Torsion and electron motion in quantum dots with crystal lattice dislocations

1999 J. Phys. A: Math. Gen. 32 571

(http://iopscience.iop.org/0305-4470/32/4/004)

J. Phys. A: Math. Gen. **32** (1999) 571–584. Printed in the UK PII: S0305-4470(99)92204-7

Torsion and electron motion in quantum dots with crystal lattice dislocations

Erik Aurell

Department of Mathematics, Stockholm University S-106 91 Stockholm, Sweden
and
PDC/KTH, S-100 44 Stockholm, Sweden

Received 4 March 1998

Abstract. The motion of a conducting electron in a quantum dot, with one or several dislocations in the underlying crystal lattice, is considered in the continuum picture, where dislocations are represented by torsion of space. The possible effects of torsion are investigated on the levels of classical motion, on non-relativistic quantum motion, and on spin–torsion coupling terms derivable in the non-relativistic limit of generalizations of the Dirac equation in a space with torsion. Finally, phenomenological spin–torsion couplings analogous to Pauli terms are considered in the non-relativistic equations. Different prescriptions of classical and non-relativistic quantum motion in a space with torsion are shown to give effects that should, in principle, be observable. Semiclassical arguments are presented to show that torsion is not relevant for the classical motion of the centre of a wavepacket. The correct semiclassical limit can instead be described as classical trajectories in a Hamiltonian given by the band energy. In the special case of a spherically symmetric band this motion reduces to straight lines, independently of local crystal orientations. By dimensional analysis the coupling constants of the possible spin–torsion interactions are postulated to be proportional to a combination of the effective mass of the electron, m_{eff}, the lattice constant, a, and $\hbar$. The level splitting is then very small with transition frequencies of the order of 1 kHz, or smaller.

1. Introduction

Quantum dots are small essentially two-dimensional conducting domains, connected to external leads by tunnel barriers such that the number of conducting electrons is quantized. The elastic mean free path and the dephasing length may, under appropriate circumstances, be much larger than the lateral size of the dots. The motion of an electron inside may therefore to a first approximation be considered as ballistic. These structures may hence in many respects be regarded as physical realizations of the quantum mechanics textbook examples of motion in two-dimensional potential wells. For recent reviews and papers, see [1–8].

The purpose of this paper is to explore a suggestion made in a book and in a series of papers by Kleinert and co-workers [9–11], which I will state compactly as follows: (a) the motion of a quantum particle in a space with torsion has several distinct features compared to free motion in flat space; (b) a crystal with defects may in the continuum picture be described as a space with torsion; (c) the motion of an electron around a defect may thus in some circumstances be modelled by the motion of a quantum particle in a space with torsion.

A continuum description of a crystal is valid at distances much larger than the lattice spacing. The low-lying electronic states in a quantum dot extend across the dot, with typical spatial scale L, while a localized defect extends over a few lattice spacings a. The scale

0305-4470/99/040571+14$19.50

separation L/a is thus in the range of 100–10 000, and it is conceivable that an effective continuum description might be appropriate.

The outline of this paper is as follows. In section 2 I review the literature on motion in spaces with torsion. The Dirac equation coupled to torsion allows for one vector and one axial vector coupling, both of which give rise to Zeeman-like couplings of spin to an axial vector in the non-relativistic limit. We also consider more phenomenologically motivated spin–torsion couplings, which yield similar terms. In section 3 I review elementary aspects of the differential geometry of physics of defects and in section 4 I discuss, on the semiclassical level, the effects of crystal torsion on electron motion. In section 5 I try to evaluate possible torsion-induced effects in quantum dots. In section 6 I summarize the results. They are negative as concerns the proposal by Kleinert that autoparallels should play a privileged role. On the semiclassical level it is possible to observe motion along geodesics, but such motion is insensitive to torsion. Motion along autoparallels and a related non-relativistic quantum mechanics could also probably be disproved by experiments. The spin–torsion coupling terms are not theoretically unsound, but lead to such very weak effects that they would be difficult to observe.

2. Classical and quantum motion in a space with torsion

In this section I use the Einstein conventions of summing over repeated indices and raising and lowering indices by the metric tensor g_{ij} and its inverse g^{ij}. For conventions pertaining to the affine connection, torsion and contorsion I follow Hehl *et al* [12], see also Schrödinger [13] and Schouten [14].

A manifold is said to carry metric and affine structure if one can compute the length of vectors in the tangent space by

$$|A|^2 = g_{ij} A^i A^j \tag{1}$$

and parallel transport of a vector along an infinitessimal distance $\mathrm{d}\vec{x}$ by

$$A^i \to A^i - \Gamma_{kj}{}^i A^j \, \mathrm{d}x^k. \tag{2}$$

The metric and the affine connection Γ are connected by the compatibility condition, that the scalar product of two arbitrary vectors is invariant under parallel transport:

$$g_{ij,k} - g_{lj}\Gamma_{ki}{}^l - g_{il}\Gamma_{kj}{}^l = 0 \tag{3}$$

which may also regarded as the statement that g is covariantly constant. The first term in (3) stands for the partial derivative $\partial g_{ij}/\partial x^k$.

The standard form of the solution of (3) is

$$g_{il}\Gamma_{kj}{}^l = g_{il}\left\{ \begin{matrix} l \\ kj \end{matrix} \right\} - K_{kji} \qquad \left\{ \begin{matrix} l \\ kj \end{matrix} \right\} = \tfrac{1}{2} g^{lm}(g_{mj,k} + g_{mk,j} - g_{kj,m}) \tag{4}$$

where we recognize the Cristoffel symbol $\left\{ \begin{matrix} l \\ kj \end{matrix} \right\}$, symmetric under the interchange of j and k. The second term in (4), K_{kji}, is known as contorsion and must be antisymmetric under the interchange of the last two indices of j and i.

