\delta\hat{V}[\beta(\mathbf{r})]\exp\{-i\mathbf{t}(\mathbf{r})\cdot\hat{\mathbf{p}}/\hbar\}\ ,\end{aligned} \tag{13}$$

where $\mathbf{t}(\mathbf{r})$ is an arbitrary vector function of $\mathbf{r}$.

The corresponding gauge group is Abelian $U_1\otimes U_1\otimes U_1$ and matrices $i\hat{p}_s/\hbar$ are the generators of a representation of the group on functions $f^{i}_{\alpha,n}$. It can be seen that for a crystal without topological defects, the gauge potential $A_1(\mathbf{r})$ in Eqs. (9) can be eliminated by the gauge transformation given in Eq. (13) with $\mathbf{t}(\mathbf{r})=\mathbf{s}(\mathbf{r})$, where $\mathbf{s}(\mathbf{r})$ is the displacement field. However, it is not possible to do this for a crystal with topological defects because in this case the displacement field is not a single-valued function of $\mathbf{r}$.

III. THE $\mathbf{k}\cdot\mathbf{p}$ HAMILTONIAN FOR CRYSTAL WITH LINEAR TOPOLOGICAL DEFECTS

Now, let us consider a crystal that contains liner topological defects such as dislocations, disclinations, and dispirations. In this case the crystal lattice is locally topologically perfect outside the defect cores and the corresponding one-electron Hamiltonian $\tilde{H}(\mathbf{p},\mathbf{r})$ is still given by Eq. (8). However, the expression for the electron wave function given in Eq. (5) is no longer valid since $\mathbf{r}'(\mathbf{r})$ is now a many-valued function of $\mathbf{r}$ and, therefore, $\Psi^{(i)}_{\mathbf{k}_{\alpha},n}(\mathbf{r}')$ cannot be used as the basic functions throughout the whole crystal.

Generally, $\mathbf{r}'(\mathbf{r})$ depends on the path along which the continuous mapping is performed starting from a reference point $\mathbf{r}_0$. Any two paths that can be continuously deformed into each other provide equivalent or, mathematically speaking, homotopic maps. These classes of homotopic maps constitute the first homotopy group based at $\mathbf{r}_0$, $\pi_1(R,\mathbf{r}_0)$, where R denotes the crystal volume space without topological defect cores, when a standard multiplication operation for paths is applied (see, for example, Refs. 17 and 18).

Thus, generally, for a crystal with topological defects the function $\mathbf{r}'(\mathbf{r})$ can be written as

$$\mathbf{r}'=\mathbf{r}'(\mathbf{r},a) , \tag{14}$$

where a is an element of $\pi_1(R,\mathbf{r}_0)$. Any two different mappings are related by a transformation operation g from the proper crystal space group G_{cr} and, therefore, we can write

$$\mathbf{r}'(\mathbf{r},a)=g(a)\mathbf{r}'(\mathbf{r},e) , \tag{15}$$

where e is the unit element of $\pi_1(R,\mathbf{r}_0)$.

To retain the general form of the electron wave function given in Eqs. (5) and (7), which is basic for finding the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian, we need to introduce a path-dependent unitary transformation of $\Psi^{(i)}_{\mathbf{k}_{\alpha},n}(\mathbf{r}')$ to compensate for the non-single-valued nature of these functions

$$\Psi(\mathbf{r})=\sum_{\alpha,n,\alpha',n',i} f^{(i)}_{\alpha,n}(\mathbf{r})U^{(i)}_{\alpha',n';\alpha,n}(\mathbf{r},a)\Psi^{(i)}_{\mathbf{k}_{\alpha'},n'}(\mathbf{r}') , \tag{16}$$

where $U^{(i)}(\mathbf{r},a)$ are unitary $\alpha n\times\alpha n$ matrices, which are continuous many-valued functions of $\mathbf{r}$. These should satisfy the condition

$$U^{(i)}(\mathbf{r},a)=U^{(j)}_{\mathrm{cr}}[g(a)]U^{(i)}(\mathbf{r},e) ; \tag{17}$$

