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Elastic Landau levels

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Abstract
In this work, we use the geometric theory of defects to investigate a continuous distribution of screw dislocations. We analyze the dynamics of a quantum particle in the presence of a density of screw dislocations. We obtain the energy levels and eigenfunctions for the particle in this background. We demonstrate that this quantum dynamics is similar to the dynamics of a charged particle in the presence of an external magnetic field. In addition, we introduce an external magnetic field and perform the calculations of the eigenfunctions and eigenvalues for the particle in this case.

1. Introduction

The first approach to the theory of defects in an elastic medium was made by the Italian school with the development of the theory of dislocations in 1900. After those initial approaches, many theories and experiments were put forward in order to describe and to observe defects in solids [1]. In recent years a series of articles, inspired by the pioneering ideas of Kröner [2] and Bilby *et al* [3], developed a geometric theory of defects. In this framework the elastic solids with topological defects can be described by Riemann–Cartan geometry [4–7].

In this formulation we use the techniques of differential geometry to describe the strain and stress induced by the defect in an elastic medium. All this information is contained in the geometric quantities (metric, curvature tensor, etc) that describe the elastic medium with defects. The boundary conditions imposed by the defect, in the elastic continuum, are accounted for by a non-Euclidean metric. In the continuum limit, the solid can be viewed as a Riemann–Cartan manifold. In general, the defect corresponds to a singular curvature or torsion (or both) along the defect line [7], where the curvature and the torsion of the manifold are associated with the topological defects, disclinations and dislocations, respectively.

There are some advantages of this geometric description of defects in solids. In contrast to the ordinary elasticity theory, this approach provides an adequate language for continuous distribution of defects [8]. The problem of the description of quantum (or classical) dynamics of particles (or quasiparticles) in the elastic medium is reduced to a problem in a curved/torsioned space. In this framework, the influence of the defects on the motion of electrons and phonons, for example, becomes reasonably easy to analyze, due to the fact that the boundary conditions imposed by the defects are incorporated into the geometry. In this geometric point of view, the quasiparticles in motion experience an effective non-Euclidean metric in an elastic medium. This change in the effective metric experienced by the quasiparticles in this medium is caused by the stress and strain provoked in the elastic medium by topological defects. The classical motion of quasiparticles in the elastic background is described by geodesics in the effective metric. The geometric theory of defects, in the continuum limit, describes the solid using a Riemann–Cartan manifold where curvature and torsion are associated with disclinations and dislocations, respectively, in the medium. The Burgers vector of a dislocation is associated with torsion, and the Frank angle of a disclination with curvature. In this theory, the elastic deformations introduced in the medium by defects are incorporated in the metric of the manifold. The quantum and classical problems in the Riemann–Cartan manifold representing a crystal with a topological defect have been extensively analyzed in recent years [14–16]. It is also worth mentioning that, two decades ago, Kawamura [17] and Bausch and co-workers [6, 19, 20] investigated the scattering of a single particle in dislocated media using a different approach and demonstrated that the equation that governs the scattering of a quantum particle by a screw dislocation is of Aharonov–Bohm type [18]. In this approach the Schrödinger equation is obtained from tight-binding microscopic theory. The Hamiltonian is derived from the usual Hamiltonian in flat space by use of a minimal coupling prescription proposed by Kibble [23] on the gauge field theory of gravity. In this description the Schrödinger equation that governs the quantum dynamics in the presence of a topological defect consists of two parts. The first part, that describes the geometric particle motion, has a covariant form. The other part has a non-covariant term, in the continuum description, which resembles those of the deformation-potential approach. In the geometric theory we obtain the same covariant terms that appear in the description of Bausch [6, 19, 20]; the non-covariant term has be included by deformation theory methods.

