Brownian motion in crystals with topological defects

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Abstract. The diffusion behaviour of a Brownian particle in a crystal with randomly distributed topological defects is analyzed by means of the continuum theory of defects combined with the theory of diffusion on manifolds. A path-integral representation of the diffusion process is used for the calculation of cumulants of the particle position averaged over a defect ensemble. For a random distribution of disclinations the problem of Brownian motion reduces to a known random-drift problem. Depending on the properties of the disclination ensemble, this yields various types of subdiffusional behaviour. In a random array of parallel screw dislocations one finds a normal, but anisotropic, diffusion behaviour of the mean-square displacement. Moreover, the process turns out to be non-Gaussian, and reveals long-time tails in the higher-order cumulants.

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1. Introduction

Dislocations and disclinations are classical examples of topological defects in condensed matter. In the following we consider a crystal with a quenched-random distribution of such defects. Our interest is in the behaviour of a Brownian particle which moves on interstitial positions of the distorted lattice. We especially work out the asymptotic long-time properties of the Brownian motion, discussed briefly in a previous communication [1].

It will be assumed that the average distance between the cores of the defects is large compared to the lattice spacing. Then, a Brownian particle predominantly stays outside the core regions, and locally sees an undisturbed lattice. Globally it feels the presence of the topological defects, e.g. by walking around a dislocation line. These considerations suggest to use the continuum theory of defects, developed by Kondo, by Bilby, Bullough, Smith, and by Kröner [2]. In this theory the limit of vanishing lattice spacing is performed, keeping track of the local orientations of the lattice. As a result, the distorted lattice is described by a Riemann-Cartan manifold where the torsion measures the defect density.

A natural basis of the further discussion is the theory of diffusion on manifolds. Similar to the procedure of Ikeda and Watanabe [3] we start from the observation that a Brownian particle locally sees a perfect lattice. This leads us to assume a standard white-noise Langevin equation for the particle position in each of the Euclidean tangent spaces of the manifold. After transformation to global coordinates we eventually establish a diffusion equation in a general covariant form. This equation depends on the defects via the metric tensor and the affine connection of the manifold. In order to perform the average over a defect ensemble, it is convenient to use a Martin-Siggia-Rose-type path-integral representation [4] of the diffusion process. The quantity of interest is the averaged propagator of the diffusion equation. Its spatial Fourier transform is a generating function of the moments of the particle position.

In a first application we consider disclinations in a two-dimensional crystal. For a single disclination the diffusion equation assumes the form of a Fokker-Planck equation with a radial drift velocity. This is plausible from the Voiterra construction [3] of a disclination where a wedge, measured by the Frank angle, is removed from the regular lattice. Consequently there is a radial decrease of the space available for a Brownian particle, generating a drift away from the disclination center. In case of a negative Frank angle the drift is towards the center. A random distribution of disclinations leads to a random-drift model where the drift velocities have a potential. For such models the mean-square displacement of a Brownian particle is known from renormalization group calculations [6]. If screening of the topological charges, i.e. of the Frank angles, is taken into account in the defect ensemble, one finds a non-universal subdiffusional behaviour. In the less physical case without screening we would expect a Sinai-type diffusion [7].

Dedicated to Professor Herbert Wagner on the occasion of his 60th birthday
Next we consider screw dislocations which naturally occur in the process of crystal growth [31]. A single straight screw dislocation line gives rise to an anisotropic diffusion equation. One finds a coupling between axial and azimuthal motions of a particle and an enhancement of its mobility in the axial direction. Both effects are due to the spiral-staircase structure of the distorted lattice and increase when the dislocation line is approached. In a random array of parallel screw dislocations any collision of the particle positions is determined by a finite number of Feynman diagrams for the self-energy of the propagator. Again we assume screening of the topological charges which now are the Burgers vectors. The mean-recur displacement then shows a net non-anisotropic diffusion behavior. However, the process is non-Gaussian, and displays long-range tails in the higher-order cumulants.

2. Continuum theory of defects

Topological defects in a crystal are in the continuum limit, described by the density of topological charges. Given this density, one wants to determine the related crystal deformations in equilibrium. One proceeds by introducing in addition to the laboratory coordinates of any point of the medium an internal frame with coordinates \(\xi(\mathbf{x})\) along the local crystallographic axes. The state of deformation then is contained in the matrix field \(B(\mathbf{x})\) defined by [2]

\[
\text{d}e = N_{\alpha\beta} \text{d}x^\alpha \text{d}x^\beta
\]

(2.1)

where summation over repeated indices is implied. Except in the defect cores \(\delta B(\mathbf{x})\) is assumed to be well-behaved and to have an inverse \(\delta B^{-1}\) with

\[
B^\alpha_\beta - \delta^\alpha_\beta = B_{\alpha\beta} \delta\eta^\beta
\]

