Diffusion in the Presence of Topological Disorder

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A general framework is presented for the discussion of Brownian motion in crystals with randomly distributed topological defects. In a two-dimensional lattice with disclinations one finds a nonuniversal subdiffusional behavior if screening in the disclination ensemble is taken into account. Without screening, a Sinai-type diffusion is expected. In a three-dimensional random array of parallel screw dislocations, a Brownian particle shows anisotropic normal diffusion. However, the process no longer is Gaussian and displays long-time tails in the fourth-order cumulants.

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It is well known that a Brownian particle in a random medium can exhibit a long-time and large-distance behavior different from that of an ordinary diffusion process [1]. Departures from the asymptotic time dependence \( \langle \Delta X(t) \rangle_0 \sim t \) of the mean-square displacement are well documented and play an important role in physical, chemical, and biological applications [2]. Here we are interested in anomalies of particle diffusion in a medium with randomly distributed topological defects, such as dislocations and disclinations.

The common feature of such defects is that locally (not too close to the defect core) the lattice looks perfect. One needs to walk around on the lattice to tell the difference between a perfect and a dislocated crystal. For the discussion of large traveling distances of a particle, it is then convenient to use the continuum theory of defects initiated by Kondo, by Bilby et al., and by Kröner [3]. This theory emerges from a lattice description in the limit of vanishing lattice spacing where, however, local angular directions are retained.

A basic concept of the continuum theory of defects is the introduction of two different frames, one with coordinates \( x^i \) in the laboratory system, and the other defined at each point in the medium with components \( \xi^\alpha \) along the local crystallographic axes. The line elements in these frames are related to each other by a matrix field \( B^i_\alpha(x) \) via

\[
dx^i = B^i_\alpha d\xi^\alpha,\tag{1}
\]

where summation over repeated indices is implied. At each \( x \) the equations \( \delta^i_\alpha B^i_\beta = \delta^i_\beta \) and \( B^i_\alpha B^i_\beta = \delta^i_\beta \) define an inverse matrix with components \( B^i_\alpha(x) \), which by \( B^i_\alpha \delta^j_\alpha = \delta^j_\beta + \beta^j_\beta \) is connected with the distortion tensor \( \beta^j_\beta(x) \) generated in the medium by the defects. For various types of defects, e.g., in an isotropic elastic medium, \( \beta^j_\beta(x) \) and, consequently, \( B^i_\alpha(x) \) are known [3].

The fact that locally (and far from any defect core) the medium behaves as a perfect crystal means that in the internal coordinate system one has a Euclidean metric tensor \( g_{\alpha\beta} = \delta_{\alpha\beta} \) and a trivial affine connection \( \Gamma^\beta_{\alpha\gamma} = 0 \). Transformation to the external coordinates then implies [3]

\[
g_{ij} = B_\gamma^i B_\beta^j \delta_{\alpha\beta}, \quad \Gamma^i_\beta = B_\alpha^i \partial_\beta B^\alpha_\beta. \tag{2}
\]

The affine connection \( \Gamma^i_\beta \) is compatible with the metric \( g_{ij} \), i.e., \( \nabla_k g_{ij} = 0 \), where \( \nabla_k \) stands for the covariant derivative \( \nabla_k g_{ij} = \partial_k g_{ij} - \Gamma^l_\beta g_{ij} - \Gamma^i_\beta g_{lj} \). However, \( \Gamma^i_\beta \) does not reduce to a Christoffel symbol, but has a nonzero torsion

\[
T^i_\beta = \frac{1}{2} \left( \Gamma^i_\beta - \Gamma^i_\beta \right) \tag{3}
\]

measuring the defect density [3].