In this work we investigate a solution, in the geometric theory of defects, that describes a continuous density of screw dislocations from the point of view of the geometric theory of defects. We propose a new expression for the metric describing continuous homogeneous distribution of parallel screw dislocations in elastic media. We obtain a metric that describes this solution and study the quantum dynamics of a single particle in this background. It is obtained that the energy eigenvalues are quantized in a way similar to the Landau quantization of a charged particle in the presence of an external magnetic field. This similarity between the quantum dynamics of a single particle, in a space with torsion, and a charged particle, in the presence of a magnetic field, is explored in this paper. In this contribution we do not consider terms in the Hamiltonian due the deformation-potential approach [6, 19, 20] but we use the geometric description to investigate the continuous distribution of screw dislocations. This paper is organized in the following way. In section 2, a continuous homogeneous distribution of parallel screw dislocation solution in a geometric theory of defects is studied, and we call this the spiral solution. In section 3, we investigate the quantum dynamics of a single particle in the presence of a continuous distribution of screw dislocations; the eigenvalues and eigenfunctions of the problem are found. In section 4, we introduce an external magnetic field and obtain the energy levels and wavefunctions in this case. Finally, in section 5, the concluding remarks are presented.

2. The spiral solution in a geometric theory of defects

In general, the defects correspond to singular curvature or torsion (or both) along the defect line [7]. We consider an infinitely long linear screw dislocation oriented along the z-axis. The three-dimensional geometry of the medium, in this case, is characterized by nontrivial torsion which is identified with the surface density of the Burgers vector in the classical theory of elasticity. In this way, the Burgers vector can be viewed as a flux of torsion. The screw dislocation is described by the following metric, in cylindrical coordinates [9, 10]:

$$\mathrm{d}s^2 = g_{ij}\,\mathrm{d}x^i\,\mathrm{d}y^j = (\mathrm{d}z + \beta\,\mathrm{d}\phi)^2 + \mathrm{d}\rho^2 + \rho^2\,\mathrm{d}\phi^2, \qquad (1)$$

where β is a parameter related to the Burgers vector b by $\beta = \frac{b}{2\pi}$. This topological defect carries torsion but no curvature. The torsion associated with this defect corresponds to a conical singularity at the origin. The only nonzero component of the torsion tensor in this case is given by the 2-form

$$T^1 = 2\pi\beta\delta^2(\rho)\,\mathrm{d}\rho \wedge \mathrm{d}\phi, \qquad (2)$$

where $\delta^2(\rho)$ is the two-dimensional delta function in flat space. The three-dimensional geometry of the medium, in this case, is characterized by nontrivial torsion, which is identified with the surface density of the Burgers vector in the classical theory of elasticity. In this way, the Burgers vector can be viewed as a flux of torsion, given by

$$\int_\Sigma T^1 = \oint_S e^1 = 2\pi\beta = b, \qquad (3)$$

where we adopt the following triad representation (1-form basis) for the metric (1):

$$e^1 = \mathrm{d}z + \beta\,\mathrm{d}\phi \qquad (4)$$

$$e^2 = \mathrm{d}\rho \qquad (5)$$

$$e^3 = \rho\,\mathrm{d}\phi, \qquad (6)$$

and the torsion 2-form is related to the triad by

$$\mathbf{T} = \mathbf{de} + \mathbf{\Gamma}^{(\mathrm{L})} \wedge \mathbf{e}, \qquad (7)$$

where $\mathbf{\Gamma}^{(\mathrm{L})}$ is the Lorentz connection, which is zero for this geometry since there is no curvature involved. This equation leads to the result (2) when we substitute (4)–(6) into it. For future comparison with the electromagnetic field strength $F_{\mu\nu}$ we write the torsion in tensor notation [11]:

$$T^a_{\mu\nu} = \partial_\mu e^a_\nu - \partial_\nu e^a_\mu - (e^b_\mu \omega^a_{\nu b} - e^b_\nu \omega^a_{\mu b}), \qquad (8)$$

where $\omega^a_{\nu b}$ is the spin connection and T^a is the 2-form component of the torsion, defined as $T^a = T^a_{\mu\nu}\mathrm{d}x^\mu \wedge \mathrm{d}x^\nu$, and the triad component $e^a = e^a_\mu\,\mathrm{d}x^\mu$. The similarity between screw dislocations and a magnetic flux was investigated in recent articles [12, 13]. This relation has a physical origin; the Burgers vector is associated with the torsion flux of the defect. This fact is demonstrated in equation (2) which shows that the torsion is zero everywhere, except on the defect. Analogously, in an infinite solenoid, the magnetic field is zero everywhere except on the solenoid. This analysis can be also obtained from comparison of equation (8) with the field strength $F_{\mu\nu}$ in the electromagnetic case. The field strength $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$, where A_μ is the vector potential, is singular on the flux line and zero in other regions of space. In the elastic case, e^a_μ, in expression (8), plays the role of a potential for torsion, since there is no torsion present in the space except on the defect, where the torsion is singular. We therefore have seen above that torsion has a behavior similar to that of the field strength in the electromagnetic case.

