Quantum mechanical motion of a particle in a dislocated crystal is formulated in terms of a path integral in a Riemannian space by using the continuum description of a deformed crystal.

Recently, Kawamura developed a theory of scattering of an electron in a crystal due to the presence of dislocations. One of the essential features of dislocated crystals is the lack of global translational symmetry although the local features of such crystals are not different from those of perfect crystals. The consequence of this feature is that locally the quantum propagation of an electron is in the form of a plane wave; namely if the phase of the wave is once determined at a lattice point, then it is also determined uniquely at other lattice points in the neighborhood. However, in a global sense, the phase of the wave is not uniquely determined in dislocated crystals. It depends on the path along which the wave propagates. Thus the mismatching of phases of waves, which have propagated along different paths, takes place at a lattice point where the waves meet each other. Detailed description of such an interesting feature is given in Kawamura's paper in the case of screw dislocations.

In this paper, we discuss this problem in a general framework by using the continuum description of deformed crystals. Suppose a particle moves in a deformed crystal, whose deformation is described in terms of a strain field \( \beta_i(x) \). Namely, when two points at \( x \) and \( x + dx \) in a perfect crystal are displaced by amounts \( u \) and \( u + du \) respectively with \( du = \beta_i(x) dx \), we call the resulting crystal a deformed crystal with a strain field \( \beta_i(x) \).

Suppose a particle moves over a small distance \( dx \) in a deformed crystal. Then the particle is considered to move over a distance \( dy \), whose components are given by

\[
dy^i = dx^i - du^i = \gamma_{i}(x) dx^i
\]

with

\[
\gamma_{i}(x) = \delta_{i} - \beta_{i}(x).
\]

in a local perfect crystal, which is obtained by relaxing the local deformation given by the strain tensor \( \beta_i(x) \). The number of atoms along each crystallographic axis which the moving particle sees is proportional to the component of the vector \( dy \) along the corresponding axis. Therefore, if the phase change of the wave function of the moving particle is governed by the number of atoms along each crystallographic axis which the particle sees as a consequence of a tight-binding Hamiltonian of the particle motion on a lattice, the distance which influences the quantum propagation is \( (dy^i)^2 \), that is,

\[
(\text{dy}^i)^2 = g_{ij}(x) dx^i dx^j
\]

where

\[
g_{ij}(x) = \gamma_{i}(x) \gamma_{j}(x)
\]

Hence we may call the deformed crystal a Riemannian space with the metric tensor \( g_{ij}(x) \) defined above. Furthermore, we define the coefficient of connexion by
\( \Gamma'(x) = \frac{\partial \gamma_i(x)}{\partial x^i} \Delta_{\mu i}(x), \) \hspace{1cm} (5)

where \( \Delta_{\mu i}(x) \) is the inverse matrix of \( \gamma_{\mu i}(x) \), namely \( \Delta_{\mu i}(x) \gamma_{\nu j}(x) \Delta_{\nu i}(x) = \delta_{\mu j}. \)

A curve whose tangential line is always parallel is given by

\[ d^2 x^i + \Gamma_i'(x) dx^i dx^i = 0, \] \hspace{1cm} (6)

which is equivalent to

\[ d\left( \frac{d y_i}{d x^i} \right) = 0, \]

which describes a straight line in the perfect crystal obtained by relaxing the local deformation of the deformed crystal.

On the assumption that the particle behaves quantum-mechanically as a free particle in the local perfect crystal, in which the displacement is given by \( dy_i \), we may construct the quantum propagation in the form of a path integral. Let us consider a path \( y(\tau) \) of the motion of the particle, starting from a given initial condition \( y(0) = y_0 \). At each instant of time \( \tau \) in the time interval \( (0, t) \), we open a gate \([y(\tau), y(\tau) + \delta y(\tau)]\). Then, the quantum mechanical amplitude of paths which go through these gates at all instants of time is given by

\[ \exp \left\{ \int_0^t d\tau \left( \frac{i}{\hbar} \left( \frac{1}{2} m \dot{x}(\tau)^2 - V(x(\tau)) \right) - i \int_0^t d\tau \left( \frac{1}{2} m \dot{x}(\tau)^2 - V(x(\tau)) \right) \right) \right\}, \] \hspace{1cm} (9)