Now, consider a test particle which is undergoing a simple random walk in a medium with topological defects. Since locally the system looks perfect (core regions excluded), the particle motion will be described in the local coordinates \( \xi^\alpha \) by an ordinary Langevin equation. After transformation to the global coordinates \( x^i \) this equation reads

\[
dx^i(t) = B^i_\alpha(\mathbf{x}(t)) \xi^\alpha(\mathbf{x}(t)), \tag{4}
\]

where \( \Lambda^\alpha(\mathbf{x}(t)) \) is a Gaussian random force with zero average and variance

\[
\langle \Lambda^\alpha(\mathbf{x}(t)) \Lambda^\beta(\mathbf{x}(t')) \rangle = 2D \delta^\alpha_\beta \delta(t - t'). \tag{5}
\]

At this stage we have to specify the interpretation of the stochastic equation (4) [4]. It turns out [5] that the Stratonovich interpretation is the only one that leads to a covariant diffusion equation.

For all types of topological defects the diffusion equation reads [5]

\[
\partial_t P(x,t) = D \Delta^T P(x,t), \tag{6}
\]

where

\[
\Delta^T = g^{ij} \nabla_i \nabla_j \nabla_i^j = \nabla_i + 2T^a_i, \tag{7}
\]

and \( g^{ij} \) is the inverse metric tensor. From the last equation it is seen that the vector \( 2T^a_i \) enters like a gauge field [6].
In (6), $P(x, t)$ is a scalar probability distribution which for a scalar observable $A(x)$ yields the expectation value
\[ \langle A \rangle(t) = \int d^d x \sqrt{g(x)} P(x, t) A(x) = \langle P(t), A \rangle. \quad (8) \]
Equation (8) provides us with a scalar product in space dimension $d$, involving the Jacobian $g = \det(g_{ij})$. With respect to this scalar product, $\Delta$ is the adjoint of the usual Laplacian $\Delta = g^{ij} \nabla_i \nabla_j$. This establishes the equivalence of our approach with the treatment of diffusion processes on manifolds by Ikeda and Watanabe [7].

We now are ready to discuss the diffusion process, averaged over a quenched random distribution of topological defects. This is conveniently done in a Martin-Siggia-Rose-type path-integral representation [8], generated from an action $J[P, Q]$ defined by
\[ \exp\{-J[P, Q]\} = \exp\left\{ -\int dt \{ Q, \left[ \partial_t - D \Delta \right] P \} \right\}. \quad (9) \]
Here, $Q(x, t)$ is an imaginary-valued response field conjugate to $P(x, t)$, and we have used the scalar product introduced in (8). The overbar means the average over an ensemble of distortion fields. These enter in (9) via the Laplacian $\Delta$ and the Jacobian $g$ in the scalar product. The quantity to be calculated is the Green function
\[ G(x, t) = \int D[P, Q] P(x, t) Q(0, 0) \exp\{-J[P, Q]\}. \quad (10) \]
Its Fourier transform $\hat{G}(q, t)$ is a generating function for the moments of the particle position $x'$, e.g.,
\[ \langle x^2 \rangle(t) = -\partial_q^2 \hat{G}(q, t)|_{q=0}. \]

In order to evaluate (10) one has to specify the type of defects and the defect ensemble. We first consider the case of disclinations, although these generate the most extreme distortion of a crystal and therefore are hard to realize. But just because of this property we expect that disclinations will produce the strongest possible anomalies in the diffusion process. As the simplest model of an ensemble we will choose a random distribution of disclination centers in a two-dimensional isotropic medium. The topological charges (Frank vectors) [9] are also assumed to be random with screening taken into account.

A single disclination at the origin generates a distortion field corresponding to a pure rotation, i.e., [9],
\[ \langle B^2 \phi \rangle = \begin{pmatrix} \cos(\Omega \phi/2\pi) & \sin(\Omega \phi/2\pi) \\ -\sin(\Omega \phi/2\pi) & \cos(\Omega \phi/2\pi) \end{pmatrix}, \quad (11) \]
where $\Omega$ is the Frank angle and $\phi = x^2/x^1$. Insertion of this field into Eqs. (2), (4) and (6), (7) yields $g = 1$ and a Fokker-Planck equation [5]
\[ \partial_t P = D \delta^{ij} \partial_i [\partial_j U] + \partial_t P, \quad (12) \]
with the drift velocity $V_i = -\partial_i U$ in which $U = \Omega \Phi$ and $\Phi(x)$ is the two-dimensional Coulomb potential.