Let us consider a small area spanned by two vectors $\mathrm{d}x_{(1)}$ and $\mathrm{d}x_{(2)}$. If we transport $\mathrm{d}x_{(2)}$ along $\mathrm{d}x_{(1)}$ it will change into (in component form) $\mathrm{d}x^i_{(2)} - \Gamma_{kj}{}^i \, \mathrm{d}x^j_{(2)} \, \mathrm{d}x^k_{(1)}$. If we move first along $\mathrm{d}x_{(1)}$ and then along $\mathrm{d}x_{(2)}$ we will hence end up with a displacement (in component form)

$$\mathrm{d}P^i_{12} = \mathrm{d}x^i_{(1)} + \mathrm{d}x^i_{(2)} - \Gamma_{kj}{}^i \mathrm{d}x^j_{(2)} \, \mathrm{d}x^k_{(1)}. \tag{5}$$

If we were, on the other hand, to make the displacements in the opposite order we would end up at

$$\mathrm{d}P^i_{21} = \mathrm{d}x^i_{(2)} + \mathrm{d}x^i_{(1)} - \Gamma_{kj}{}^i \mathrm{d}x^j_{(1)}\,\mathrm{d}x^k_{(2)}. \tag{6}$$

The difference between these displacements is a vector, which measures by how much the circuit fails to close if direction vectors are parallel transported around the perimeter of the area spanned by $\mathrm{d}x_{(1)}$ and $\mathrm{d}x_{(2)}$

$$\mathrm{d}B^i = \mathrm{d}P^i_{12} - \mathrm{d}P^i_{21} = \Gamma_{kj}{}^i\big(\mathrm{d}x^j_{(1)}\,\mathrm{d}x^k_{(2)} - \mathrm{d}x^j_{(2)}\,\mathrm{d}x^k_{(1)}\big). \tag{7}$$

The parentheses in (7) is the area element $\mathrm{d}A_{12}{}^{jk}$ spanned by $\mathrm{d}x_{(1)}$ and $\mathrm{d}x_{(2)}$. The part of Γ antisymmetric in interchange of j and k is called torsion, and has hence the following relation to $\mathrm{d}B$ (in component form follows):

$$\mathrm{d}B^i = -S_{kj}{}^i\,\mathrm{d}A_{12}{}^{kj} \qquad S_{kj}{}^i = \Gamma_{[kj]}{}^i. \tag{8}$$

Torsion is therefore a third-order tensor, and it may be connected to contorsion by

$$K_{ijk} = -S_{ijk} + S_{jki} - S_{kij} \tag{9}$$

from which it is seen that the required antisymmetricity of K (in the last two indices) follows from the antisymmetricity of S (in the first two indices). As a final consistency check one may antisymmetrize Γ using the decomposition of (4):

$$\begin{aligned}\Gamma_{[kj]}{}^i &= \left\{ \begin{matrix} i \\ [kj] \end{matrix} \right\} - K_{[kj]}{}^i = 0 - \tfrac{1}{2}\big(K_{kj}{}^i - K_{jk}{}^i\big) \\ &= \tfrac{1}{2}\big(S_{kj}{}^i - S_{jk}{}^i\big) = S_{kj}{}^i. \end{aligned} \tag{10}$$

The symmetric part of $\Gamma_{kj}{}^i$ under interchange of k and j thus contains both the Cristoffel symbol and a symmetrized combination of the antisymmetric part; this explains the distinction between contorsion and torsion.

The geodesics on a manifold are given by

$$\frac{\mathrm{d}^2x^i}{\mathrm{d}\tau^2} + \left\{ \begin{matrix} i \\ jk \end{matrix} \right\} \frac{\mathrm{d}x^j}{\mathrm{d}\tau}\frac{\mathrm{d}x^k}{\mathrm{d}\tau} = 0 \qquad \text{(geodesics)}. \tag{11}$$

The intuitive concept of free motion seems, however, to imply that velocity vectors change according to the law of parallel transport, and such curves are called autoparallels:

$$\frac{\mathrm{d}^2x^i}{\mathrm{d}\tau^2} + \Gamma_{kj}{}^i \frac{\mathrm{d}x^j}{\mathrm{d}\tau}\frac{\mathrm{d}x^k}{\mathrm{d}\tau} = 0 \qquad \text{(autoparallels)}. \tag{12}$$

The interesting observation stressed by Kleinert is then that in a space with torsion geodesics and autoparallels do not coincide. It is not obvious which of the two is the most natural extrapolation from ordinary classical mechanics. For different points of view, see, on the side of autoparallels, Kleinert [9–11], and on the side of geodesics Hehl *et al* [12], Audretsch [23], and the recent papers of Lämmerzahl [24] and Barros e Sá [15].

In any case, from the viewpoint of Hamiltonian dynamics autoparallels have peculiar features. One of the simplest examples is motion on a two-dimensional surface with constant diagonal metric and constant torsion. The torsion tensor has then only two independent non-zero components, namely S_{121} and S_{122}, which together specify a direction in the plane, $\vec{b} = (S_{121}, S_{122})$. It is here straightforward to integrate equations (12): they describe motion at constant speed, but where the direction of velocity changes so as to be orthogonal to $\vec{b}$. In other words, kinetic energy in the ordinary sense is conserved, but momentum and phase space volume is not. In these respects motion along autoparallels in a space with torsion is similar to a mechanical system with non-holonomic constraints [16, 17] (for analytic and numerical

investigations of a clarifying concrete example, see [18–20]), an analogy also used extensively by Kleinert.

The difference between autoparallels and geodesics carries over to the quantum mechanics of a non-relativistic scalar particle. The gradient of a scalar is a vector, and the covariant derivative of this vector involves the connection, so that the contraction of two covariant derivatives acting on a scalar is

$$g^{ij} D_i D_j \psi = g^{ij} D_i \partial_j \psi = \left(g^{ij} \partial_i \partial_j - g^{ij} \Gamma_{ij}{}^{l} \partial_l\right)\psi. \tag{13}$$

The usual generalization of the kinetic term in the Schrödinger equation involves, on the other hand, the Laplace–Beltrami operator

$$\frac{1}{\sqrt{g}}\left(\partial_i g^{ij} \sqrt{g} \partial_j\right)\psi = \left(g^{ij} \partial_i \partial_j - g^{ij} \left\{ \begin{matrix} l \\ ij \end{matrix} \right\} \partial_l\right)\psi \tag{14}$$

which is self-adjoint with respect to the standard scalar product $\langle \eta | \psi \rangle = \int \sqrt{g} \eta^* \psi$.

The difference between (13) and (14) is a gradient

$$K_i{}^{il} \partial_l \psi = -2 S^l \partial_l \psi \qquad S_l = S_{li}{}^{i} \tag{15}$$

which, as remarked by Kleinert, is not in general self-adjoint, at least not with respect to the same scalar product. Quantum dynamics governed by (13) is therefore not necessarily unitary. This somewhat disturbing property can be compared with the fact that the phase space volume in the usual sense is not conserved by classical motion along autoparallels.

The problem of geodesics versus autoparallels can also finally be considered, albeit a little indirectly, for relativistic spin-$\frac{1}{2}$ particles. To define spinors in general relativity one needs a system of local intertial frames ξ^α_X, each defined in the neighbourhood of some spacetime point X. The transformation matrix between ξ^α_X and a chosen, in general non-inertial, local coordinate system at X is called a vierbein

$$V^\alpha{}_\mu = \left(\frac{\partial \xi^\alpha_X(x)}{\partial x^\mu}\right)_{x=X}. \tag{16}$$

The first index of the vierbein denotes a direction in the local inertial frame, and is hence lowered and raised with the Minkowski metric η. The second index, in contrast, denotes a direction in the tangent space at X, in a basis determined by the coordinate system x^μ, and is therefore raised and lowered with the metric tensor g.