Katanaev [8] demonstrated that solutions of the geometric theory of defects yield the solutions of the same problems in the nonlinear elasticity theory. Moreover, the metric that describes a defect solution is an exact solution and the linear elasticity is obtained taking the appropriate limits. In this paper we use the geometric theory of defects to describe a continuous distribution of parallel screw dislocations. We choose the geometric approach developed by Katanaev and Volovich for defects in solids. We consider a cylindrically symmetric distribution of parallel screw dislocations and we assume that they are uniformly distributed in the elastic medium. Since the space that describes a single screw dislocation is locally flat, it makes sense to construct a new solution to the 'Einstein' equations corresponding to a collection of parallel screw dislocations. In this way we obtain the following metric:

$$\mathrm{d}s^2 = (\mathrm{d}z + \Omega\rho^2\,\mathrm{d}\varphi)^2 + \mathrm{d}\rho^2 + \rho^2\,\mathrm{d}\varphi^2, \qquad (9)$$

with the following density of the Burgers vector: $\Omega = b_i\sigma/2$, where σ is the area density of dislocations. This metric describes a continuous distribution of screw dislocations. The torsion is uniformly distributed in all space. Now we investigate the geometrical properties of this space. We choose the following triad representation (1-form basis) for the metric (9):

$$e^1 = \mathrm{d}z + \Omega\rho^2\,\mathrm{d}\phi \tag{10}$$

$$e^2 = \mathrm{d}\rho \tag{11}$$

$$e^3 = \rho\,\mathrm{d}\phi. \tag{12}$$

Using this fact we obtain the flux of torsion associated with this space:

$$\int_\Sigma T^1 = \oint_S e^1 = 2\pi\Omega\rho^2, \tag{13}$$

where we have used that $T^1_{\rho\phi} = -T^1_{\phi\rho} = 2\Omega$. Note that the torsion is uniform in all space. This fact will be used in the next section to analyze the similarities of this uniform torsion space with a uniform magnetic field.

3. Quantum dynamics in the presence of the spiral dislocation

In this section we investigate the quantum dynamics of a single particle moving in the background described by (9). In recent years the problem of the quantum dynamics of a single particle in the presence of a dislocation field was investigated by several authors using different approaches. The study of quantum scattering of electrons by a screw was investigated by Kawamura [17] who, using a tight-binding approach, demonstrated that scattering is of Aharonov–Bohm [18] type. Bausch, Schmitz and Turski [6, 19–21] investigated the dynamics of a quantum particle in the presence of a single screw/edge dislocation. They derived the Schrödinger equation from the tight-binding microscopic Hamiltonian and obtained no bound states for a quantum particle in the field of screw dislocation. In this description the Schrödinger equation, that governs the quantum dynamics in the presence of a topological defect, consists of two parts. The first part that describes the geometric particle motion has a covariant form. The other part has a non-covariant term, in the continuum description, which resembles those of the deformation-potential approach. This non-covariant terms introduce in the Schrödinger equation a repulsive potential that contributes an asymmetry in scattering amplitude. Using a geometric description, the defect is represented by a metric and the Schrödinger equation is written using the Laplace–Beltrami operator in this space. We will consider a Hamiltonian for a neutral particle which includes the topological information on the medium in its kinetic part derived from the Laplace–Beltrami operator for metric (1). We consider the absence of external field. The Hamiltonian that describes a quantum particle in a non-Euclidean background is given by

$$H = \frac{1}{2\mu\sqrt{g}}\left(-\mathrm{i}\hbar\frac{\partial}{\partial x^i}\right)\sqrt{g}g^{ij}\left(-\mathrm{i}\hbar\frac{\partial}{\partial x^j}\right), \tag{14}$$

where μ is mass of the particle. In this way the Schrödinger equation for an electron in the presence of a single screw dislocation is given by

$$-\frac{\hbar^2}{2m}\left\{\partial_z^2 + \frac{1}{\rho}\partial_\rho(\rho\partial_\rho) + \frac{1}{\rho^2}(\partial_\phi - \beta\partial_z)^2\right\}\Psi = E\Psi. \tag{15}$$