Qualitatively, the appearance of a drift velocity is plausible in view of the Volterra construction [9] of a disclination. For positive $\Omega$ the disclination is created by cutting out an angular section from the unperturbed lattice and gluing together the lips of the cut. The distorted lattice then is allowed to relax into a state of elastic equilibrium, leading to symmetry with respect to the defect center. As a consequence of this operation, the space available for a Brownian particle is (compared with the regular lattice) increasingly reduced with increasing distance from the disclination center. Since this happens in an isotropic way, we expect the appearance of a radial drift velocity away from the center. If $\Omega$ is negative, the direction of the drift velocity obviously is reversed.

For a distribution of disclinations we assume
\[ U(x) = \int d^2 y \Phi(x - y) \rho(y), \quad (13) \]
where $\rho(x) = \sum \Omega \delta(x - x_\nu)$ is a topological charge density. The defect ensemble is taken to be Gaussian with zero mean and an isotropic and translationally-invariant second moment which includes the possibility of screening of the topological charges [5]. Equation (13) thus is complemented by
\[ \hat{\Phi}(q) = \frac{1}{q^2}, \quad \hat{\rho}(q)\hat{\rho}(p) = \gamma \frac{q^2}{q^2 + m^2}(2\pi)^2 \delta(q + p), \quad (14) \]
where $m$ is the inverse screening length. The factor $q^2$ in the numerator of the noise spectrum arises from the requirement of neutrality of the topological charges in each realization, $\hat{\rho}(0) = 0$, provided $m$ is finite. In the (probably less physical) case $m = 0$, the ensemble describes an array of completely uncorrelated disclinations.

According to (12)–(14) the general case of randomly distributed disclinations is equivalent to a random-drift model. Such systems have repeatedly been discussed in the literature [10], including the case of present interest where the velocities have a potential. In the limit $q^2 \ll m^2$ the velocity correlation function of our model becomes
\[ \langle V_i(q) V_j(p) \rangle = \gamma D^2/m^2(q_i q_j/q^2)(2\pi)^2 \delta(q + p). \]

A renormalization-group analysis of this system has been worked out by Kravtsov, Lerner, and Yudson [10]. They showed that $d_c = 2$ is just the upper critical dimension in which the coupling constant $u = \gamma/4\pi m^2$ is not renormalized. As a consequence, one finds the nonuniversal subdiffusive behavior
\[ \langle x^2 \rangle(t) \sim t^{1-\gamma/(8\pi m^2)}. \quad (15) \]

The case $m = 0$ yields
\[ \langle V_i(q) V_j(p) \rangle = \gamma D^2(q_i q_j/q^4)(2\pi)^2 \delta(q + p) \]
and has been considered by Bouchaud, Comtet, Georges, and Le Doussal [10]. Now the upper critical dimension is $d_c = 4$, and the coupling constant $u = \gamma/4\pi \mu^2$, with $\mu$ being an inverse scaling length, is driven by renormalization to a strong-coupling regime. The authors, however,
offer some heuristic arguments leading to a Sinai-type diffusion behavior

$$\langle x^2(t) \rangle \sim (\ln t)^2. \tag{16}$$

Equation (16) represents an even stronger deviation from normal diffusion than the result (15). This is to be expected since unscreened disclinations generate the most extreme distortion of the ideal lattice. Since a tightly bound pair of disclinations with opposite Frank angles can form an edge dislocation [11], we furthermore expect that (15) also is valid in an appropriate ensemble of edge dislocations.

As another application we now consider Brownian motion in an array of parallel screw dislocation lines which intersect the transverse plane at random positions. The topological charges in this case are Burgers vectors oriented parallel to the dislocation lines [9]. Their magnitudes are also assumed to be random, again with screening taken into account. This type of topological disorder naturally occurs in the process of crystal growth from a melt [12].

