Electron-state effect induced by helical structure of metal nanowires formulated by path integrals in Riemann space

H. Kato* and H. Yashiro
Yamanashi University, Faculty of Engineering, 4-3-11 Takeda, Kofu, 400-8511 Yamanashi, Japan
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Thin nanowires of a metal have a multishell structure in which several deformed helical shells are stacked. The purpose of this paper is to give a perspective on the electron state in a helical nanowire based on the Riemann geometrical formulation of quantum mechanics within the continuum approximation of a wire. The helical configuration of atoms in the wires results in a sort of vector potential, and the electron state is modulated by the winding number and the shear modulus of the shell. The energy dispersion curve depends on the imbalance of the slide and distortion angles of the wire.

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Recently, quantized conductance at room temperature has been investigated through the metallic nanowires formed at the elongated point contact.1–3 Especially, in the nanowire of gold, the relation between the conductance and the atomic configuration is clarified by the combination of the measurements of the conductance by the STM and the structure by the TEM.2 At thin nanowires the existence of the Multi Helical Shell structure (MHS) is confirmed through these experiments,4,5 whose helical structure is enhanced as the diameter of a wire decreases. The same helical structure is also discussed regarding the wires of Ti,6 Pt,7 Pb, and Al.8 This structure is considered widely present at the metal wire. A shell in MHS is formed by the lattice with a shear strain, which affects the radius and pitch of the helix.4

A study about the electron state in a helical wire pointed out a possibility of shifts and crosses of the energy dispersion curve, which affect the channel number of the conductance.9 This discussion treats the effect of torsion around the wire axis but neglects the slide along the axis. One of the purposes of this paper is to propose a model about the electron state in a helical wire which is affected by both the torsion and slide along the wire axis. An electron motion in the crystal with a dislocation has been discussed by applying a Riemann geometrical formulation.10 Because of the similarity of the structure between the dislocation in a crystal and the helical wire, we apply a Riemann geometrical formulation to discuss the electron state in a helical wire.

We introduce the hypothesis that the electron state is expressed by a localized base even in a deformed wire. This localized base reduces to the Wannier basis when the deformation is relaxed. Then, the local motion of an electron from the ith site to the jth site is determined independently from the global structure of the wire and the motion is reduced to a free electron in a relaxed space without deformation. If we denote the location of the ith site in the deformed space by \( \mathbf{x}_i \) and \( \xi_i \) in the relaxed space, the transition matrix satisfies the relation \( \langle \mathbf{x}_j(t_f) | \mathbf{x}_i(t_i) \rangle = \langle \xi_j(t_f) | \xi_i(t_i) \rangle \). Here, \( t_i \) and \( t_f \) are times to occupy the initial and final sites. Using continuum approximation to the sites, the motion of an electron in the potential \( U \) at the relaxed space is governed by a Lagrangian

\[
L = \frac{m}{2} \left( \frac{d\xi}{dt} \right)^2 - U, \tag{1}
\]

with an effective mass \( m \). Here, the site index is abbreviated because of the continuum approximation. The potential \( U \) is introduced to entrap the electron in a wire, which is assumed to be the well potential given by

\[
U(\xi) = \begin{cases} 0 & \text{inside of the wire} \\ \infty & \text{outside of the wire} \end{cases} \tag{2}
\]

If we use the rectangular coordinate, the transition matrix \( G = \langle \xi(t_f) | \xi(t_i) \rangle \) is expressed in the path-integral formulation as follows:

\[
G = \int \mathcal{D}\xi(t) \exp \left[ \frac{i}{\hbar} \int_0^T L(\dot{\xi}, \xi) dt \right]. \tag{3}
\]

Here, the symbol \( \mathcal{D}\xi(t) \) stands for the path-integration and \( T = t_f - t_i \). The motion of an electron is related to the square of infinitesimal distance \( d\xi^2 \). If the relation between \( d\xi \) and \( d\mathbf{x} \) is determined, the motion of an electron can be expressed by a quadratic form of displacement vector \( d\mathbf{x} \) in a deformed space. This quadratic form is the fundamental form of Riemann geometry and is the starting point of its quantization.10

