PHYSICAL REVIEW
LETTERS

VOLUME 80 16 MARCH 1998 NUMBER 11

Single-Particle Quantum States in a Crystal with Topological Defects

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(Received 27 May 1997)

The influence of frozen-in topological defects in a crystal on the long-wavelength quantum states of a particle is considered. In the continuum limit of a conveniently defined tight-binding model one is led to a covariant Schrödinger equation on a Riemann-Cartan manifold. When the tight-binding transfer energies are assumed to depend on the local lattice deformations caused by the defects, additional noncovariant terms are generated in the Hamiltonian. These terms generate bound states of the particle to edge dislocations and enhance the scattering of particles on screw dislocations. [S0031-9007(98)05432-5]

PACS numbers: 02.40.Ky, 61.72.Lk, 72.10.Fk

The dynamics of a particle on a Riemann-Cartan manifold, i.e., a manifold with curvature and torsion, has attracted much interest in various branches of physics ranging from general relativity to solid state physics. In gravitation theory the curvature and torsion of space are generated by the mass and spin degrees of freedom of the matter fields; see, e.g., Ref. [1]. Solid and liquid crystals with topological defects in the continuum limit can also be described by a Riemann-Cartan manifold where now the curvature and torsion fields are proportional to the topological charge densities of the defects [2,3]. For instance, the Burgers vector of a dislocation gives rise to a torsion and the Frank angle of a disclination to a curvature of the manifold.

We recently have analyzed the classical diffusion of a Brownian particle on a Riemann-Cartan manifold representing a crystal with frozen-in topological defects [4]; see also Ref. [5]. In an identical setting we now want to establish a general framework for the discussion of the long-wavelength quantum states of a single particle, e.g., an electron. A major advantage of our approach is that it reconciles some seemingly incompatible results of previous investigations.

On the basis of the deformation potential approximation (see, e.g., Ref. [6]), Lifshitz and Pushkarov found an infinite number of bound states of a particle to an edge dislocation [7]. By similar arguments Kosevich pointed out the possible existence of bound states to screw dislocations [8]. On the other hand, in a purely geometric approach Kawamura observed Aharonov-Bohm–type interference effects in the scattering process of a particle on a screw-dislocation line [9]. In that treatment no binding potential shows up to dislocations of any kind, although the physics of the deformation potential method is claimed to be incorporated [10]. Our expositions will clarify the relation of the two different approaches including their physical implications.

Guided by the picture of a classical random walk of a particle in a topologically distorted crystal, we start off in the quantum case from a tight-binding model on a d-dimensional lattice which coherently is deformed due to the presence of frozen-in topological defects. With the notations $\boldsymbol{n}$ for the position vectors of the lattice sites and $\boldsymbol{a}(\boldsymbol{n})$ for the vectors pointing from $\boldsymbol{n}$ to the nearest-neighbor sites of $\boldsymbol{n}$ our model Hamiltonian reads

$$H = -\frac{1}{2}\sum_{\boldsymbol{n}} a^d \sum_{\boldsymbol{a}(\boldsymbol{n})} t(\boldsymbol{a}(\boldsymbol{n})) \times [\varphi^\dagger(\boldsymbol{n} + \boldsymbol{a}(\boldsymbol{n}))\varphi(\boldsymbol{n}) + \varphi^\dagger(\boldsymbol{n})\varphi(\boldsymbol{n} + \boldsymbol{a}(\boldsymbol{n}))]. \quad (1)$$

0031-9007/98/80(11)/2257(4)$15.00

Here a^d is the volume of the unit cell of the undistorted lattice, $t(\boldsymbol{a}(\boldsymbol{n}))$ is the transfer energy along the bond $\boldsymbol{a}(\boldsymbol{n})$, and $\varphi^\dagger$, φ are the particle creation and annihilation operators obeying the commutation (or anticommutation) relations

$$[\varphi(\boldsymbol{n}), \varphi^\dagger(\boldsymbol{m})] = \frac{1}{a^d}\,\delta_{\boldsymbol{n},\boldsymbol{m}}\,. \tag{2}$$