Parallel transport and covariant differentiation of a spinor in the direction α of the local inertial frame are determined by the vierbeins as

$$\mathcal{D}_\alpha \psi = V_\alpha{}^\mu (\partial_\mu + \Gamma_\mu)\psi \qquad \Gamma_\mu = \tfrac{1}{2} \sigma^{\beta\gamma} V_\beta{}^\nu V_{\gamma\nu;\mu} \tag{17}$$

where $\sigma^{\beta\gamma}$ are the basis elements of infinitesimal Lorentz transformations in the spinor representation, and the semicolon in the last factor stands for covariant differentiation of the vierbein according to

$$V_{\gamma\nu;\mu} = V_{\gamma\nu,\mu} - \left\{ \begin{matrix} \kappa \\ \mu\nu \end{matrix} \right\} V_{\gamma\kappa}. \tag{18}$$

The Dirac equation in a space with curvature is then

$$\mathrm{i}\hbar \gamma^\alpha \mathcal{D}_\alpha \psi + mc\mathbf{1}\psi = 0. \tag{19}$$

For a classical discussion of these matters, see [21]. For a thoroughly modern discussion from the mathematical point of view, see [22].

When we also allow torsion of space we enter into less well chartered territory. One possible way to proceed is to take as building blocks the vierbeins directly, allowing for $V^\alpha{}_{\mu,\nu}$

not necessarily being equal to $V^{\alpha}{}_{\nu,\mu}$. The minimal formal change in the Dirac equation is then to perform the covariant differentiation in (18) using the full affine connection instead of the Cristoffel symbol. However, we also now have torsion as an independent tensor. By contractions we can form a vector $S^l = S^l{}_m{}^m$ and an axial vector $\tilde{S}^l = \epsilon^{lmno} S_{mno}$. The simplest relativistically covariant additional terms in (19) are hence

$$\left(\mathrm{i}C\overline{h}S_\alpha\gamma^\alpha + D\overline{h}\tilde{S}_\alpha\gamma_5\gamma^\alpha\right)\psi \tag{20}$$

where C and D are dimensionless numerical constants. In fact, performing the covariant differentiation in (18) with the affine connection will not bring in any more terms except those in (20). The Dirac equation coupled to torsion by the simplest vector and axial vector couplings and covariant differentiation is thus

$$\mathrm{i}\overline{h}\gamma^\alpha\mathcal{D}_\alpha\psi + \left((C-1)\mathrm{i}\overline{h}S_\alpha\gamma^\alpha + \left(D+\tfrac{1}{6}\right)\overline{h}\tilde{S}_\alpha\gamma_5\gamma^\alpha\right)\psi + mc\mathbf{1}\psi = 0 \tag{21}$$

where the covariant derivative $\mathcal{D}_\alpha$ is defined by (17) and (18). If we also put the constraint that (21) should be derivable by variation from a real action, we are led to the specific choice $C = 1, D = 0$, which is often referred to in the literature as the Dirac equation minimally coupled to torsion [12, 23–25].

I will in the following neglect time components of the spacetime torsion vector S_l. The only non-vanishing component of the axial vector $\tilde{S}_l$ is then $\tilde{S}_0$, which, if we look at it in three dimensions, transforms as a pseudo-scalar. The axial vector coupling in (21) then has the following non-relativistic limit [24]:

$$\mathrm{i}\left(D+\tfrac{1}{6}\right)\frac{\overline{h}^2}{m}\tilde{S}_0\left(\vec{\sigma}\cdot\vec{\partial}\right)\psi \tag{22}$$

where $\vec{\sigma}$ is the vector of Pauli matrices and the derivative acts on the wavefunction to the right.

The vector coupling in (21) is, on the other hand, completely analogous to the coupling to an external electromagnetic field. It will thus, in the non-relativistic limit, give rise to an effect like the coupling of spin and magnetic field

$$\frac{(C-1)}{2}\frac{\overline{h}^2}{m}(\vec{\nabla}\times\vec{S})\cdot\vec{\sigma}\,\psi \tag{23}$$

where $\vec{S}$ denotes the vector of spatial components of the four-dimensional torsion vector.

In summing up this section we see that the equations for autoparallels (12) and the putatitive generalization of the Schrödinger operator as the contraction of two covariant derivatives formed with the affine connection (13) are the odd ones out. Neither arises as the limit of the Dirac equation minimally coupled to torsion, which only gives a spin–torsion coupling reminiscent of a Pauli term, the standard Laplace–Beltrami operator and geodesics.

3. Torsion: continuum representation of defects

The description of defects in crystal lattices in the continuum picture with tools from differential geometry has a distinguished history, described in the 1980 Les Houches lectures of Kröner [26], which also give a good introduction.

The basic idea is quite simple. A crystal is supposed to carry only isolated defects, such that around most points locally one has a perfect lattice. The lattice locally around a point, if continued without defects or deformations indefinitely, may be considered as the tangent space of the crystal at this point. The local lattice directions provide a basis for this space. A vector in the tangent space can then be identified with moving a certain number of lattice units in each direction. Parallel transport of a vector from lattice point P to lattice point Q means that we identify the vector of, say, n_i steps in crystal direction i at P with the vector of

an equal number of steps in the same lattice direction at Q. Since the local lattice directions may change from point to point in the crystal, a vector can change under parallel transport if measured in an external frame of reference.

We can then consider the following process. Take two lattice vectors n_1 and n_2 in directions i_1 and i_2. Transport the pair first along n_1, then along n_2, $-n_1$ and $-n_2$. If the crystal is perfect the circuit closes and we are back at the point where we started.

If, however, the circuit has circled a dislocation line, we are not back at the point of departure. Dislocations lines in three-dimensional crystals are characterized by a vector $\vec{t}$ tangential to the line, and a vector $\vec{b}$ describing the mismatch if we circle the dislocation line in the positive sense determined by $\vec{t}$.

That is, if we introduce a vector $\mathrm{d}A_j$ normal to and equal in length to the area spanned by n_1 and n_2, then the mismatch when going around the circuit is linearly related to $\mathrm{d}A$ by

$$\mathrm{d}b^i = \alpha^{ji}\,\mathrm{d}A_j \tag{24}$$

where α is the density of dislocation lines with $\vec{t}$ in the j direction and $\vec{b}$ in the i direction [26].