In Fig. 1, the outer shell with radius \( R \) (a), which is a component of the multi-shell structure, and its unfolding diagram (b) are shown. The helical shell is characterized by two angles, \( \alpha_R \) and \( \beta_R \). The slide along the \( z \)-axis is determined.
by angle \( \alpha_R \), which is related to the absolute value of the Burgers vector \( b=2\pi R \tan \alpha_R \). The torsion around the \( z \)-axis is subjected by angle \( \beta_R \), which determines the pitch of the helix \( \zeta_{tr} = 2\pi R/\tan \beta_R \). In Fig. 1(b), the length of the chiral vector is denoted by an arrow with a symbol \( C \), whose size is measured along the circumference of a wire represented by \( C=2\pi R=d \cos(\beta_R-\alpha_R)/\cos \beta_R \) with \( d \) as a size of the shell along the crystal lattice.4

Using the cylindrical coordinates, the relation between a displacement of an electron in a helical wire \( dx = (dr, d\theta, dz) \) and that in a relaxed space \( d\xi = (dx, d\theta, dz) \) is given by

\[
d\xi = (1 + B) \cdot dx.
\]

Using relation (5) we transform the path of \( \xi \) into the path of \( x \) in Eq. (3). For this transformation we need the Jacobian of functional10 \( J=E(\xi(t))/\alpha(t) \), which is given by

\[
J = \exp \left[ -\int_{t_i}^{t_f} \frac{1}{i} \frac{\partial}{\partial r} \text{tr}(B) dt \right].
\]

Then the Lagrangian \( L \) in Eq. (3) becomes as follows:

\[
L = \frac{m}{2} \left[ \dot{r}^2 + \frac{1}{\cos \gamma} \left( \cos \alpha \dot{\theta} \theta + \sin \alpha \dot{\beta} \right)^2 \right] - \frac{\hbar}{2m} \left( \frac{\partial}{\partial r} \text{tr}(B) \right) - U - \Delta V_1.
\]

Here, \( \Delta V \) is a quantum correlation defined by

\[
\Delta V_1 = -\frac{\hbar^2}{8m} \frac{1}{r^2},
\]

which is related to the Weyl ordering of operators in the cylindrical coordinates.11,12

A classical Hamiltonian \( H_c \) of the system is obtained by the Legendre transformation on Eq. (7), whose explicit form is given by

\[
H_c = \frac{1}{2m} \left( p_r - \frac{\hbar}{i} \frac{\partial \text{tr}(B)}{\partial r} \right)^2 + \left( \cos \alpha \frac{p_\theta}{r} + \sin \alpha p_z \right)^2 + U + \Delta V_1,
\]

where \( p_r \), \( p_\theta \), and \( p_z \) are momentums conjugate to \( r \), \( \theta \), and \( z \), respectively.

On the other hand, according to the procedure of quantization by use of the path-integral method,12,13 a quantum Hamiltonian which reduces to the Lagrangian (7) is obtained by the Weyl ordering of the classical Hamiltonian (9) with the momentum operators,

\[
p_r = \frac{\hbar}{i} \left( \frac{\partial}{\partial r} + \frac{1}{r} + \frac{\gamma}{2} \tan \gamma \right), \quad \frac{\hbar}{i} \frac{\partial}{\partial \theta}, \quad \frac{\hbar}{i} \frac{\partial}{\partial z},
\]

with \( \gamma = \gamma/2 \). The quantum Hamiltonian \( H \) of an electron in a helical wire is given by

\[
H = -\frac{\hbar^2}{2m} \left( \frac{1}{r} + \frac{\gamma'}{\tan \gamma} \right)^2 - \frac{2}{r^2} + \frac{2\gamma'}{\cos^3 \gamma}.
\]

When \( \alpha_R = 0 \), the Hamiltonian \( H \) is a \( \gamma \) number, this Hamiltonian subjects the motion of an electron in the vector potential

\[
A = \frac{\alpha_R}{R} r^2 p_r e_\theta.
\]

This vector potential is equivalent to that of a uniform magnetic field and we can expect the Aharonov-Bohm effect on the motion around the circumference of a wire.

\[
E(\theta) = E(0) \cos \gamma.
\]