where $U^{(i)}_{\mathrm{cr}}[g(a)]$ is the matrix of an irreducible representation Γ_i of the crystal space group corresponding to the element $g(a)$. A substitution of Eq. (16) into the Schrödinger equation for the overlapping function $f^{(i)}_{\alpha,n}(\mathbf{r})$ gives the following general $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian $\hat{H}(\mathbf{k},\mathbf{r})$ for an electron in a crystal with linear topological defects:

$$\begin{aligned}\hat{H}(\mathbf{k},\mathbf{r})=H\{&\hat{\mathbf{p}}'(\mathbf{r},a)\\&-i\hbar[\nabla+\hat{\mathbf{A}}(\mathbf{r})],\hat{V}'[\mathbf{r},a,\beta(\mathbf{r},a)]\}\end{aligned} , \tag{18}$$

where

$$\begin{aligned}&\hat{\mathbf{A}}(\mathbf{r})=\hat{\mathbf{A}}_1(\mathbf{r})+\hat{\mathbf{A}}_2(\mathbf{r}) ,\\&\hat{\mathbf{A}}_1(\mathbf{r})=\beta^{T}(\mathbf{r},a)\hat{\mathbf{p}} ,\\&\hat{\mathbf{A}}_2(\mathbf{r})=\exp\{-i\mathbf{s}(\mathbf{r},a)\cdot\hat{\mathbf{p}}/\hbar\}\mathbf{U}^{+}(\mathbf{r},a)\\&\qquad\times[\nabla\mathbf{U}(\mathbf{r},a)]\exp\{i\mathbf{s}(\mathbf{r},a)\cdot\hat{\mathbf{p}}/\hbar\} ;\end{aligned} \tag{19}$$

here $\mathbf{U}(\mathbf{r},a)=U^{(1)}(\mathbf{r},a)\otimes U^{(2)}(\mathbf{r},a)\otimes\ldots\otimes U^{(k)}(\mathbf{r},a)$ is the matrix of the direct product of matrices $U^{(i)}(\mathbf{r},a)$. Taking into account the conditions given in Eqs. (15) and (17) and the definition of the path-dependent distortion tensor $\beta_{ij}(\mathbf{r},a)=-\partial r'_i(\mathbf{r},a)/\partial r_j$, it can be easily seen that in spite of the path dependencies of $\hat{\mathbf{A}}_1(\mathbf{r})$ and $\hat{\mathbf{A}}_2(\mathbf{r})$ their sum $\hat{\mathbf{A}}(\mathbf{r})$ is path independent and can be written as

$$\begin{aligned}\hat{\mathbf{A}}(\mathbf{r})=&\beta^{T}(\mathbf{r},e)\hat{\mathbf{p}}+\exp\{-i\mathbf{s}(\mathbf{r},e)\cdot\hat{\mathbf{p}}/\hbar\}\\&\times\mathbf{U}^{+}(\mathbf{r},e)[\nabla\mathbf{U}(\mathbf{r},e)]\exp\{i\mathbf{s}(\mathbf{r},e)\cdot\hat{\mathbf{p}}/\hbar\} .\end{aligned} \tag{20}$$

The matrices $\hat{\mathbf{p}}'(\mathbf{r},a)$, $\hat{V}'(\mathbf{r},a)$, and $\hat{V}'[\mathbf{r},a,\beta(\mathbf{r},a)]$ in Eq. (18) are given by the unitary transformation of $\hat{\mathbf{p}}$, $\hat{V}$, and $\hat{V}'[\beta(\mathbf{r},a)]$:

$$\begin{aligned}&\hat{\mathbf{p}}'(\mathbf{r},a)=\mathbf{U}^{+}(\mathbf{r},a)\hat{\mathbf{p}}\mathbf{U}(\mathbf{r},a) ,\\&\hat{V}'(\mathbf{r},a)=\mathbf{U}^{+}(\mathbf{r},a)\hat{V}\mathbf{U}(\mathbf{r},a) ,\\&\delta\hat{V}'_0(\mathbf{r},a)=\mathbf{U}^{+}(\mathbf{r},a)\delta\hat{V}[\beta(\mathbf{r},a)]\mathbf{U}(\mathbf{r},a) .\end{aligned} \tag{21}$$