In order to reveal the long-wavelength quantum states of the particle, one has to expand the φ operators depending on $\boldsymbol{a}(\boldsymbol{n})$ in (1) to second order in the lattice constant a of the undistorted lattice. This is most easily done for a simple cubic lattice for which the set of vectors $\boldsymbol{a}(\boldsymbol{n})$ can be written in terms of two subsets as

$$\{\boldsymbol{a}(\boldsymbol{n})\} = \{\boldsymbol{a}_\alpha(\boldsymbol{n}), -\boldsymbol{a}_\alpha(\boldsymbol{n} - \boldsymbol{a}_\alpha(\boldsymbol{n}))\}, \qquad \alpha = 1, \ldots, d\,, \tag{3}$$

with the components

$$a^i_\alpha(\boldsymbol{n}) = aB^i_\alpha(x)\,. \tag{4}$$

The matrix field $B^i_\alpha(x)$ is determined by the distortion tensor $\beta_i{}^j(x)$ of the defects via the relations $B^\alpha_i B^j_\alpha = \delta_i{}^j$, $B^\alpha_i B^i_\beta = \delta^\alpha{}_\beta$, and $B^\alpha_i \delta^j_\alpha = \delta_i{}^j + \beta_i{}^j$. It also provides the continuum description of the distorted crystal by a Riemann-Cartan manifold with the metric tensor and affine connection [2]

$$g_{ij} = B^\alpha_i B^\beta_j \delta_{\alpha\beta}, \qquad \Gamma_{ij}{}^k = B^k_\alpha \partial_i B^\alpha_j\,, \tag{5}$$

and the notation g^{ij} for the inverse of g_{ij}. The covariant derivative ∇_i implied by the affine connection in (5) commutes with the metric since $\nabla_k g_{ij} \equiv \partial_k g_{ij} - \Gamma_{ki}{}^l g_{lj} - \Gamma_{kj}{}^l g_{il} = 0$. Whereas the gradient of some scalar Φ 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

$$\nabla^T_i \equiv \nabla_i + 2T_{ij}{}^j \tag{6}$$

with the torsion tensor

$$T_{ij}{}^k \equiv \tfrac{1}{2}(\Gamma_{ij}{}^k - \Gamma_{ji}{}^k)\,, \tag{7}$$

which measures the defect density [2]. For practical calculations it is convenient to use the form $(1/\sqrt{g})\partial_i\sqrt{g}$ for the operator (6) where g is the Jacobian of the metric tensor (5). The distortion tensor and consequently the quantities (5)–(7) are explicitly known for the most familiar topological defects [2].

We now consider the continuum limit of the Hamiltonian (1) for a model with a distortion-independent transfer energy $t = \hbar^2/(2ma^2)$ where m is an effective mass of the particle. This allows one to express H in terms of the operator $S(a) \equiv \sum_{\boldsymbol{a}(\boldsymbol{n})} \varphi(\boldsymbol{n} + \boldsymbol{a}(\boldsymbol{n}))$ which will be expanded up to second order in a. In (1) the lowest-order result $S(0) = 2d\varphi(x)$ merely leads to a constant energy shift for the particle, and the first-order term vanishes by inversion symmetry, valid to linear order in a [due to (3)]. For the second-order coefficient $S''(0)/2$ Eqs. (4)–(7) imply the expression

$$\begin{aligned}\sum_\alpha B^i_\alpha B^j_\alpha \partial_i\partial_j\varphi \;+\; \sum_\alpha B^i_\alpha(\partial_i B^j_\alpha)\partial_j\varphi \\ = g^{ij}\partial_i\partial_j\varphi \;-\; g^{ik}\Gamma_{ik}{}^j\partial_j\varphi \\ = g^{ij}[\nabla^T_i\nabla_j \;-\; 2T_{ik}{}^k\nabla_j]\varphi\,,\end{aligned} \tag{8}$$

which equipped with a factor a^2 has to be inserted into (1). After passage from the lattice sum including the factor a^d to an integral over the invariant volume element $d^dx\sqrt{g(x)}$, a few partial integrations and use of the identity $\partial_i\sqrt{g} = \Gamma_{ik}{}^k\sqrt{g}$ lead to the result

$$H = -\frac{\hbar^2}{2m}\int d^dx\,\sqrt{g}\,\varphi^\dagger[\,g^{ij}\nabla^T_i\nabla_j + (\,g^{ij}\nabla^T_i T_{jk}{}^k)]\varphi\,, \tag{9}$$

where, corresponding to (2), the operators $\varphi, \varphi^\dagger$ obey the commutation relations

$$[\varphi(x), \varphi^\dagger(y)] = \frac{1}{\sqrt{g(x)}}\,\delta(x - y)\,. \tag{10}$$