FIG. 2. Dispersion relation of the electron energy when \( \alpha_R = 17^\circ, \beta_R = 14^\circ \) (a), \( \alpha_R = 0^\circ, \beta_R = 14^\circ \) (b), and \( \alpha_R = 17^\circ, \beta_R = 0^\circ \) (c). Thin curves for \( \alpha_R = \beta_R = 0^\circ \) are also depicted for the sake of comparison. The meaning of the indexes is discussed in the text.
If the wave function $\psi(r, \theta, z)$ is separated into $\psi(r, \theta, z) = \chi(r) e^{i(n + k z)}$ with $k$ as a wave number along the $z$-axis and $n$ an integer (which is determined by the boundary condition about $\theta$), the energy eigenvalue $E$ is decided by the eigenvalue problem of the function $\chi(r)$:

$$
\left( \frac{d}{dr} + a \right)^2 \chi + \left( \frac{1}{r} + \frac{\gamma^2}{2} \tan \gamma \right) \left( \frac{d}{dr} + a \right) \chi + \frac{2Em}{\hbar^2} \chi + \Delta V \chi = 0.
$$

(17)

Here, $a = \partial \mathcal{V}(B)/\partial r$ and $\Delta V = \Delta V_1 - \Delta V_2$. Because of the well potential given by Eq. (2), the function $\chi(r)$ must satisfy the boundary conditions: $\lim_{r \to 0} r \chi'(R) = 0$ and $\chi(R) = 0$.

By means of a numerical analysis on a discretized representation of Eq. (17), we obtain the eigenvalue of $E$ and summarize it in Fig. 2. There are three cases where different values of $\alpha_R$ and $\beta_R$ are given: (a) $\alpha_R = 17^\circ$, $\beta_R = 14^\circ$, (b) $\alpha_R = 0^\circ$, $\beta_R = 14^\circ$, and (c) $\alpha_R = 17^\circ$, $\beta_R = 0^\circ$. The thin curves are for the case of $\alpha_R = 0^\circ$ and $\beta_R = 0^\circ$, which are given for the sake of comparison. In Fig. 2(a), the solid and thin curves are almost aligned with each other and cannot be distinguished. This means that when the slide and the torsion are almost aligned with each other and cannot be distinguished.

When the parameters $\alpha_R$ and $\beta_R$ vanish, the function $\chi(r)$ reduces to $J_n(z_{np}r/R)$ where $J_n$ is the Bessel function of nth order and $z_{np}$ is its zero point, i.e., $J_n(z_{np}) = 0 (n = 1, 2, 3, \cdots)$. The index labeled for each curves in Fig. 2 is a pair of these values of $\alpha_R$ and $\beta_R$. When there is an imbalance between the values of $\alpha_R$ and $\beta_R$, the dispersion relation shifts along the axis of the wave number $k$. The shift increases with the value of the index $n$, so that a possible crossing will occur between the dispersion curves. As already discussed, if the Fermi level is located at this crossing point, the channel number of conduction will be affected. Even though the value of the reported $\gamma_R$ or imbalance is small, the externally applied torsion involves a large imbalance and the electron state will be affected.

If the wire is composed of a single shell with radius $R$, the wave function becomes a two-dimensional function of $\theta$ and $z$ and given by $\psi(\theta, z) = e^{i(n + k z)}$ ($n = 0, 1, 2, \cdots$). The energy eigenvalue $E_{sh}$ of a two-dimensional electron on a shell is expressed by

$$
E_{sh} = \frac{\hbar^2}{2mR^2} \left[ \frac{n^2}{q_R} \cos^2 \gamma_R + kR - \frac{n}{q_R} \cos (\beta_R + \alpha_R) \sin \gamma_R \right]^2
$$

(18)

with $q_R = \sin^2 \alpha_R + \cos^2 \beta_R$. The electron state on a single helical shell is a one-dimensional wave which is quantized by an integer $n$ and propagates along the wire axis with a wave number $k$. From Eq. (18), we can recognize that the dispersion curve shifts when $\alpha_R$ and $\beta_R$ is imbalance or $\gamma_R \neq 0$ and its shift depends on the integer $n$. This dependence of the index $n$ is similar to that appearing in Fig. 2 for a solidity wire.

In this paper we have given a model in which a helical structure of a nanowire is characterized by two parameters, the slide angle $\alpha_R$ and the torsion angle $\beta_R$, and the motion of an electron in a helically deformed wire is mapped onto a locally free motion in a space without the deformation. A global structure of a helical wire is taken into account on a Hamiltonian with an effective vector potential due to a helical curvature. According to this model, a possible shift and crossing of the energy dispersion curves is discussed, which depends on the imbalance of the angles $\alpha_R$ and $\beta_R$.

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8*Electronic address: katoh@yamanashi.ac.jp