These matrices are dependent on the path a, but their combinations in the Hamiltonian given in Eq. (18) are path independent since the initial Hamiltonian given in Eq. (2) is invariant with respect to transformations from the crystal space group. The Hamiltonian given in Eq. (16) is invariant under the following gauge transformation:

$$\begin{aligned}&f(\mathbf{r})\to\mathbf{T}(\mathbf{r})f(\mathbf{r}) ,\\&\hat{\mathbf{A}}(\mathbf{r})\to\mathbf{T}(\mathbf{r})\hat{\mathbf{A}}(\mathbf{r})\mathbf{T}^{-1}(\mathbf{r})-[\nabla\mathbf{T}(\mathbf{r})]\mathbf{T}^{-1}(\mathbf{r}) ,\\&\hat{\mathbf{p}}'(\mathbf{r},a)\to\mathbf{T}(\mathbf{r})\hat{\mathbf{p}}'(\mathbf{r},a)\mathbf{T}^{-1}(\mathbf{r}) ,\\&\hat{V}'_0(\mathbf{r},a)\to\mathbf{T}(\mathbf{r})\hat{V}'_0(\mathbf{r},a)\mathbf{T}^{-1}(\mathbf{r}) ,\\&\delta\hat{V}'[\mathbf{r},a,\beta(\mathbf{r},a)]\to\mathbf{T}(\mathbf{r})\delta\hat{V}'[\mathbf{r},a,\beta(\mathbf{r},a)]\mathbf{T}^{-1}(\mathbf{r}) ,\end{aligned} \tag{22}$$

where

$$\mathbf{T}(\mathbf{r})=[T^{(1)}(\mathbf{r})\otimes T^{(2)}(\mathbf{r})\otimes\ldots\otimes T^{(k)}(\mathbf{r})]\exp\{i\mathbf{t}(\mathbf{r})\cdot\hat{\mathbf{p}}/\hbar\} ,$$

and $T^{(i)}(\mathbf{r})$ are arbitrary unitary matrices whose dimensions are determined by the dimensions of the irreducible representations Γ_i and whose matrix elements should be single-valued functions of $\mathbf{r}$.

Using the gauge invariance property, we can eliminate the potential $\hat{\mathbf{A}}(\mathbf{r})$ in any single connected area of the crystal by a gauge transformation with

$$T^{(i)}(\mathbf{r})=U^{(i)}(\mathbf{r},e)\ ,\quad \mathbf{t}(\mathbf{r})=\mathbf{s}(\mathbf{r},e)\ . \tag{23}$$

This means that the gauge field $F_{kl}(\mathbf{r})$, which is defined a standard way,

$$F_{kl}(\mathbf{r})=\frac{\partial \hat{A}_l(\mathbf{r})}{\partial r_k}-\frac{\partial \hat{A}_k(\mathbf{r})}{\partial r_l}+i[\hat{A}_k(\mathbf{r}),\hat{A}_l(\mathbf{r})] \tag{24}$$

is zero outside the topological defects.

Thus, the gauge field is confined within the topological defect cores and influences the electrons in the volume of crystal only through the gauge potential which extends beyond it.

To find the gauge potential field $\mathbf{A}(\mathbf{r})$ from Eq. (20) we need to know explicit expressions for $U^{(i)}(\mathbf{r},a)$. The choice of $U^{(i)}(\mathbf{r},a)$ is restricted only by the condition given in Eq. (17), and the related extent of freedom in the choice of $U^{(i)}(\mathbf{r},a)$ reflects the freedom in the initial gauge. Finding explicit expressions for $U^{(i)}(\mathbf{r},a)$ in a general case of a crystal with a given number of topological defects of given types is not a simple task, since there is no one-to-one correspondence between the topological defect types and the elements of the crystal space group $g(a)$, $a\in\pi_1(R,\mathbf{r}_0)$. In particular, the same $g(a)$ may correspond to linear topological defects with different winding indexes. Moreover, the general approach based on the analyses of the algebraic structure of the group of homotopy classes in the space of degeneracy fails to classify the topological defects in crystals and other ordered media with broken translational symmetry since it is necessary to take into account the nonlocal compatibility conditions and at present no adequate mathematical apparatus for this exists.[18,19] However, it is possible to find an expression for $U^{(i)}(\mathbf{r},a)$ provided the mapping $\mathbf{r}'(\mathbf{r},a)$ is known. To do this let us represent an element of the crystal proper space group in the form