The solution of this equation can be obtained using the ansatz

$$\Psi = C\mathrm{e}^{\mathrm{i}\ell\phi}\mathrm{e}^{\mathrm{i}kz}R(\rho), \tag{16}$$

where C is a normalization constant and k is a constant. Substituting equation (16) into the Schrödinger equation, we obtain the following radial equation:

$$\{\rho\,\partial_\rho(\rho\partial_\rho) - (\ell - \beta k)^2 + (\mathcal{E}^2 - k^2)\rho^2\}R(\rho) = 0, \tag{17}$$

where $\mathcal{E}^2 = \frac{2mE}{\hbar^2}$. This equation is a Bessel differential equation whose regular solutions are given by

$$R^{\mathrm{Reg}}_{\ell K}(\lambda\rho) \propto (\pm 1)^\ell J_{|\ell-\beta k|}(\lambda\rho), \tag{18}$$

where $m^2 = (\ell - \beta k)^2$ and $\lambda^2 = \mathcal{E}^2 - k^2$. The 'plus sign' corresponds to the case $\ell \geqslant -[\beta k]$ and the 'minus sign' corresponds to the case $\ell < -[\beta k]$. Here $[x]$ means the largest integer less than or equal to x.

Note that equation (17) is an Aharonov–Bohm type equation that agrees with previous results of Kawamura [17] where the Burgers vector plays the role of a magnetic flux. Using the geometric approach of Katanaev and Volovich we also obtain that the equations that govern scattering of electrons by screw dislocations are of Aharonov–Bohm type. The difference of the approach using the equation obtained by Bausch *et al* [6, 19–21] from that used in this contribution is due to the fact that we do not consider the deformation-potential contribution in the Hamiltonian; in this way we do not include in equation (15) a potential repulsive term.

Now, we focus on the interest of this paper, the study of quantum dynamics of an electron in the presence of a continuous distribution of parallel screw dislocations. The study of electrons in the presence of many screw dislocations can be investigated when we consider a continuous distribution of parallel screw dislocations. In section 2, we obtain a geometric description of a medium that contains a continuous distribution of parallel screw dislocations. In this way, we use the geometric description to obtain the Hamiltonian of a single particle in the presence of a continuous distribution of screw dislocations. In the space of the continuous distribution of parallel screw dislocations (9) the Hamiltonian (14) of a single particle is given by

$$H = -\frac{\hbar^2}{2\mu}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) + \frac{1}{\rho^2}\left(\frac{\partial}{\partial\varphi} - \Omega\rho^2\frac{\partial}{\partial z}\right)^2 + \frac{\partial^2}{\partial z^2}\right]. \tag{19}$$

In this way, we write the Schrödinger equation for this system in the following form:

$$\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2} - 2\Omega\frac{\partial}{\partial\varphi}\frac{\partial}{\partial z} + (1+\Omega\rho^2)\frac{\partial^2}{\partial z^2} + \frac{2\mu E}{\hbar^2}\right]\Psi = 0. \tag{20}$$

We use the following ansatz for the solution of the Schrödinger equation:

$$\Psi(\rho,\varphi,z) = R(\rho)\mathrm{e}^{\mathrm{i}m\varphi}\mathrm{e}^{\mathrm{i}kz}, \tag{21}$$

where m is an integer number. Substituting the ansatz (21) in equation (20), the Schrödinger equation assumes the following form:

$$\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\left(\rho\frac{\mathrm{d}R}{\mathrm{d}\rho}\right) - \frac{m^2}{\rho^2} - k^2\Omega^2\rho^2 R + \beta' R = 0, \tag{22}$$

with $\beta' \equiv \frac{1}{4k\Omega}(2k\Omega m - k^2 + \frac{2\mu E}{\hbar^2})$. Using the following change of variables:

$$\xi \equiv k\Omega\rho^2, \tag{23}$$

equation (22) is transformed into

$$\xi\frac{\mathrm{d}^2R}{\mathrm{d}\xi^2} + \frac{\mathrm{d}R}{\mathrm{d}\xi} - \frac{m^2}{4\xi}R - \frac{\xi}{4}R + \beta' R = 0. \tag{24}$$