For a single screw dislocation, parallel to the $x^3$ axis, and going through the origin of the $x^1$, $x^2$ plane, the distortion tensor in an isotropic elastic medium has the nonzero components [3]

$$\beta^3_1 = -\partial U, \quad \beta^3_2 = \partial U. \tag{17}$$

with $U = b\Phi$ where $b$ is the magnitude of the Burgers vector, and $\Phi(x^1, x^2)$ again is the two-dimensional Coulomb potential. The matrix field $B_i^j(x)$, corresponding to (17), leads via Eqs. (2), (3) and (6), (7) to the Jacobian $g = 1$ of the metric tensor and to the diffusion equation

$$\partial_i P = D (\partial^j \partial_j + \partial^2) P + D [\delta^{ij}(\partial_j U)(\partial_i U) + \partial^2_j \partial^i \partial_j U] P.$$

(18)

Here and in the following we use the notation $x = (x^1, x^2), z = x^3, \partial^i = \partial_i, \partial^2 = \partial_1 + \partial_2$, and $\epsilon^{ij} = -\epsilon^{ji}$ with $i, j = 1, 2$ and $\epsilon^{12} = 1$. For an ensemble of parallel screw dislocations (18) will be supplemented again by Eqs. (13) and (14), where in this case $\rho(x) = \sum \beta_i \delta(x - x_i)$ means the density of Burgers vectors.

In the functional representation (9), we now make the ensemble average explicit by introducing the action

$$K[P, Q, U] = \int dt \int dz \int d^2 x \{ D [\partial_i - D(\partial^2 + \partial^2)] P + D(\partial_i, Q) [2\epsilon^{ij}(\partial_j U)\partial_i + \delta^{ij}(\partial_j U)(\partial_i U)\partial_i] P \}
+ \frac{1}{2} \int d^2 x \int d^2 y U(x) C^{-1}(x - y) U(y). \tag{19}$$

with $C(q) = \gamma / q^2(q^2 + m^2)$. Then, $J[P, Q]$ can be replaced by $K[P, Q, U]$ in the definition (10) of the Green function $G(x, z, t)$ with an additional functional integration over $U(x)$.

According to (19) a diagrammatic expansion of the Fourier transform $\hat{G}(q, k, \omega)$ involves the propagator $G_0(q, k, \omega) = 1/[i\omega + D(q^2 + k^2)]$, the correlator $C(q)$, a three-point vertex $\sim k$, and a four-point vertex $\sim k^2$. We eventually will be interested in cumulants of the particle position containing finite powers in $z$. Therefore, we only need to calculate contributions to the self-energy $\Sigma(q, k, \omega) = \hat{G}_0^{-1}(q, k, \omega) - \hat{G}^{-1}(q, k, \omega)$ with a finite power in $k$, i.e., two-point vertex diagrams with a finite number of interaction vertices [5]. In this sense the model turns out to be exactly solvable.

For the mean-square displacement of the particle we find an anisotropic normal diffusion, enhanced in the $z$ direction. The latter is plausible since the locally isotropic random steps globally lead to a climbing up or down of the particle on the spiral staircases of the screw dislocations. This effect is not strong enough to generate a superdiffusive (at least logarithmic) correction in the $z$ direction. However, anomalies do show up in higher cumulants of the particle position. For the fourth-order cumulants we find [5] $\langle x^4 \rangle_c = 0$ and

$$\langle x^2 z^2 \rangle_c \sim \langle z^4 \rangle_c \sim t \ln t \tag{20}$$

for $t \to \infty$. Thus, topological disorder can give rise to a non-Gaussian random-walk process. A measure of the deviation from Gaussian behavior is relative cumulants which exhibit long-time tails, e.g., $\langle z^4 \rangle_c / \langle z^2 \rangle^2 \sim (\ln t)/t$. It should be possible to see these anomalies experimentally or in a simulation.

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