$$g=g_1^{n_1}g_2^{n_2}g_3^{n_3}g_4^{n_4}g_5^{n_5}g_6^{n_6}\ , \tag{25}$$

where g_i are generators of the group and n_i are corresponding integer powers. The first three generators, g_1,g_2,g_3, are primitive translations which generate all the translations compatible with the crystal lattice and the other three, g_4,g_5,g_6, are primitive rotations (these can also include nonprimitive translations for nonsymmorfic groups) which generate all rotations from the point group of the crystal. For crystals with low symmetrical lattices some of the primitive rotations in Eq. (25) may be equal to the identity transformation, e. For a given mapping $\mathbf{r}'(\mathbf{r},a)$, we can ascribe to a point of the crystal $\mathbf{r}$ and to a mapping path a an element h of the group of proper affine transformations of Euclidean space, Aff(3), in the following way:

$$h(\mathbf{r},a)=\{\mathbf{s}(\mathbf{r},a),\ \mathbf{A}^{-1}(\mathbf{r}a)\}\ , \tag{26}$$

where $\mathbf{s}(\mathbf{r},a)=\mathbf{r}'(\mathbf{r},a)-\mathbf{r}$ is the displacement vector corresponding to point $\mathbf{r}$ of the crystal, and $\mathbf{A}(\mathbf{r},a)$ is a 3×3 real matrix with a positive determinant whose matrix elements are given by $A_{ij}(\mathbf{r},a)=\partial r_i'(\mathbf{r},a)/\partial r_j$. The matrix $\mathbf{A}(\mathbf{r},a)$ may be written in the form $\mathbf{A}(\mathbf{r},a)=\mathbf{R}(\mathbf{r},a)\mathbf{M}(\mathbf{r},a)$, where $\mathbf{M}(\mathbf{r},a)=[\mathbf{A}(\mathbf{r},a)\mathbf{A}^T(\mathbf{r},a)]^{1/2}$, and $\mathbf{R}(\mathbf{r},a)$ is an orthogonal matrix corresponding to a rotation of Euclidean space. This allows a natural continuous mapping of the nine-dimensional group Aff(3) into the six-dimensional Euclidean group $E(3)$:

$$\begin{aligned}h(\mathbf{r},a)&=\{\mathbf{s}(\mathbf{r},a),\ \mathbf{A}(\mathbf{r},a)\}\\&\to d(\mathbf{r},a)=\{\mathbf{s}(\mathbf{r},a),\mathbf{R}(\mathbf{r},a)\}\ .\end{aligned} \tag{27}$$

An element $d(\mathbf{r},a)$ of the Euclidean group can be written in the form

$$\begin{aligned}d(\mathbf{r},a)=&\exp\{s_1(\mathbf{r},a)G_1\}\exp\{s_2(\mathbf{r},a)G_2\}\\&\times\exp\{s_3(\mathbf{r},a)G_3\}\\&\times\exp\{s_4(\mathbf{r},a)G_4\}\exp\{s_5(\mathbf{r},a)G_5\}\\&\times\exp\{s_6(\mathbf{r},a)G_6\}\ ,\end{aligned} \tag{28}$$

where G_i are generators of the Euclidean group and $s_i(\mathbf{r},a)$ ar real number parameters. The generators G_i can be chosen in the form $G_i=\ln(g_i)$, for $g_i\neq e$. If $g_i=e$ for some i the corresponding G_i can be taken in an arbitrary way with the only restriction being that it should not be equal to G_{i+1} or G_{i-1}. For this choice of generators the parameters in Eq. (28) can be found in the following natural way. For $i=1,2,3$, the parameters $s_i(\mathbf{r},a)$ are equal to the corresponding components of the displacement vector $\mathbf{s}(\mathbf{r},a)$ and for $i=4,5,6$, the parameters are $s_i(\mathbf{r},a)=\varphi_i(\mathbf{r},a)/2\pi$, where $\varphi_i(\mathbf{r},a)$ are the angles of the corresponding rotations about the axes of the primitive rotations g_4,g_5,g_6. Using such a representation we can obtain an explicit form of $U^{(i)}(\mathbf{r},a)$ in Eq. (17):