The Hamiltonian (9) is manifestly covariant; i.e., it has the same form for arbitrary types and configurations of topological defects. This reflects the purely geometric particle motion on the lattice in the present case. In a gradient expansion of the Hamiltonian covariance alone would allow an undetermined coupling constant in the potential part. This is reminiscent of a proper choice for the prefactor of the curvature term in a quantum system on a Riemann manifold [11].

The expression $g^{ij}\nabla^T_i\nabla_j$ in the kinetic part of (9) is identical to the Laplace-Beltrami operator $(1/\sqrt{g})\partial_i\sqrt{g}\,g^{ij}\partial_j$ and in general differs from the operator $g^{ij}\nabla^T_i\nabla^T_j$ entering the diffusion equation on a manifold [4]. Also, our Hamiltonian is self-adjoint in contrast to the operator $g^{ij}\nabla_i\nabla_j$ favored by Kleinert [12].

The potential energy in (9) is proportional to the divergence of the torsion vector $T^i \equiv g^{ij}T_{jk}{}^k$ which is the only nontrivial scalar of the manifold in addition to the scalar curvature R. Whereas one finds $\nabla^T_i T^i = 0$ for screw dislocations and $\nabla^T_i T^i \neq 0$ for edge dislocations, the condition $R = 0$ is valid for both types of dislocations [2]. As an example of a defect with $R \neq 0$ we mention a kind of disclination defined by a distortion field $B^\alpha_i(x)$ which describes local rotations of the lattice [12] and implies $\nabla^T_i T^i = R/4$.

In case of a three-dimensional crystal with a single screw-dislocation line along the z axis with Burgers vector $\boldsymbol{b} = b\boldsymbol{e}_z$, Eq. (9) leads in terms of cylinder coordinates to the Schrödinger equation

$$\begin{aligned}i\hbar\partial_t\psi(x,t) = -\frac{\hbar^2}{2m}\left[\Delta + \frac{b}{\pi r^2}\left(\partial_\phi\partial_z + \frac{b}{4\pi}\,\partial_z^2\right)\right] \\ \times\,\psi(x,t)\,,\end{aligned} \tag{11}$$

where Δ stands for the usual Laplacian in Euclidean space. According to Kawamura [9] this equation

converts an incident (stationary) wave $\psi_0(r,\phi,z) = \exp[-i(qr\cos\phi - kz + \phi kb/2\pi)]$ with transverse and longitudinal wave numbers q, k into an Aharonov-Bohm scattering wave $\psi_s(r,\phi,z)$ which obeys the condition $\psi_0(0,\phi,z) + \psi_s(0,\phi,z) = 0$ [13], and for $r \to \infty$ and $\phi \neq \pi$ has the asymptotic behavior $\psi_s(r,\phi,z) = (2\pi iqr)^{-1/2}\exp[i(qr + kz)]f(\phi)$ with the scattering amplitude

$$f(\phi) = \sin(kb/2)\,\frac{e^{i(k/|k|)(\phi-\pi)/2}}{\cos(\phi/2)}\,. \tag{12}$$

However, ψ_0 and ψ_s are independent stationary states of (11) so that the general solution is given by the superposition $\psi(r,\phi,z) = \psi_0(r,\phi,z) + [1 - \psi(0,0,0)]\psi_s(r,\phi,z)$. Here, the value $\psi(0,0,0)$ should be considered as a parameter which, due to the breakdown of the continuum approximation at $r = 0$, has to be determined by a lattice calculation. The term $\propto\psi(0,0,0)$ reduces the Aharonov-Bohm interferences, and in the worst case $\psi(0,0,0) = \psi_0(0,0,0)$ suppresses them completely. It will be shown below that a screw dislocation in general is dressed by a repulsive potential $V(r) \propto 1/r^2$ which implies $\psi(0,\phi,z) = 0$ but also considerably modifies the scattering amplitude (12).

