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Scattering of electrons on screw dislocations

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A previously established general framework for the description of long-wavelength quantum states of electrons in a crystal with topological defects is used to discuss the scattering of electrons on a screw dislocation. The corresponding Schrödinger equation contains contributions of the type of a vector potential as well as of a repulsive scalar potential. Together they give rise to modified Aharonov-Bohm interferences in the scattering amplitude, for which the far-field expression is calculated exactly. [S0163-1829(99)01121-2]

In connection with investigations of residual low-temperature resistivities, the scattering cross section of electrons on a screw dislocation has been calculated in Born approximation by Hunter and Nabarro,[1] and in a partial-wave expansion by Stehle and Seeger.[2] Both approaches use the defect-free crystal as a reference system, and the screw dislocation was represented by a deformation potential.[3] In a continuum version, the latter was expected to give an adequate description of the long-wavelength scattering waves.

More recently it has been pointed out by Kawamura[4] that the topological nature of a screw dislocation invalidates assumption of an ideal lattice structure at arbitrary distances from the dislocation core. Correspondingly, an incoming electron cannot be described by a simple plane wave. In the continuum limit of a tight-binding model, defined on a lattice with a built-in screw dislocation, Kawamura derived a Schrödinger equation with only a kinetic term in the Hamiltonian. The Fourier transform of this equation with respect to the axial coordinate of the dislocation is reminiscent of that for an electron moving in the vector potential of a magnetic flux line. Accordingly, Kawamura predicted Aharonov-Bohm interferences[5] in the scattering process of an electron on a screw dislocation. However, due to the assumption of constant transfer energies in the tight-binding model, Kawamura misses a long-ranged repulsive potential which can compete with the kinetic terms, and which dominates lattice corrections of the Hamiltonian in the core region.[6]

In a recent general treatment of the long-range quantum states of an electron in a crystal with topological defects[7] we also used the tight-binding approximation as an intermediate step. For constant transfer energies this led in the continuum limit to a covariant Schrödinger equation which, in the language of the continuum theory of defects,[8] lives on a Riemann-Cartan manifold. Additional noncovariant terms show up in this equation when the transfer energies, i.e., the tunneling rates of the particle, are assumed to depend on the local lattice deformations caused by the defects.

Applied to the case of a single straight screw dislocation, the covariant part immediately reproduces Kawamura's form of the Schrödinger equation. The noncovariant contributions, arising from the most natural and most simple deformation dependence of the transfer energies, include a repulsive potential which has the same long-distance behavior as the covariant kinetic terms. This invalidates any kind of perturbation expansion for the scattering amplitude which therefore in the following is calculated without such approximations.

Before continuing, we mention an alternative way to derive the Schrödinger equation for a particle moving in a medium with topological defects.[9] This approach uses the idea of a gauge-field theory of topological defects,[10] and in principle allows to avoid the tight-binding approximation.

Within our approach[7] we have explicitly derived the Schrödinger equation for a spinless electron moving in a simple-cubic crystal with a single screw-dislocation line along the z axis. In terms of cylinder coordinates $x=(\mathbf{r},z)$, with $\mathbf{r}=(r\cos\phi,r\sin\phi)$, the result reads

$$i\hbar\partial_t\psi(x,t)=-\frac{\hbar^2}{2m}\left(\frac{1}{r}\partial_r r\partial_r+\frac{1}{r^2}\partial_\phi^2+\partial_z^2+\frac{b}{\pi r^2}\partial_\phi\partial_z-\frac{b^2}{2\pi^2a^2r^2}\right)\psi(x,t), \qquad (1)$$

where m is the effective mass of the electron, $b=\mathbf{b}\cdot\mathbf{e}_z$ is the magnitude of the Burgers vector of the dislocation, and a is the lattice constant of the undistorted lattice. The Hamiltonian H in this equation has the same form as that used by Stehle and Seeger,[2] but will here be split in a different way into a kinetic and a potential part.