$$\begin{aligned}U^{(i)}(\mathbf{r},a)=&\exp\{s_1(\mathbf{r},a)\ln(U_{\mathrm{cr}}^{(i)}[g_1])\}\exp\{s_2(\mathbf{r},a)\ln(U_{\mathrm{cr}}^{(i)}[g_2])\}\exp\{s_c(\mathbf{r},a)\ln(U_{\mathrm{cr}}^{(i)}[g_3])\}\\&\times\exp\{s_4(\mathbf{r},a)\ln(U_{\mathrm{cr}}^{(i)}[g_4])\}\exp\{s_5(\mathbf{r},a)\ln(U_{\mathrm{cr}}^{(i)}[g_5])\}\exp\{s_6(\mathbf{r},a)\ln(U_{\mathrm{cr}}^{(i)}[g_6])\}\ .\end{aligned} \tag{29}$$

Since the first three generators g_1,g_2,g_3 are primitive translations, we can easily find that $\ln(U_{\mathrm{cr}}^{(i)}[g_i])=-ik_i$, where k_i are the corresponding components of the electron wave-vector operator (or quasimomentum operator) $\mathbf{k}$, which acts on the overlapping wave functions $f_{\alpha,n}^{(i)}$ in the following way:

$$(\mathbf{k})_{\alpha,n,i;\alpha',n',i'}=\mathbf{k}_\alpha\delta_{\alpha,\alpha'}\delta_{n,n'}\delta_{i,i'}\ . \tag{30}$$

A substitution of Eq. (30) into Eq. (28) allows it to be rewritten as

$$U^{(i)}(\mathbf{r},a)=\exp\{-i\mathbf{s}(\mathbf{r},a)\mathbf{k}\}$$
$$\times\exp\{\varphi_4(\mathbf{r},a)\ln(U_{\mathrm{cr}}^{(i)}[g_4])/2\pi\}$$
$$\times\exp\{\varphi_5(\mathbf{r},a)\ln(U_{\mathrm{cr}}^{(i)}[g_5])/2\pi\}$$
$$\times\exp\{\varphi_6(\mathbf{r},a)\ln(U_{\mathrm{cr}}^{(i)}[g_6])/2\pi\}\ . \qquad (31)$$

Finally, it follows from Eqs. (15), (25), and (29) that the choice of $U^{(i)}(\mathbf{r},a)$ in the form given in Eq. (31) satisfies the condition given in Eq. (17). Thus, a substitution of Eq. (31) into Eq. (19) allows us to find explicit expressions for the gauge potential field $\mathbf{A}(\mathbf{r})$ in the general case of a crystal containing any liner topological defects. In addition, it follows from Eq. (31) that the gauge group related to the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian given in Eq. (18) is actually the Euclidean group $E(3)$. For this group the general gauge transformations given in Eq. (22) should be restricted to six-parameter gauge transformations,

$$\mathbf{T}(\mathbf{r})=[T^{(1)}(\mathbf{r})\otimes T^{(2)}(\mathbf{r})\otimes\ldots\otimes T^{(k)}(\mathbf{r})]$$
$$\times\exp\{i\mathbf{t}(\mathbf{r})\mathbf{k}\{\ \exp\{i\mathbf{t}(\mathbf{r})\hat{\mathbf{p}}/\hbar\}\ ,$$
$$T^{(i)}(\mathbf{r})=\exp\left\{\frac{\tau_6(\mathbf{r})\ln(U_{\mathrm{cr}}^{(i)}[g_6])}{2\pi}\right\}$$
$$\times\exp\left\{\frac{\tau_5(\mathbf{r})\ln(U_{\mathrm{cr}}^{(i)}[g_5])}{2\pi}\right\} \qquad (32)$$
$$\times\exp\left\{\frac{\tau_4(\mathbf{r})\ln(U_{\mathrm{cr}}^{(i)}[g_4])}{2\pi}\right\}\ ,$$

where $\tau_4(\mathbf{r})$, $\tau_5(\mathbf{r})$, $\tau_6(\mathbf{r})$, and $\mathbf{t}(\mathbf{r})$ are arbitrary single-valued functions of $\mathbf{r}$.