(2.2)

The assumption that the lattice looks locally perfect means that the internal frames have a Euclidean metric tensor \(\eta^\alpha\eta^\beta = \delta^\alpha\beta\), and a trivial affine connection \(\Gamma^\kappa_\alpha\beta = 0\). Transformed to the laboratory system, this implies [2]

\[
\delta\eta^\alpha = B^\alpha_\rho \delta x^\rho + \Gamma^\alpha_\beta_\rho \delta x^\beta \delta x^\rho
\]

(2.3)

The affine connection \(\Gamma^\alpha_\beta_\rho\) is compatible with the metric tensor \(\eta^\alpha\eta^\beta\) since with the notation \(\delta\eta^\alpha\) for the covariant derivative

\[
T^\alpha_\beta_\rho = \Gamma^\beta_\rho_\alpha + \Gamma^\alpha_\beta_\rho - \Gamma^\gamma_\beta_\alpha \eta^\gamma_\rho = 0.
\]

(2.4)

However, \(T^\alpha_\beta_\rho\) has a nonzero torsion

\[
T^\alpha_\beta_\rho = \Gamma^\beta_\rho_\alpha - \Gamma^\alpha_\beta_\rho
\]

(2.5)

and therefore does not reduce to a Christoffel symbol. We mention that the curvature tensor

\[
R^\kappa_\alpha_\beta_\rho = \Gamma^\kappa_\alpha_\beta_\gamma \eta^\gamma_\rho - \Gamma^\kappa_\alpha_\beta_\rho = T^\kappa_\alpha_\beta_\rho + T^\kappa_\beta_\alpha_\rho - T^\kappa_\rho_\alpha_\beta
\]

(2.6)

vanishes for dislocations but is nonzero for dislocations. This follows from the representation

\[
R^\kappa_\alpha_\beta_\rho = B^\kappa_\alpha_\beta \eta^\rho - B^\kappa_\alpha_\rho \eta^\beta
\]

(2.7)

and the fact that \(B\) is multi-valued for dislocations [5]. According to the properties (2.4) and (2.5) the deformed crystal is, in the continuum limit, represented by a Riemann-Cartan manifold. The internal Euclidean frames can be considered as tangent spaces to this manifold. A crucial point now is the observation that the torsion \(T^\alpha_\beta_\rho(\mathbf{x})\) directly measures the density of defects [2]. This follows from the identity

\[
\sum\delta \eta^\alpha \eta^\beta = \frac{d}{dS} B_{\alpha\beta} \eta^\rho - \frac{d}{dS} R_{\alpha\beta\rho}(\mathbf{x}) \delta\eta^\rho
\]

(2.8)

where \(d\rho\) is the antisymmetric surface element on \(S\) and \(B^\alpha_\beta\) is the total Burgers vector of the defect lines enclosed by the boundary of \(S\). Equation (2.8) arises from (2.3) and (2.5) by use of Stokes' theorem.

In order to determine the field \(B^\alpha_\beta(\mathbf{x})\), for a given density of Burgers vectors. Eqs. (2.3), (2.5), and (2.8) need to be supplemented by an additional principle. For defects causing small deformations this is provided by the equilibrium conditions of linear elasticity theory. In terms of the distortion tensor

\[
\delta \eta^\alpha = B^\alpha_\beta \delta x^\beta - \delta x^\alpha
\]

(2.9)

with the symmetrized elastic constants \(C_{ijkl}\) of the defect-free crystal. Here the positions of indices are irrelevant since \(\delta x = \delta x + O(\beta)\). Linearization of (2.8) in \(\beta\) implies [2]

\[
\delta \eta^\alpha = B^\alpha_\beta \delta x^\beta - \delta x^\alpha
\]

(2.10)

where \(\delta x^\alpha\) is the Lie-Christoffel tensor, and \(\eta^\alpha\) is the density of Burgers vectors, such that

\[
(\delta x^\alpha) \eta^\alpha = 0
\]

(2.11)

with \(\delta x^\alpha = \delta x^\alpha - \delta x^\alpha\). The solution of eqs. (2.10) and (2.11) for a single straight screw dislocation in an isotropic elastic medium is well known [2] and is represented in Chapter 8.