After adding and subtracting a term $(\hbar^2/2m)(b/2\pi r)^2\partial_z^2$ in Eq. (1), the separation $\psi(\mathbf{r},z,t)=\exp(-iEt/\hbar)\exp(ikz)\chi(\mathbf{r})$ leads to the equation

$$\left[\frac{1}{r}\partial_r r\partial_r+\frac{1}{r^2}(\partial_\phi+i\alpha)^2-\beta^2\frac{1}{r^2}+q^2\right]\chi(\mathbf{r})=0. \qquad (2)$$

Here $\alpha\equiv kb/(2\pi)$ and $\beta^2\equiv[2-(ka)^2](b/2\pi a)^2$ formally enter as the strengths of a vector and of a scalar potential, and q is determined by $E=(\hbar^2/2m)(q^2+k^2)$. The scalar potential just arises from the deformation-dependent transfer energies and is repulsive, since the continuum limit implies $ka<1$, i.e., $\beta^2>0$.

If in Eq. (2) α and β temporarily are considered as independent parameters, then the case $\beta=0$ just corresponds to the model discussed by Kawamura.[4] For the corresponding scattering problem he adopted the Aharonov-Bohm solution[5]

$$\chi_\alpha(\mathbf{r})=\sum_{\nu=-\infty}^{\infty}(-i)^{\kappa(\nu)}J_{\kappa(\nu)}(qr)e^{i\nu\phi}, \qquad (3)$$

where $J_{\kappa(\nu)}$ is a Bessel function with $\kappa(\nu)\equiv\sqrt{(\nu+\alpha)^2}$. Asymptotically, for $r\to\infty$, one finds (after a minor correction in Ref. 5)

$$\chi_\alpha(\mathbf{r})\to e^{-i(qr\cos\phi+\alpha\phi)}+\frac{e^{ikr}}{(2\pi iqr)^{1/2}}\sin(\pi\alpha)\frac{e^{i(\alpha/2|\alpha|)(\phi-\pi)}}{\cos(\phi/2)}, \qquad (4)$$

which shows that Eq. (3) describes a wave function, coming in from the positive x axis.

In the context of our approach,[7] the case $\beta=0$ originates from the covariant part of the Hamiltonian where the Laplace-Beltrami operator determines the kinetic energy. The potential $\propto\beta^2$ stems from noncovariant terms in the Hamiltonian, which follows from distortion-dependent transfer energies in a tight-binding model.[7] It is purely repulsive and has, in a similar form, been proposed by Kosevich[11] on a phenomenological basis.

Since this potential is of the same order as the vector-potential terms in Eq. (2), it is not advisable to use a perturbation expansion in β. Instead, we use the full Green function $G(\mathbf{r},\mathbf{r}')=\langle\mathbf{r}|1/(H-E-i\epsilon)|\mathbf{r}'\rangle$ to write the exact solution of Eq. (2) in the form

$$\chi(\mathbf{r})=\chi_\alpha(\mathbf{r})-\beta^2\frac{\hbar^2}{2m}\int d^2r'\,G(\mathbf{r},\mathbf{r}')\frac{1}{r'^2}\chi_\alpha(\mathbf{r}'). \qquad (5)$$

For the Green function one finds

$$G(\mathbf{r},\mathbf{r}')=\Theta(r'-r)F(\mathbf{r},\mathbf{r}')+\Theta(r-r')F(\mathbf{r}',\mathbf{r}), \qquad (6)$$

where, in terms of Bessel and Hankel functions $J_{\lambda(\mu)},H^{(1)}_{\lambda(\mu)}$ with $\lambda(\mu)=\sqrt{(\mu+\alpha)^2+\beta^2}$,

$$F(\mathbf{r},\mathbf{r}')=i\frac{m}{\hbar^2}\sum_{\mu=-\infty}^{\infty}J_{\lambda(\mu)}(qr)H^{(1)}_{\lambda(\mu)}(qr')e^{i\mu(\phi-\phi')}. \qquad (7)$$