IV. PROPERTIES OF THE k·p HAMILTONIAN

Let us first check that the Hamiltonian given in Eq. (18) produces no field for an electron in a topologically imperfect lattice with zero atomic potential.

Indeed, in this case for a given star of wave vectors $\{\mathbf{k}_\alpha\}$ compatible with the symmetry of the lattice only one irreducible representation of the space group exists whose basic functions are plane waves $\Psi_{\mathbf{k}_\alpha}(\mathbf{r})=\exp\{i\mathbf{k}_\alpha\mathbf{r}\}$. The matrix of the momentum operator is $(\hat{\mathbf{p}})_{\alpha,n,i;\alpha',n',i'}=\hbar(\mathbf{k}_\alpha+\mathbf{q})\delta_{\alpha,\alpha'}\delta_{n,n'}\delta_{i,i'}$, where $\mathbf{q}$ is a vector of the reciprocal crystal lattice. Thus, $\hat{\mathbf{p}}$ does not mix different irreducible representations of the crystal space group and, therefore, the gauge transformation given in Eq. (32) with $\mathbf{t}(\mathbf{r})=\mathbf{s}(\mathbf{r},a)$, $\tau_i(\mathbf{r})=\varphi_i(\mathbf{r},a)$ is possible since it does not depend on the path a. This transformation eliminates the gauge potential $\hat{\mathbf{A}}(\mathbf{r})$ everywhere in the crystal.

Now, let us study in some more detail the case of a crystal which contains only dislocations. For this case the elements of the crystal space group $g(a)$ in Eq. (15) are translations on the Burgers vector $\mathbf{b}(a)$ and the corresponding matrices $U^{(i)}(\mathbf{r},a)$ can be taken in the form

$$U^{(i)}(\mathbf{r},a)=\exp\{-i\mathbf{s}(\mathbf{r},a)\cdot\mathbf{k}\}\ . \qquad (33)$$

This allows us to find from Eq. (19) a general expression for gauge potential $\hat{\mathbf{A}}(\mathbf{r})$ in the crystal with dislocations

$$\hat{\mathbf{A}}(\mathbf{r})=i\beta^T(\mathbf{r})(\hat{\mathbf{p}}/\hbar-\mathbf{k}_\alpha)\ , \qquad (34)$$

where $\mathbf{k}_\alpha$ is a multiplication operator $(\mathbf{k}_\alpha)_{\alpha,n,i;\alpha',n',i'}=\mathbf{k}_\alpha\delta_{\alpha,\alpha'}\delta_{n,n'}\delta_{i,i'}$. It also follows from Eq. (19) that the matrices of operators $\hat{\mathbf{p}}'$ and $V'(\mathbf{r})$ in this case are equal to their original forms $\hat{\mathbf{p}}'=\hat{\mathbf{p}}$, $\hat{V}'(\mathbf{r})=\hat{V}(\mathbf{r})$.

Thus, for a crystal with dislocations the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian can be generally found from the usual $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian for a perfect crystal by substitutions

$$\nabla\rightarrow\nabla+\hat{\mathbf{A}}(\mathbf{r})\ ,\quad \hat{V}_0\rightarrow\hat{V}_0+\delta\hat{V}(\mathbf{r})\ , \qquad (35)$$

where $\hat{\mathbf{A}}(\mathbf{r})$ is given in Eq. (34) and describes the changes in the kinetic energy operator while $\delta\hat{V}(\mathbf{r})$ describes the changes in the potential energy operator. Using Eqs. (2) and (3) we can write the explicit expression for the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian for a crystal with dislocations in the following way:

$$\hat{H}(\nabla,\mathbf{r})=\sum_{l,q}\hat{P}_l\{\hat{M}_{lq}+\delta\hat{M}_{lq}(\mathbf{r})\}\hat{P}_q+\hat{V}_0+\delta\hat{V}(\mathbf{r})\ , \qquad (36)$$

where $\mathbf{P}=\hat{\mathbf{p}}-i\hbar(\nabla+\hat{\mathbf{A}})$ and matrices $\hat{M}_{lq}$ and $\delta\hat{M}_{lq}(\mathbf{r})$ are

$$\hat{M}_{lq}=\frac{\delta_{lq}}{2m}+\frac{i}{4m^2c^2}\sum_s e_{slq}\hat{\sigma}_s\hat{V}_0\ ,$$
$$\delta\hat{M}_{lq}(\mathbf{r})=\frac{i}{4m^2c^2}\sum_s e_{slq}\hat{\sigma}_s\delta\hat{V}(\mathbf{r})\ . \qquad (37)$$