Assuming for the radial eigenfunctions the form

$$R(\xi) = \mathrm{e}^{-\frac{\xi}{2}}\xi^{\frac{|m|}{2}}u(\xi), \tag{25}$$

which satisfies the usual asymptotic requirements and finiteness at the origin for the bound state, we have

$$\xi\frac{\mathrm{d}^2u}{\mathrm{d}\xi^2} + (1+|m|-\xi)\frac{\mathrm{d}u}{\mathrm{d}\xi} + \left(\beta' - \frac{|m|+1}{2}\right)u = 0. \tag{26}$$

We find that the solution of equation (26) is the degenerate hypergeometric function

$$u(\xi) = F\left(-\beta' + \frac{|m|+1}{2}, |m|+1, \xi\right). \tag{27}$$

In order to have normalization of the wavefunction, the series (27) must be a polynomial of degree n; therefore,

$$-\beta' + \frac{|m|+1}{2} = -n,$$

where n is an integer number. With this condition, we obtain the discrete values for the energy, given by

$$E = \hbar\omega_{\mathrm{el}}\left(n + \frac{|m|}{2} + \frac{m}{2} + \frac{1}{2}\right) + \frac{k^2\hbar^2}{2\mu} \tag{28}$$

where $\omega_{\mathrm{el}} \equiv \frac{2\hbar k\Omega}{\mu}$. Note that in this result we obtain a bound state of a single particle in the presence of the continuous homogeneous distribution of parallel screw dislocations. This is in contrast with the scattering of one particle in the presence of a screw dislocation [6, 12, 17, 19–21] where the problem is similar to the Aharonov–Bohm problem of a quantum particle in the presence of magnetic solenoid, where no bound state were found. The free particle in the presence of a density of screw dislocations presents energy levels quantized similarly to the Landau levels exhibited by a charged particle in the presence of a uniform field. In this way, it is explicit that the uniform torsion exhibited by a distribution of defects plays the role of a uniform magnetic field. Like in recent articles, the influence of a topological defect in the Landau levels was investigated [15, 16, 24]. In the present case the presence of a defect density provokes the energy quantization in Landau-like levels. These levels we called elastic Landau levels.

4. Quantum dynamics in the presence of a magnetic field

In this section, we analyze the quantum dynamics of a charged particle moving in an elastic medium with a uniform density of screw dislocations subjected to an external magnetic field. The Hamiltonian that describes a quantum particle in the presence of an external magnetic field in a non-Euclidean background is given by

$$H = \frac{1}{2\mu\sqrt{g}}\left(-\mathrm{i}\hbar\frac{\partial}{\partial x^i} - \frac{e}{c}A_i\right)\sqrt{g}g^{ij}\left(-\mathrm{i}\hbar\frac{\partial}{\partial x^j} - \frac{e}{c}A_j\right), \tag{29}$$

where μ is the mass of the particle. Now, we consider an external magnetic field given by

$$\vec{B} = B\hat{e}_z, \tag{30}$$

and the vector potential associated with the field configuration is $A_\varphi = \frac{B\rho}{2}$. Now, using a Hamiltonian that describes a quantum particle in the presence of an external magnetic field (29) we obtain the following expression:

$$H = -\frac{\hbar^2}{2\mu}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) + \left(\frac{1}{\rho}\frac{\partial}{\partial\varphi} - \rho\Omega\frac{\partial}{\partial z} - \frac{\mathrm{i}e}{\hbar c}\frac{B\rho}{2}\right)^2 + \frac{\partial^2}{\partial z^2}\right]. \tag{31}$$