For the case of an edge dislocation line along the z axis of a three-dimensional isotropic elastic medium with Burgers vector $\boldsymbol{b}$ Eq. (9) leads, contrary to the quite different result in [9], to the Schrödinger equation

$$i\hbar\partial_t\psi(x,t) = -\frac{\hbar^2}{2m}\left\{\Delta - \frac{b}{2\pi(1-\nu)r}\left[(1-2\nu)(\sin\phi)(\Delta - \partial_z^2) - \frac{1}{r}\left(\partial_r\partial_\phi\cos\phi + r\partial_r\frac{1}{r}\cos\phi\,\partial_\phi\right)\right] + \frac{1}{2}[\boldsymbol{b}\times\nabla\delta(\boldsymbol{r})]_z\right\}\psi(x,t)\,, \tag{13}$$

where ν is the Poisson ratio, $\boldsymbol{r} \equiv (r\cos\phi, r\sin\phi)$, and $\nabla \equiv \partial/\partial\boldsymbol{r}$. Elastic stability requires $-1 < \nu < 1/2$ and consequently rules out the singular cases $\nu = 1/2, 1$ in (13). The appearance of the parameter ν in the Schrödinger equation is to be expected because the lattice deformations are determined by the elastic properties of the crystal. Accidentally this is not the case for the screw-dislocation result (11) due to the isotropy of the distortion field around the dislocation line.

One of the most interesting physical questions in the present case is whether (13) allows the formation of bound states of the particle to the defect. The answer to this question is negative since in dimension $d = 2$ an attractive δ potential as well as its derivative are known to have no bound states [14]. This also rules out the possibility of bound states for the above-mentioned disclinationlike defects for which one finds $\nabla_i^T T^i = (\Omega/2)\delta(\boldsymbol{r})$ with a Frank angle Ω. 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 [15].

In general, the transfer energies $t(\boldsymbol{a}(\boldsymbol{n}))$ are not constant but will depend on the local lattice deformations caused by the defects. The simplest model of such a dependence follows by replacing the lattice constant a in the deformation-independent transfer energies by the actual lengths of the vectors $\boldsymbol{a}(\boldsymbol{n})$. Because of (4) this leads for the first subset in (3) to the expression

$$t_\alpha(x) = \frac{\hbar^2}{2ma^2}\,\frac{1}{\delta_{ij}B^i_\alpha(x)B^j_\alpha(x)}\,, \tag{14}$$

which, within the following approximations, also applies to the second subset in (3). It is important to use the Euclidean metric in (14) since the bond lengths in the lattice have to be measured by an observer in the laboratory system. As a consequence, insertion of (14) into the model (1) leads to additional noncovariant terms in the kinetic and in the potential parts of the Hamiltonian (9).

In the case of a single edge dislocation the additional potential energy in the Schrödinger equation (13) reads, to lowest order in the distortion tensor $\beta_i{}^j(x)$,

$$V(r,\phi) = -\frac{\hbar^2}{2ma^2}\,4\,\mathrm{Tr}(\beta) = \frac{\hbar^2}{2ma^2}\,\frac{1-2\nu}{1-\nu}\,\frac{2b\sin\phi}{\pi r}\,. \tag{15}$$

For wave numbers $q, k \ll a^{-1}$, and for $r \neq 0$ this potential dominates all correction terms to the Laplacian in (13) including those arising from (14) in the kinetic energy. Therefore, in leading order the Hamiltonian of the system reduces to $H(k,\boldsymbol{p},\boldsymbol{r}) = (\hbar k)^2/2m + \boldsymbol{p}^2/2m + V(\boldsymbol{r})$ where $\boldsymbol{p}$ means the operator $(\hbar/i)\partial/\partial\boldsymbol{r}$.