The Jacobian is the determinant of the matrix whose \((i\tau)(j\tau')\) component is \( \delta y^i(\tau) / \delta x^i(\tau') \). Here we suppose that the indices of rows and columns are the pairs \((i, \tau)\). By using the formula \( \det(A + B) = \det A \cdot \det(1 + A^{-1}B) = \det A \cdot \exp \left[ \text{Tr}(\log(1 + A^{-1}B)) \right] = \det A \cdot \exp \left[ \text{Tr}(A^{-1}B) - (1/2) \text{Tr}(A^{-1}BA^{-1}B) \right] + \ldots \), we obtain the following expression of the Jacobian:

\[ J = \prod_{0 < \tau < t} \gamma(x(\tau)) \] \hspace{1cm} (10)

\[ \times \exp \left\{ \int_0^t d\tau \left( \frac{1}{2} m \dot{x}(\tau)^2 - V(x(\tau)) \right) \right\} \]

where \( \gamma(x) \) is the determinant of the \( 3 \times 3 \) matrix \( \gamma_{\mu i}(x) \) and \( \Gamma'_i(x) - \Gamma_i'(x) \) is a torsion tensor. Thus we arrive at the final expression for the amplitude of the quantum propagation of a particle starting from the initial condition \( x(0) = x_0 \) and arriving at \( x(t) = x \) at time \( t \) in the form of a path integral

\[ G(x, x_0; t) = \int_{x(0) = x_0} \cdots \int_{x(t) = x} \prod_{0 < \tau < t} \left\{ \delta x^i(\tau) \delta x^i(\tau') \delta x^i(\tau') \right\} \]

\[ \times \prod_{0 < \tau < t} \gamma(x(\tau)) \] \hspace{1cm} (10)

\[ \times \exp \left\{ \int_0^t d\tau \left( \Gamma_i'(x(\tau)) - \Gamma_i'(x(\tau)) \right) \dot{x}^i(\tau) \right\} \]

\[ \times \exp \left\{ \int_0^t \frac{1}{2} m / 2 g_{\mu i}(x(\tau)) \dot{x}^i(\tau) \dot{x}^i(\tau') \right\} \] \hspace{1cm} (10)
The argument above can be applied immediately to the diffusion process in a distorted lattice. Suppose a particle performs a random walk on the lattice. The particle jumps from one site to a neighbouring site with constant frequency even if the distance between the neighbouring sites is changed by the deformation of the lattice. The diffusion process in the continuum limit of the lattice corresponds to the situation of the above argument. The conditional probability of finding the particle in the interval \([x', x + dx]\) at time \(t\) with the condition that the particle was at \(X_0\) at time \(t=0\) is just
\[
G(x, X_0; t) = \exp\left\{\frac{i}{\hbar} \int_0^t \left[ \frac{m}{2} \left( \dot{x}_1^2 + \dot{x}_2^2 + \dot{x}_3^2 \right) - eA_1(x)\dot{x}_1 - eA_2(x)\dot{x}_2 - eA_3(x)\dot{x}_3 \right] dt \right\},
\]
which can be alternatively written as
\[
G(x, x_0; t) = \int_{x_0}^x \int_0^t \prod_{0 < \tau < t} \delta x_1(\tau) \delta x_2(\tau) \delta x_3(\tau) \left\{ -\dot{x}_1^2(\tau) - \dot{x}_2^2(\tau) - \dot{x}_3^2(\tau) \right\} dt.
\]

The latter expression implies the following: First draw a path in the \((x^1, x^2)\)-plane, which starts at \(x^1(0) = x_0^1, x^2(0) = x_0^2\). Then perform the path integral over \(x^3(\tau)\) \(0 < \tau < t\) with the constraints \(x^3(0) = x_0^3\) and \(x^3(t) = x_3\) and \(\int_0^t dt\{ \dot{x}_1(\tau) = \dot{x}_1(x(\tau)) + \dot{x}_1(\tau) \beta_{13}(x(\tau)) \} \). We then perform the path integral over \(x^1(\tau)\) and \(x^2(\tau)\) \(0 < \tau < t\). Furthermore by introducing the delta-function, we arrive at a rather familiar form
\[
G(x, x_0; t) = \frac{1}{(2\pi\hbar)^3} \int_0^t dt \int_{-\infty}^{\infty} dQe^{iQ},
\]

which can be alternatively written as
\[
G(x, x_0; t) = \int_0^t \prod_{0 < \tau < t} \delta x_1(\tau) \delta x_2(\tau) \delta x_3(\tau) \left\{ -\dot{x}_1^2(\tau) - \dot{x}_2^2(\tau) - \dot{x}_3^2(\tau) \right\} dt.
\]
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6) K. Kondo, RAAG Memoirs 3 (1962), 163.
8) See for example, L. D. Faddeev and A. A. Slavnov, Gauge Fields: Introduction to Quantum Field Theory (Benjamin, London, 1980).