The procedure described here is, of course, identical to that used to define the torsion tensor in section 2 so one may introduce a crystal torsion field as

$$S_{kj}{}^{i} = -\tfrac{1}{2}\epsilon_{kjm}\alpha^{mi} \tag{25}$$

where ϵ is the totally antisymmetric Levi-Civita tensor and summation of repeated indices is understood.

In simple three-dimensional crystals with one atom per Bravais cell there are two qualitative types of dislocations: screw dislocations where $\vec{b}$ is parallel to $\vec{t}$ and edge dislocations where $\vec{b}$ is normal to $\vec{t}$ [26–28]. In the first case the dislocation tensor α has only diagonal elements, while in the second case it has only off-diagonal elements.

The totally antisymmetric trace of the crystal torsion field vanishes for edge dislocations since

$$\epsilon^{kji}S_{kji} = -\alpha^{l}{}_{l}. \tag{26}$$

On the other hand, for screw dislocations the contracted torsion vector vanishes since

$$S_i = S_{il}{}^{l} = -\tfrac{1}{2}\epsilon_{ilm}\alpha^{ml}. \tag{27}$$

S_i can hence be looked upon as a vector dual to the antisymmetric part of the dislocation density tensor. For edge dislocations it is normal to both $\vec{b}$ and $\vec{t}$, and equal to half of $\vec{b}$ in length.

4. Geodesics versus autoparallels in crystal space

A crystal space with dislocations but without interstitial defects carries torsion but not curvature [26]. Geodesics in this space means simply straight lines in the frame of reference of an external observer. Autoparallels, on the other hand, means motion which is always in the same direction with respect to the local crystal directions.

The following discussion will be on the level of a semiclassical model. The basic idea is to take a wavepacket, a superposition of Bloch states, and assume that the crystal changes on length scales much larger than the spread of the wavepacket. To construct the Bloch states I can therefore take the crystal lattice close to a given point where the wavepacket is centred and extend it indefinitely in all direction without deformations or defects. This corresponds to the tangent lattice in the sense of section 3. If I go far enough from the point the real lattice and the tangent lattice will differ, but at those distances the amplitude of the wavepacket is assumed vanishingly small, so this difference will be ignored.

More quantitatively, the wavepacket is built from Bloch states with wavevectors in a domain of size Δk around $\boldsymbol{k}$. We assume that Δk is small compared to the dimensions of the Brillouin zone, and that $1/\Delta k$ is small compared to the scale L on which the lattice changes orientation appreciably. In real space the wavepacket is then located in a domain of size $1/\Delta k$ around a centre, which is denoted by $\boldsymbol{r}$.

In the absence of external electric and magnetic fields the equations of motion for the centre of the wavepacket in an undistorted crystal are [27]

$$\dot{\boldsymbol{r}} = \boldsymbol{v}_n(\boldsymbol{k}) = \frac{1}{\hbar}\frac{\partial \mathcal{E}_n(\boldsymbol{k})}{\partial \boldsymbol{k}} \qquad \hbar\dot{\boldsymbol{k}} = 0 \tag{28}$$

where $\hbar\boldsymbol{k}$ is the crystal momentum and $\mathcal{E}_n(\boldsymbol{k})$ is the energy of the state with wavevector $\boldsymbol{k}$ in the nth band. Equation (28) describes motion in a straight line. This picture is valid as long as dispersion effects are not important,

$$t \ll t_{\text{disp}} \sim \frac{\hbar}{(\partial^2 \mathcal{E}_n(\boldsymbol{k}))/\partial \boldsymbol{k}^2 (\Delta k)^2}. \tag{29}$$

To see the effects of the changing crystal before dispersion sets in too strongly we must demand that L is much less than the distance the wavepacket traverses during time t_{disp}, that is

$$\frac{1}{\Delta k} \ll L \ll L_{\text{disp}} \qquad L_{\text{disp}} = \frac{\partial \mathcal{E}_n(\boldsymbol{k})/\partial \boldsymbol{k}}{\partial^2 \mathcal{E}_n(\boldsymbol{k})/\partial \boldsymbol{k}^2}\frac{1}{(\Delta k)^2}. \tag{30}$$

As we will see later, for realistic values of Δk the bounds in (30) are a little tight, but for the present discussion it is sufficient that there are, in principle, some scales of time where the wavepacket is still localized on a length scale much less than L, but has moved a distance much larger than L. In this intermediate regime one can thus pose the problem of whether the wavepacket would follow geodesics or autoparallels or some other curves in crystal space.

Let the motion of the centre of the wavepacket be parametrized by $(x^*(t), \boldsymbol{k}(t))$, both from now on given in a coordinate system fixed in space. The changing orientation of the crystal can then be described by postulating that the band energy $\mathcal{E}_n(\boldsymbol{k}, x)$ is a slowly varying function of x. As the wavepacket moves in the crystal from position $x^*(0)$ at 0 to position $x^*(t)$ at t it acquires a phase of $\exp(\mathrm{i}(S[x^*(t), \boldsymbol{k}(t)])/\hbar)$ where

$$S[x^*(t), \boldsymbol{k}(t)] = \int_0^t [\hbar\boldsymbol{k}(t)\cdot\dot{x}^*(t) - \mathcal{E}_n(\boldsymbol{k}(t), x^*(t))]. \tag{31}$$

The actual path is determined by the condition that S should be stationary under variations. It is obvious that if we introduce the momentum $\boldsymbol{p} = \hbar\boldsymbol{k}$ and the Hamiltonian function $H(\boldsymbol{p}, x) = \mathcal{E}_n(\boldsymbol{p}/\hbar, x)$ the centre will follow the classical trajectories of H.

Let us assume for simplicity that the band energy has the structure $\mathcal{E}_n(\boldsymbol{k}) = \frac{1}{2}\hbar^2 m_{ij}^{-1}\boldsymbol{k}^i\boldsymbol{k}^j$, where m_{ij} is the effective mass tensor, which has principal axes $\hat{n}^{(1)}, \ldots, \hat{n}^{(d)}$ and effective masses in those directions $m_1, \ldots, m_d$. The changing orientation of the crystal is effected by letting the principal axes depend on x. The classical Hamiltonian is then

$$\sum_i \frac{1}{2m_i}(\boldsymbol{p}\cdot\hat{n}^{(i)}(x))^2 = \sum_{jk} g_{jk}(x)\boldsymbol{p}^j\boldsymbol{p}^k \qquad g_{jk}(x) = \sum_i \frac{1}{2m_i}\hat{n}_j^{(i)}(x)\,\hat{n}_k^{(i)}(x). \tag{32}$$

The wavepacket will hence follow the geodesics with respect to the metric g_{ij} induced by the crystal orientations and the band structure.