Insertion of Eq. (3), and of Eqs. (6) and (7) into Eq. (5), and use of the asymptotic form

$$H^{(1)}_\lambda(qr)\to\sqrt{\frac{2}{\pi qr}}e^{i(qr-\lambda\pi/2-\pi/4)} \qquad (8)$$

for $r\to\infty$, leads to the behavior

$$\chi(\mathbf{r})-\chi_\alpha(\mathbf{r})\to-i\beta^2\frac{1}{\sqrt{2\pi iqr}}e^{iqr}\sum_{\mu=-\infty}^{\infty}e^{i[\mu\phi-\lambda(\mu)\pi/2]}\times\sum_{\nu=-\infty}^{\infty}(-i)^{\kappa(\nu)}\int_0^{2\pi}d\phi'\,e^{i(\nu-\mu)\phi'}\times\int_0^\infty\frac{d\rho}{\rho}J_{\lambda(\mu)}(\rho)J_{\kappa(\nu)}(\rho). \qquad (9)$$

The integral over ϕ' yields $2\pi\,\delta_{\mu\nu}$, which makes the sum over ν trivial. Subsequent use of the identity

$$\int_0^\infty\frac{d\rho}{\rho}J_\lambda(\rho)J_\kappa(\rho)=\frac{2}{\pi(\lambda^2-\kappa^2)}\sin\left[\frac{\pi}{2}(\lambda-\kappa)\right] \qquad (10)$$

leads, together with Eq. (4), to the final result:

$$\psi(\mathbf{r})\to e^{-i(qr\cos\phi+\alpha\phi-kz)}+f(\phi)\frac{e^{i(qr+kz)}}{\sqrt{2\pi iqr}} \qquad (11)$$

with the scattering amplitude

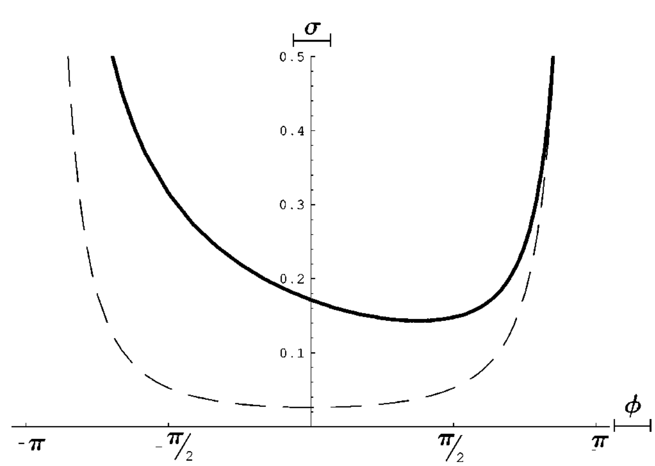

FIG. 1. Scattering cross section, following from Eq. (12) for $ka=qa=0.7$ and $b=a$. The dashed line represents Kawamura's result for the same values of the parameters.

$$f(\phi)=\sin(\pi\alpha)\frac{e^{i(\alpha/2|\alpha|)(\phi-\pi)}}{\cos(\phi/2)}-2\sum_{\mu=-\infty}^{\infty}e^{i\mu\phi}(e^{-i\pi\kappa(\mu)}-e^{-i\pi\lambda(\mu)}), \qquad (12)$$

which corrects the expression given in Ref. 7. The related differential scattering cross section per unit length of the dislocation line $d\sigma/d\phi=1/(2\pi q)|f(\phi)|^2$ is plotted in Fig. 1 for the values of α and β, given below Eq. (2). Also shown is the result for the artificial case $\beta=0$, i.e., for the cross section calculated by Kawamura.[4] In both cases the far-field approximation to ψ breaks down close to $\phi=\pi$, which will lead to quantitative corrections in these regions.[5] The essential result, however, is that the inclusion of the repulsive deformation potential obviously breaks the symmetry $\phi\rightarrow-\phi$ in Kawamura's differential cross section, reflecting the chiral nature of the screw dislocation.

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