The potential $V(\boldsymbol{r})$ as given by (15) has a long-ranged attractive section in the plane transverse to the dislocation line. As pointed out by Lifshitz and Pushkarov [7] this implies the existence of 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 [16]. This means that in terms of the classical Hamiltonian $N = h^{-2}\int d^2p\; d^2r\,\Theta[E - H(k,\boldsymbol{p},\boldsymbol{r})]$ which, solved for E, leads to the result

$$E_N(k) = \frac{(\hbar k)^2}{2m} - \left(\frac{b}{2\pi a}\,\frac{1-2\nu}{1-\nu}\right)^2\frac{\hbar^2}{2ma^2}\,\frac{1}{N}\,. \tag{16}$$

The coefficient of the $1/N$ term specifies the phenomenological coupling constant in the treatment by Lifshitz and

Pushkarov [7]. Corrections to the quasiclassical approximation give rise to higher-order terms in $1/N$.

In the case of a screw dislocation the potential arising from (14) turns out to be

$$V(r) = \frac{\hbar^2}{2ma^2}\, 2\ \mathrm{Tr}(\beta\beta^T) = \frac{\hbar^2}{2ma^2}\,\frac{b^2}{2\pi^2 r^2}\,. \qquad (17)$$

A potential of this form with an undetermined prefactor has also been found in a phenomenological approach by Kosevich [8] who argues that in some semiconductors the prefactor might be negative 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.

There is, however, a significant contribution of the potential (17) to the scattering properties of a particle on a screw dislocation, especially in case of an incident wave vector with $k = 0$ which, according to (11), does not even see the dislocation. In order to support the Aharonov-Bohm interferences, the regime $k \gg q$ should be chosen for the incident wave vector. Then, for consistency, one has to add in (11) the term $V(r)[1 + (1/2)(a\partial_z)^2]\psi(x,t)$ generated by (14). Stationary solutions of the resulting Schrödinger equation can be expanded in terms of the exact eigenfunctions $J_{|\lambda|}(qr)\exp(i\mu\phi)\exp(ikz)$ where $J_{|\lambda|}$ is a Bessel function with $\lambda^2 = (\mu + kb/2\pi)^2 + (b^2/2\pi^2a^2)[1 + (1/2)(ka)^2]$, and μ is an integer. For an incident wave of the previous form ψ_0 this leads to $\psi = \psi_0 + \psi_s$ where ψ_s looks as before, however, with the new scattering amplitude

$$f(\phi) = -\frac{b^2}{2\pi^2a^2}\left[1 - \frac{(ka)^2}{2}\right]e^{-i(kb-\pi)/2} \times \sum_{\mu=-\infty}^{\infty} \frac{e^{i\mu(\phi-\pi)}}{\lambda(\mu)}\left[\frac{1 - e^{-i[\lambda(\mu)-\mu-kb/2\pi]\pi}}{\lambda(\mu) - \mu - kb/2\pi} + \frac{1 - e^{-i[\lambda(\mu)+\mu+kb/2\pi]\pi}}{\lambda(\mu) + \mu + kb/2\pi}\right]. \qquad (18)$$

Partial waves with different μ, i.e., different angular momenta, interfere in the differential scattering cross section (per unit length of the dislocation line) $d\sigma/d\phi = (2\pi q)^{-1}|f(\phi)|^2$. The latter is even in ϕ and, by numerical evaluation of (18), turns out to increase monotonically from $\phi = 0$ to $\phi = \pi$ where it has an artificial singularity due to the far-field approximation for ψ_s [13]. Qualitatively this behavior is similar to that following from (12), however, without a reduction of the scattering part due to a nonzero value of $\psi(0,0,0)$ in the present case.

As a final remark we point out that our approach differs from most of the previous discussions of the problem by a systematic use of the continuum theory of defects [2] and by imposing covariance of the model with constant transfer rates. The inclusion of a dependence of these rates on the lattice deformations necessarily leads to noncovariant terms in the Hamiltonian since in the opposite case $t(x)$ should be a scalar and therefore must depend on x through the quantities $\nabla_i T^i(x)$ and $R(x)$. These, however, vanish everywhere in the crystal except at the cores of the defects.

We gratefully acknowledge helpful discussions with Rolf Burghaus, Georg Foltin, Arnold M. Kosevich, and Valery Pokrovski. This work has been supported by the Deutsche Forschungsgemeinschaft under SFB 237 and by the KBN (Poland) Grant No. 2 P03B 117 12.

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