In the special case of a spherically symmetric band structure the effective mass tensor is proportional to the identity. The Hamiltonian is then $\frac{1}{2}m_{\text{eff}}^{-1}\boldsymbol{p}^2$, and the dependence of the crystal orientations drop out. In the last idealized case we would thus predict motion along straight lines which are geodesics and not autoparallels in crystal space.

To end the discussion we must also take into account that lattice directions in real crystals are changed by the presence of dislocations. These are local scatterers, and we have to check whether the coherence of the wavepacket can be maintained over such distances that the lattice orientations change appreciably. Suppose that the strength of the perturbation is U and that it has support over a typical distance of the lattice spacing a. The wavepacket passes over the defect during a time T_{scatter} of about $\hbar/(\Delta k|(\partial\mathcal{E}_n(\boldsymbol{k}))/\partial\boldsymbol{k}|)$, while the natural time scale of the action of the scattering potential on the wavepacket is $\hbar/U$. If we assume scattering to any state on the energy shell with equal probability, we have

$$P_{\text{scatter on shell}} \sim (a\Delta k)^d (a\boldsymbol{k})^d \left(\frac{\Delta k}{\boldsymbol{k}}\right)\left(\frac{U T_{\text{scatter}}}{\hbar}\right)^2. \tag{33}$$

Equation (33) is an overestimate, but probably not very much so. A derivation of (33) using standard first-order perturbation theory is given below in appendix A.

Consider now an array of dislocation lines with surface density n, and a wavepacket moving in a plane perpendicular to the lines. As it traverses a distance L it will, in general, encounter $Ln/\Delta k$ defects, and the total probability of being scattered by any of them is

$$P_{\text{scatter along } L} \sim \left(L\frac{1}{\Delta k}n\right)(a\Delta k)^d \left(\frac{U}{\Delta k(\partial\mathcal{E}_n(\boldsymbol{k}))/\partial\boldsymbol{k}}\right)^2 (a\boldsymbol{k})^d \left(\frac{\Delta k}{\boldsymbol{k}}\right). \tag{34}$$

We want this probability to be much less than one. A surface dislocation density of n leads to a crystal torsion field of strength na, since each dislocation contributes a Burgers' vector of length a. The crystal directions can change appreciably over a length L if the line integral of torsion is of order one, that is $naL \sim 1$. The two estimates are compatible if

$$(a\Delta k)^{d-1}(a\boldsymbol{k})^d \left(\frac{U}{\Delta k(\partial\mathcal{E}_n(\boldsymbol{k}))/\partial\boldsymbol{k}}\right)^2 \left(\frac{\Delta k}{\boldsymbol{k}}\right) \ll 1. \tag{35}$$

We are interested in the case $d = 2$. Assuming for simplicity $\mathcal{E}_n(\boldsymbol{k}) \sim \frac{1}{2}m_{\text{eff}}\boldsymbol{k}^2$ we have

$$(a\boldsymbol{k})^3 \left(\frac{U}{\mathcal{E}_n(\boldsymbol{k})}\right)^2 \ll 1 \qquad (d = 2). \tag{36}$$

This bound can evidently only be satisfied, and then only for sufficiently large crystal momenta $\boldsymbol{k}$, if the effective scattering potential U is much less than the largest kinetic energies in the band. Condition (36) is a serious point. If U is not sufficiently small then scattering is the leading effect and considerations pertaining to fine points of the continuum picture, which we pursue here, are simply irrelevant to electron motion in quantum dots. We remark in contrast that in the three-dimensional situation (35) becomes

$$(a\Delta k)(a\boldsymbol{k})^4 \left(\frac{U}{\mathcal{E}_n(\boldsymbol{k})}\right)^2 \ll 1 \qquad (d = 3) \tag{37}$$

which can always be satisfied, if Δk is small enough.

5. Possible torsion effects in quantum dots

I will now consider the following possible types of effects: (a) classical motion; (b) non-relativistic quantum motion; (c) spin–torsion coupling terms derivable from the non-relativistic limit of the Dirac equation minimally coupled to torsion; (d) phenomenological spin–torsion couplings appropriate for the situation of quantum dots.

When classical or semiclassical descriptions are valid, the electronic motion in the dot is effectively two dimensional. Let the two directions of the dot be 1 and 2 and the third vertical

direction 3. For points (a) and (b) we only need to consider the possible effects of elements S_{121} and S_{122} of the crystal torsion matrix, i.e. only edge dislocations, while for (c) and (d) we also need to consider screw dislocations.

It is convenient to express torsion in the lattice unit a. Kröner discusses a crystal with one edge dislocation per every 10×10 atoms, all Burgers vectors of all dislocations oriented the same way. In this situation crystal torsion would be $0.01/a$, and one would have to move a distance $100a$ to see to change the lattice directions change appreciably. It is not clear whether this example is realistic, the surface defect density being about 10^{17} m^{-2}. As the standard set-up I will thus consider one a dislocation per every 100×100 atoms. Torsion would then be $10^{-4}/a$, and one would have to move a distance of $10^4 a$ to change the crystal orientations. Crystals with lower dislocation densities could surely be fabricated, but then we would need macroscopic quantum dots to see the possible effects of crystal torsion.

With quantum dots of micron size the bounds on dispersion from section 4 can be satisfied. We would see the lattice orientations change when we move from one side of the dot to the other, i.e. $L \sim 10^4 a$. If we choose the spread of the wavepacket Δk to be about $10^{-3}/a$. then $1/\Delta k \ll L \ll L_{\text{disp}}$ with an order of magnitude at the lower inequality and two orders of magnitude at the upper inequality. The semiclassical argument predicts that wavepackets follow classical trajectories in a Hamiltonian given by the band energy as functions of crystal momentum. This structure stems from solving for the Bloch states in the crystal potential—information which is not contained in the continuum description of the crystal as a metric space with curvature and torsion. In the general case neither geodesics nor autoparallels in crystal space therefore have any particular relevance to the problem. In the special case of a spherically symmetric band structure we do, however, recover motion along straight lines, i.e. geodesics in crystal space. Motion along autoparallels would, on the other hand, be on curved paths as in the example discussed in section 2. If the approximation of a spherically symmetric band structure is a sufficiently good one, and if the local scattering potentials are weak enough that the wavepacket does not lose coherence, then the difference between geodesics and autoparallels could, in principle, be observable.