To find an effective-mass Hamiltonian, second-order perturbation theory can be applied to Eq. (36), which gives

$$\hat{H}^{\mathrm{eff}}_{n,n'}(\nabla,\mathbf{r})=\hat{H}^{(1)}_{n,n'}(\nabla,\mathbf{r})$$
$$+\sum_m\frac{\hat{H}^{(2)}_{n,m}(\nabla,\mathbf{r})\hat{H}^{(2)}_{m,n}(\nabla,\mathbf{r})}{E_m-E_n}\ , \qquad (38)$$

where $\hat{H}^{(1)}_{n,n'}(\nabla,\mathbf{r})$ and $\hat{H}^{(2)}_{n,n'}(\nabla,\mathbf{r})$ are the diagonal and nondiagonal parts of $\hat{H}(\nabla,\mathbf{r})$, respectively. For a simple band extremum with inversion symmetry we can find an expression for the effective-mass Hamiltonian with an accuracy up to terms proportional to β, ∇^2, and $\beta\nabla$ and neglecting the terms containing higher powers of β and ∇ or coordinate derivatives of β:

$$\hat{H}^{\mathrm{eff}}_{n,n'}(\nabla,\mathbf{r})=\hat{H}^{\mathrm{eff}(0)}_{n,n'}(\nabla+\hat{\mathbf{A}}_2,\mathbf{r})+\sum_{i,j}\varepsilon_{ij}D^{ij}_{n,n'}\ , \qquad (39)$$

where part, $\hat{\mathbf{A}}_2(\mathbf{r})=-i\beta^T(\mathbf{r})k_\alpha$, of the gauge potential contributes to the kinetic energy in $\hat{H}^{\mathrm{eff}}_{n,n'}(\nabla,\mathbf{r})$ while the part $\hat{\mathbf{A}}_1(\mathbf{r})=i\beta^T(\mathbf{r})\hat{\mathbf{p}}/\hbar$ contributes to the deformation potential tensor $D^{ij}_{n,n'}$:

$$D^{ij}_{n,n'}=\frac{\partial\left\{\delta\hat{V}+\sum_{l,q}(\hat{\mathbf{A}}_{1,l}\hat{M}_{lq}\hat{\mathbf{p}}_q+\hat{\mathbf{p}}_l\hat{M}_{lq}\hat{\mathbf{A}}_{1,q})\right\}_{n,n'}}{\partial\varepsilon_{ij}}\ . \qquad (40)$$

The effective gauge potential $\hat{\mathbf{A}}_2(\mathbf{r})$ is magnetic-field-like and the corresponding flux confined inside a dislocation line, of the effective magnetic field given in Eq. (24), is determined by the scalar product of the dislocation

Burgers vector $\mathbf{b}$ and wave vector $\mathbf{k}_\alpha$:

$$\Phi=\int_S dS_j e_{jkl}\hat{F}_{kl}=-\frac{(\mathbf{k}_\alpha\cdot\mathbf{b})}{2\pi}\Phi_0\ , \tag{41}$$

where $\Phi_0=i/2\pi$ is the flux quantum and the integral is over the defect core cross section area S. For the case of a dislocation with Burgers vector equal to a primitive lattice translation and a band extremum at the edge of Brillouin zone the scalar product $(\mathbf{k}\cdot\mathbf{b})$ can take values $n\pi$, where n is an integer. Therefore, it follows from Eq. (41) that in this case the flux confined inside the dislocation core can take only integer or half-integer values. In the first case, the gauge potential does not affect electrons in a crystal, but in the latter case the flux should strongly influence the election motion and the shallow bound states in the crystal volume.

V. CONCLUSIONS

In this paper we have found a general expression for the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian for crystals with linear topological defects. This expression contains gauge potential terms which generally correspond to a non-Abelian gauge group. The gauge field is confined inside the defect cores and can influence the motion of free carriers as well as shallow bound states in the vicinity of defect lines.

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