The radial Schrödinger equation associated with this Hamiltonian (31) is obtained using the ansatz (21) and assumes the following form:

$$\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\left(\rho\frac{\mathrm{d}R}{\mathrm{d}\rho}\right) - \frac{m^2}{\rho^2}R + \left[2K\Omega m - k^2 + \frac{2\mu E}{\hbar^2}\right]R + K^2\Omega^2\rho^2 R = 0, \tag{32}$$

where $K \equiv k + \frac{eB}{2\hbar\Omega c}$. Now, we use the change of variables $\xi = K\Omega$, and obtain the following equation:

$$\xi\frac{\mathrm{d}^2R}{\mathrm{d}\xi^2} + \frac{\mathrm{d}R}{\mathrm{d}\xi} - \frac{m^2}{4\xi}R - \frac{\xi}{4} + \beta' R = 0, \tag{33}$$

where $\beta' \equiv \frac{1}{4K\Omega}(2K\Omega m - k^2 + \frac{2\mu E}{\hbar^2})$.

Assuming for the radial wavefunction the form $R(\xi) = \mathrm{e}^{-\frac{\xi}{2}}\xi^{\frac{|m|}{2}}u(\xi)$, we obtain that $u(\xi)$ satisfies the following equation:

$$\xi\frac{\mathrm{d}^2u}{\mathrm{d}\xi^2} + (1+|m|-\xi)\frac{\mathrm{d}u}{\mathrm{d}\xi} + \left(\beta' - \frac{|m|+1}{2}\right)u = 0. \tag{34}$$

In this form, the solution of equation (34) is the degenerate hypergeometric function

$$u(\xi) = F\left(-\beta' + \frac{|m|+1}{2}, |m|+1, \xi\right). \tag{35}$$

The torsion and the magnetic field appear formally on the same footing in the Hamiltonian. But that does not imply the similarity of torsion and magnetic field; in the present case the torsion introduces a spiral structure in the medium absent in the magnetic field case. In fact that is a consequence of the fact that the gauge groups for the magnetic field case and the screw dislocation are essentially different [21].

The series (35) is a polynomial of degree n, if the following condition is obeyed:

$$-\beta' + \frac{|m|+1}{2} = -n, \tag{36}$$

where n is an integer number. In this form, using equation (36) the energy levels are given by

$$E = \hbar\left(\omega_{\mathrm{el}} + \omega_{\mathrm{c}}\right)\left(n + \frac{|m|}{2} + \frac{m}{2} + \frac{1}{2}\right) + \frac{k^2\hbar^2}{2\mu}, \tag{37}$$

where $\omega_{\mathrm{c}} = \frac{eB}{\mu}$ i.e. ($\omega = eB/\mu$) is the cyclotronic frequency. We observe that expression (37) is again similar to the Landau levels.

5. Concluding remarks

We analyzed the uniform density of screw dislocations and investigated the similarities between a uniform torsion provoked by a continuous homogeneous distribution of parallel screw dislocations in elastic media and a uniform magnetic field. We obtain the metric that describes this distribution of screw dislocations. The torsion 2-form is calculated and we demonstrated that it is similar to the magnetic field 2-form. On the basis of these similarities we investigated the quantum dynamics of a free particle in the presence of a density of screw dislocations. This analysis demonstrates that a uniform torsion is responsible for an analog Landau quantization. We also consider the introduction of an external magnetic field and the quantum dynamics of a single particle in the presence of a continuous homogeneous distribution of parallel screw dislocations. The energy spectrum and eigenfunctions are obtained and we observe that the presence of magnetic field introduces an additive effect in the spectrum. This fact can be seen in equation (37) where ω_{el} and ω_{c} are two positive quantities which add together. The torsion and the magnetic field appear formally on the same footing in the Hamiltonian. But that does not imply similarity of the torsion and magnetic field; in the present case the torsion introduces a spiral structure in the medium absent in the magnetic field case. In fact that is a consequence of the fact that the gauge groups for the magnetic field case and the screw dislocation are essentially different [21]. A complete study of this problem should include a potential originating from deformation-potential theory [6, 19–22]. This will be done in a more detailed forthcoming publication.

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