The scale separation is even more favourable for a description in terms of a non-relativistic quantum particle. Consider the ground state or a low-lying excited state in the example discussed previously. If the prescription (13) were correct, they would be solutions to the eigenvalue equation

$$\left(-\frac{\hbar^2}{2m_{\text{eff}}}\nabla^2 + \sum_i U(x - x_i) + \frac{\hbar^2}{m_{\text{eff}}} S^l \partial_l\right)\psi = E\psi \tag{38}$$

where U is the scattering potential from dislocations at points x_i and S^l is the crystal torsion vector, which in the example under discussion would be about $10^{-4}/a$. The derivative ∂_l acting on a low-lying state is also about $10^{-4}/a$ if the lateral size of the dot is in the micron range. Hence the perturbation $S^l \partial_l$ is of the order of $10^{-8}/a^2$, which is comparable to the energy gap between the ground state and the low-lying states of (38). As discussed above in section 2 this perturbation breaks Hermiticity, and hence leads, if large enough, to complex eigenvalues, i.e. states exponentially decaying or growing in time. On a conceptual level the problem is primarily the exponentially growing modes. One might imagine that the defects could perhaps excite certain electronic states in the dot, and that for some transient time the growth rates of those states could be described by the eigenvalues of (38). This picture does not look very plausible physically, and could probably be ruled out by experiments, at least on a qualitative level.

Let us now turn to possible spin–torsion couplings. The most straightforward, but also certainly the smallest, are the non-relativistic limits of the vector and axial vector couplings

in the Dirac equation, (23) and (22). In the first case we have the curl of the torsion vector. Let us assume that the torsion varies in a controlled manner in the plane of the dot. We only have to consider edge dislocations, since the vector $\vec{S}$ vanishes for a screw dislocation. When the density of edge dislocations varies normally to the vector $\vec{S}$ we would have an effective coupling analogous to the Zeeman effect, with an effective magnetic field pointing in the vertical direction (out of the plane of the dot). In the axial vector case we only have to consider screw dislocations, $\tilde{S}_0$ being the sum of densities of screw dislocations in all directions.

We can also discuss more phenomenological spin–torsion coupling terms. In the physical situation of a quantum dot the vertical direction is determined by the gradient of dopant concentration. We can therefore form a combination of torsion and the vertical direction vector which transforms as an axial vector, namely $\hat{S}^l = \epsilon_i{}^{jk}\hat{n}_3^i S_{jk}{}^l$. This is just the vector $\vec{b}$ which results from circling a dislocation in the 12-plane, i.e. $\hat{S}$ could have elements both in and out of the plane. We then consider a term like $\kappa\hat{S}\cdot\vec{\sigma}$. Torsion has the physical dimension of inverse length, hence κ should have dimension mass$\cdot$(length)^3 (time)$^{-2}$. The only combination of Planck's constant $\hbar$, the lattice constant a and the effective electron mass $m_{\rm eff}$, which has this dimension is $\hbar^2/am_{\rm eff}$. This coupling can be compared dimensionally with (23) and (22), which have the bare electron mass instead of $m_{\rm eff}$ and a spatial derivative instead of $1/a$.

The energy splitting of two states with spin, respectively parallel and antiparallel to $\hat{S}$, will then be κ times the average value of $\hat{S}$ in lattice units. With the standard case of one dislocation per 100×100 atoms this gives

$$\Delta E_{\rm torsion} \approx \frac{\kappa}{10^4 a}. \tag{39}$$

The frequency of the transition is hence

$$\nu_{\rm torsion} \sim 10^{-4}\frac{\hbar}{m_{\rm eff}a^2} \approx 100\ \text{Hz} \tag{40}$$

where, for simplicity, I have estimated $m_{\rm eff}$ with the electron rest mass and a to be 1 Å. The two terms derivable from the Dirac equation discussed above are even smaller, approximately by a factor of a/L.

6. Conclusions

In this paper I have taken up a suggestion of Kleinert that the motion of a classical quantum particle in a space with torsion could be relevant to describe some properties of a crystal with defects. I have focused on the example of electron motion in quantum dots, since these systems most nearly realize the textbook example of electron motion in potential wells.

In a space with torsion there are two different privileged classical motions, geodesics and autoparallels. A semiclassical analysis carried out in section 4 indicates that at some scales of space and time geodesic motion could be observed, if the band energy structure is spherically symmetric, and the local scattering potential from dislocations sufficiently weak. The last condition is very stringent in two-dimensional geometries such as quantum dots, and local scattering is in fact likely to be the dominant effect. A continuum description of the motion of an electron in a crystal with dislocations is therefore probably not very useful in two dimensions. Assuming nevertheless, for the sake of the argument, that the local scattering potential is weak, the conditions for the distinction between geodesics and autoparallels could probably be realized experimentally. These issues are discussed in section 5. If the band energy structure is not spherically symmetric the problem is more complicated and neither geodesics nor autoparallels would follow from the semiclassical argument.

The distinction between geodesics and autoparallels carry over to the quantum mechanics of a non-relativistic particle, i.e. to the proper generalization of the Schrödinger equation to a space with torsion. The analogy with geodesics would be the Laplace–Beltrami operator, while the analogy with autoparallels would be another differential operator introduced by Kleinert. The difference between the two operators can be relatively large, and hence observable. Since it breaks Hermiticity, it leads to modes exponentially growing or decaying in time, an effect which should be falsifiable by experiments.

The spin–torsion coupling terms, both those derivable from the Dirac equation and more phenomenological ones, are all very small and give transitions with frequencies of 1 kHz, or below.

Hence we conclude that whatever the motion of a classical or quantum particle in a space with torsion should be, the issue has little bearing on electron motion in quantum dots. The semiclassical motion of wavepackets can, in favourable cases, be arranged to be along geodesics, i.e. along straight lines, but autoparallels are never relevant. Bound electronic states in a quantum dot may to some degree of accuracy be described as the eigenstates of the Laplacian with Dirichlet boundary conditions, but the alternative introduced by Kleinert has eigenstates that are exponentially growing or decaying in time, and this contradicts the very notion of stationary bound states in the dot. The spin-coupling terms are not in contradiction with theoretical arguments, nor with conceivable experiments. But their effects are so weak that it would be very difficult to observe them.

Acknowledgments

I thank Nuno Barros e Sá, Ingemar Bengtsson, Alexander Grishin, Dmitri Leites, Paolo Muratore-Ginanneschi, Arne Nordmark, and Per Salomonson for discussions. This work was supported by the Swedish Natural Science Research Council through grant S-FO-1778-302.

Appendix. Computation of the wavepacket-defect cross section

The wavepacket interacts with the defect during a time of about

$$T_{\text{scatter}} = \frac{\hbar}{\Delta k|(\partial \mathcal{E}_n(\boldsymbol{k}))/\partial \boldsymbol{k}|}. \tag{A1}$$

It is therefore convenient to regard the defect as a time-dependent perturbation, switched on before $-T_{\text{scatter}}$ and switched off after T_{scatter}. For definitiveness take $V(x,t) = V(x)\exp(-1/(2\sigma^2)(t/T_{\text{scatter}})^2)$ with σ some number which will eventually be taken to infinity.

Let us take a lattice of large finite size Λ with the isolated defect centred at the origin. The values of the wavevector k then come in integer multiples of $2\pi/\Lambda$. The time-dependent Bloch states are denoted by $\Psi^{(0)}_{n,k}(x)$, and are normalized by $\int_{\Lambda^d} |\Psi^{(0)}_{n,k}(x)|^2 = 1$. The wavepacket formed by Bloch waves from the nth band is given by $\sum_k \Psi^{(0)}_{n,k} a^{(0)}_k$, where the amplitudes are normalized by $\sum_k |a^{(0)}_k|^2 = 1$.

When the wavepacket has passed over the defect, i.e. after the perturbation has been switched off, we have to first order in the perturbation the out state

$$\Psi(\text{out}) = \sum_k \Psi^{(0)}_{n,k}\left(a^{(0)}_k + \sum_l U_{kl} a^{(0)}_l\right) \qquad U_{kl} = -\frac{\mathrm{i}}{\hbar}\int_{-\infty}^{\infty} V_{kl}(t)\,\mathrm{e}^{\mathrm{i}(E_k - E_l)/\hbar t} \tag{A2}$$

where $V_{kl}(t)$ is the time-dependent matrix element between the time-independent Bloch states k and l. The time dependence of the Bloch states have been written out explicitly in the matrix

element in (A2). The difference between $\Psi(\mathrm{out})$ and the unperturbed wavepacket at the same time is $\delta\Psi(\mathrm{out}) = \sum_{kl} \Psi^{(0)}_{n,k} U_{kl} a^{(0)}_l$. It is orthogonal to the unperturbed state. The absolute square of $\delta\Psi$ hence represents the probability to be in an out state orthogonal to the unperturbed wavepacket.

I disregard scattering out of the band. Then, for pairs of states such that $|E_k - E_l| \gg \overline{h}/(T_{\mathrm{scatter}})$ the transition probability amplitude U_{kl} will be very small. Inserting the definition of T_{scatter} this means that only wavevectors in a thin shell of thickness about Δk around the surface given by $E_k = E_{\boldsymbol{k}}$ are scattered. The matrix element is

$$V_{kl}(t) = \langle k|V|l\rangle \exp\bigl(-\tfrac{1}{2}\sigma^2 (t/T_{\mathrm{scatter}})^2\bigr) \tag{A3}$$

where $\langle k|V|l\rangle = \int (\Psi^{(0)}_{n,k})^*(x)\, V(x)\, \Psi^{(0)}_{n,l}(x)\, \mathrm{d}x$. If both wavevectors are within Δk of $\boldsymbol{k}$ then, because $1/\Delta k$ is assumed much larger than a,

$$\langle k|V|l\rangle = \left(\frac{a}{\Lambda}\right)^d U \qquad |k-l| \sim \Delta k \tag{A4}$$

where U is some measure of the strength of the potential. In general, if $|l\rangle$ is in the wavepacket we can always for the same reason substitute $\langle k|V|l\rangle$ with $\langle k|V|\boldsymbol{k}\rangle$. We now have

$$U_{kl} = -\frac{\mathrm{i}}{\overline{h}} \langle k|V(x)|l\rangle \exp\left(-\frac{1}{2}\left(\sigma T_{\mathrm{scatter}}\left(\frac{E_k - E_l}{\overline{h}}\right)\right)^2\right)\sqrt{2\pi\sigma^2 T^2_{\mathrm{scatter}}}. \tag{A5}$$

The total probability of scattering is

$$|\delta\Psi|^2 = \sum_{nkl} U^*_{nk} U_{nl} (a^{(0)}_k)^* a^{(0)}_l. \tag{A6}$$

Let the amplitudes be given as $a^{(0)}_k = [(2\pi)^{d/2}/\Lambda^{d/2}] f_0(k)$, where the smooth function $f_0(k)$ is normalized by $\int_{\Lambda^d} |f_0(k)|^2 = 1$. For definitiveness take $f_0(k)$ to be a Gaussian centred at $\boldsymbol{k}$ with width Δk:

$$f_0(k) = \exp\left(-\frac{1}{2}\left(\frac{k-\boldsymbol{k}}{\Delta k}\right)^2\right)\bigl(\pi(\Delta k)^2\bigr)^{-d/4}. \tag{A7}$$

We now wish to compute $\sum_l U_{nl} a^{(0)}_l$ where n is anywhere on the shell of scattered wavevectors. We have to separate components of wavevector l parallel and orthogonal to $\frac{\partial \mathcal{E}_n(\boldsymbol{k})}{\partial \boldsymbol{k}}$. By expanding

$$E_n - E_l = (E_n - E_{\boldsymbol{k}}) - \frac{\partial \mathcal{E}_n(\boldsymbol{k})}{\partial \boldsymbol{k}}(l_\parallel - \boldsymbol{k}_\parallel) \tag{A8}$$

and using the definition of T_{scatter} from (A1) we have

$$\begin{aligned}\sum_l U_{nl} a^{(0)}_l = -\frac{\mathrm{i}}{\overline{h}} \langle n|V(x)|\boldsymbol{k}\rangle \sqrt{2\pi\sigma^2 T^2_{\mathrm{scatter}}}\left(\frac{\Lambda}{2\pi}\right)^{d/2} \bigl(\pi(\Delta k)^2\bigr)^{-d/4}\bigl(2\pi(\Delta k)^2\bigr)^{d/2} \\ \times\sqrt{\frac{1}{\sigma^2+1}}\exp\left(-\frac{1}{2}\frac{\sigma^2}{\sigma^2+1}\left(\frac{T_{\mathrm{scatter}}(E_n - E_{\boldsymbol{k}})}{\overline{h}}\right)^2\right).\end{aligned} \tag{A9}$$

The contribution to (A6) from a given wavevector n can therefore be written as

$$\begin{aligned}\left|\sum_l U_{nl} a^{(0)}_l\right|^2 = \left(\frac{|\langle n|V|\boldsymbol{k}\rangle| T_{\mathrm{scatter}}}{\overline{h}}\right)^2 \frac{\sigma^2}{\sigma^2+1}(\Delta k)^d (2\pi)^{d/2+1} 2^{d/2} \\ \times\left(\frac{\Lambda}{2\pi}\right)^d \exp\left(-\frac{1}{2}\frac{2\sigma^2}{\sigma^2+1}\left(\frac{T_{\mathrm{scatter}}(E_n - E_{\boldsymbol{k}})}{\overline{h}}\right)^2\right).\end{aligned} \tag{A10}$$

When we sum over n we can take out a value $\boldsymbol{n}$ such that $E_{\boldsymbol{n}} = E_{\boldsymbol{k}}$, and then integrate parallel to $\partial E/\partial \boldsymbol{n}$. That will give a term $\sqrt{(2\pi(\sigma^2+1)\hbar^2)/(2\sigma^2 T_{\text{scatter}}^2(\partial E/\partial \boldsymbol{n})^2)}$. Incorporating the partial derivative in a delta function we can hence write

$$|\delta\Psi|^2 = \sqrt{\frac{\sigma^2}{\sigma^2+1}}(\Delta k)^{d+1}(2\pi)^{d/2+2}2^{d/2-1}\left(\frac{T_{\text{scatter}}}{\hbar}\right)^2\left|\frac{\partial E}{\partial \boldsymbol{k}}\right| \times\left(\frac{\Lambda}{2\pi}\right)^{2d}\int \delta(E_n - E_{\boldsymbol{k}})|\langle n|V|\boldsymbol{k}\rangle|^2\,\mathrm{d}n. \tag{A11}$$

Here we can take the limit of σ going to infinity and we have thus removed the spurious time dependence of the perturbation.

By an order-of-magnitude estimate we take $|\langle n|V|\boldsymbol{k}\rangle| = U(a/\Lambda)^d$ for all states n on the energy shell given by $E_n = E_{\boldsymbol{k}}$. We can then take the matrix element outside the integral $\int \delta(E_n - E_{\boldsymbol{k}})\,\mathrm{d}n$, which is the density of states at energy $E_{\boldsymbol{k}}$. If we further assume that $E_n = \frac{1}{2}m_{\text{eff}}n^2$, then the density of states is equal to $(\Omega_d \boldsymbol{k}^d)/2E_{\boldsymbol{k}}$, where Ω_d is the area of the unit sphere in d dimensions. We can finally take out from (A11) the combination $\Delta k|\partial E/\partial \boldsymbol{k}|1/(2E_{\boldsymbol{k}})$ which can be rewritten more simply as $\Delta k/\boldsymbol{k}$, and this gives (33).

If we would instead have assumed that the matrix element is only non-zero between states in the wavepacket, we would then have estimated the integral in (A11) by $\int_{|n-\boldsymbol{k}|\leqslant\Delta k}\delta(E_n - E_{\boldsymbol{k}})\,\mathrm{d}n$ which is about $(\Delta k)^{d-1}/|\partial E/\partial \boldsymbol{k}|$. The probability of being scattered from one wavepacket to another is hence

$$P_{\text{scatter within }\Delta k} \sim (a\Delta k)^{2d}\left(\frac{UT_{\text{scatter}}}{\hbar}\right)^2 \tag{A12}$$

which can also be derived by straightforward dimensional analysis, since the probability density of the wavepacket is about $(\Delta k)^{2d}$.

References

[1] Kirk W P and Reed M A (eds) 1992 *Nanostructures and Mesoscopic Systems* (San Diego, CA: Academic)
[2] Kastner M A 1992 *Rev. Mod. Phys.* **64** 849
[3] Baranger H U, Jalabert R A and Stone A D 1993 *Chaos* **3** 665
[4] Tomsovic S and Heller E 1993 *Phys. Rev. Lett.* **70** 1405
[5] Marcus C M *et al* 1997 *Chaos Solitons Fractals* **8** 1261
[6] Mathur H, Gkcedag M and Stone A D 1995 *Phys. Rev. Lett.* **74** 1855
[7] Agam O, Wingreen N, Altshuler B, Ralph D C and Tinkham M 1997 *Phys. Rev. Lett.* **78** 1956
(Agam O, Wingreen N, Altshuler B, Ralph D C and Tinkham M 1996 Chaos, interactions and nonequilibrium effects in the tunneling spectra of small metallic particles *Preprint* cond-mat/9611115)
[8] Bruus H, Lewenkopf C H and Mucciolo E R 1996 *Phys. Rev.* B **53** 9868
[9] Kleinert H 1995 *Path Integrals in Quantum Mechanics, Statistics and Polymer Physics* (Singapore: World Scientific)
[10] Kleinert H and Fiziev P 1996 *Europhys. Lett.* **35** 241
[11] Kleinert H 1996 Quantum equivalence principle (Cargese Summer School lectures) *Preprint* quant-ph/9612040
Kleinert H 1998 *Acta Phys. Pol.* B **29** 1033
(Kleinert H 1997 Nonholonomic mapping principle for classical and quantum mechanics in spaces with curvature and torsion *Preprint* APS E-print aps1997sep03 002)
Fiziev P and Kleinert H 1995 Anholonomic transformations of mechanical action principle *Proc. Workshop Variational and Local Methods in the Study of Hamiltonian Systems* ed Ambrossetti and Dell'Antonio (Singapore: World Scientific) pp 166–77
(Fiziev P and Kleinert H 1996 *Preprint* gr-cq/9605046)
[12] Hehl F W, van der Heyde P and Kerlick G D 1976 *Rev. Mod. Phys.* **48** 393
[13] Schrödinger E 1960 *Space-Time Structures* (Cambridge: Cambridge University Press)
[14] Schouten J A 1954 *Ricci Calculus* (Berlin: Springer)

[15] Barros e Sá N 1997 Autoparallels from a variational principle *Stockholm University Preprint*
[16] Arnold V I, Kozlov V V and Neishtadt A I 1988 *Dynamical Systems III* (Berlin: Springer)
[17] Poincaré H 1901 *C. R. Acad. Sci., Paris* **132** 369–71
[18] Bondi H 1986 *Proc. R. Soc.* A **405** 265
[19] Garcia A and Hubbard M 1988 *Proc. R. Soc.* A **418** 165
[20] Nordmark A, Essén H and Lesser M 1997 Unidirectional spin and nonholonomic dynamics *Proc. 3rd EUROMECH Solid Mechanics Conf. (Stockholm)* (*Proc. R. Soc.* to appear)
[21] Weinberg S 1972 *Gravitation and Cosmology* (New York: Wiley)
[22] Berline N, Getzler E and Vergne M 1991 *Heat Kernals and Dirac Operators* (Berlin: Springer)
[23] Audretsch J 1981 *Phys. Rev.* D **24** 1470
[24] Lämmerzahl C 1997 Constraints on space-time torsion from Hughes–Drever experiments *Preprint* gr-qc/9704047 (*Phys. Lett.* A to appear)
[25] Hehl F-W and Datta B K 1971 *J. Math. Phys.* **12** 1334
[26] Kröner E 1981 Continuum theory of defects *Physics of Defects (Les Houches XXXV)* ed R Balian (Amsterdam: North-Holland)
[27] Ashcroft N W and Mermin N D 1976 *Solid State Physics* (Philadelphia, PA: Sauders)
[28] Kittel C 1976 *Introduction to Solid State Physics* 5th edn (New York: Wiley)