Disclinations in general create strong deformations in a crystal and therefore are treated in a different way. The Volterra construction suggests to define a disclination by a matrix field \(B(\mathbf{x})\) corresponding to a pure rotation \([5]\). In general the matrix \(B = (B_{\alpha\beta})\) can be written as

\[
B = S \cdot R
\]

where \(S\) describes a stretching and \(R\) a rotation. Consequently, \(S = S \cdot R^T\), so that \(S = D^T R^{-1} = (u_{ij})\). For a single disclination in equilibrium stretching distortions will occur which increase with growing distance from the center of rotation. We will, however, consider random distributions of disclinations in a two-dimensional plane crystal where these large-scale distortion fields essentially cancel. With regard to that we adopt the above definition, and write

\[
R(x) = \exp(\lambda x)
\]

(2.12)

with \(\varepsilon = r^2\), \(\varepsilon_{12} = 1\). Again the position of indices is irrelevant since in the present case \(\eta^\alpha = \delta^\alpha_\beta\).

Insertion of (2.13) into (2.7) yields

\[
R_{\alpha\beta} = \varepsilon_{12} (\delta^\alpha_\beta - \delta^\beta_\alpha) + \varepsilon_{12} \lambda
\]

(2.14)

so that, parallel to (2.8), one finds the relation \([5]\)

\[
\frac{d}{ds} R_{\alpha\beta} = \varepsilon_{12} \frac{d}{ds} \delta^\alpha_\beta + \varepsilon_{12} \lambda
\]

(2.15)

which connects the curvature with the Frank angle \(\Omega\). For a disclination, centered at the origin, (2.15) implies...
From (3.7) it also follows that $\beta^T$ is the adjoint of the usual Laplacian $\Delta \equiv g^{ij} \mathcal{D}_i \mathcal{D}_j$ with respect to the scalar product
\begin{equation}
\langle X(t), \mathcal{O} \rangle \equiv \int d^d x \sqrt{g(x)} X(x) Y(x),
\end{equation}
defined for scalar quantities $X(x)$, $Y(x)$.

Our interest is in expectation values of the type (3.6), averaged over a quenched random distribution of defects. Such averages are most conveniently performed in a Martin-Siggia-Rose-type path-integral representation [4] of the diffusion process. Effectively, one proceeds by defining an action $J[P, \mathcal{O}]$ via
\begin{equation}
\exp \left[ - J[P, \mathcal{O}] \right] = \exp \left[ - \int dt \mathcal{D} Q_{\tau} \overline{[\mathcal{O}_\tau - D \mathcal{Q}]} P \right]
\end{equation}
where $DQ_{\tau,0}$ is an imaginary valued response field conjugate to $P(\tau,0)$. In (3.11) the scalar product (3.10) has been used, and the overbar means the average over a defect ensemble. All informations of interest can now be extracted from the Green function
\begin{equation}
G(x, \tau) = \int D[P, \mathcal{O}] P(x, \tau) \mathcal{O}(0,0) \exp \left[ - J[P, \mathcal{O}] \right].
\end{equation}
In fact, its Fourier transform $\tilde{G}(q, t)$ is the generating function for the moments of the particle position. As an example,
\begin{equation}
\langle x^2 \rangle(t) = -\frac{2}{q^2} \tilde{G}(q, t)_{q \to 0}.
\end{equation}

The next step therefore is to evaluate $G(x, \tau)$ for specified defects and for a conveniently chosen ensemble of such defects.

4. The case of disclinations

According to (2.13) and the related discussion, we have, for a single disclination with Frank angle $\Omega$ at the origin of the two-dimensional plane,
\begin{equation}
B(x) = \exp \left[ \Omega \arctan \frac{x^2}{x^1} \right].
\end{equation}
Via (2.3) and (3.5) this implies $g = 1$, and
\begin{equation}
D^{ij} = D^{ij}, \quad V^i = D \frac{\Omega}{2\pi} \overline{x^1 x^i} = -D^{ij} \delta_i U
\end{equation}
for the drift velocity and the diffusion tensor, $P(x, t)$ has been introduced as a scalar probability distribution which for some observable $A(x)$ in space dimension $d$ yields the expectation value
\begin{equation}
\langle A(x) \rangle(t) = \int d^d x \sqrt{g(x)} P(x, t) A(x).
\end{equation}
The covariance of (3.4) follows by use of the identity
\begin{equation}
\delta_{ij} \sqrt{g} \Gamma_{ij} \Gamma_{ij} = \delta_{ij} \sqrt{g} \Gamma_{ij}
\end{equation}
which can be derived from the representation $g = \exp \left[ \text{Tr} \ln g_{ij} \right]$. In fact, (3.7) allows to convert (3.4) into the manifestly covariant form
\begin{equation}
\delta_{ij} P = D \Delta_{ij} P
\end{equation}
where
\begin{equation}
\Delta_{ij} \equiv g^{ij} \mathcal{D}_i \mathcal{D}_j, \quad \mathcal{D}_i \equiv V_i + 2T_{ij}.
\end{equation}

\begin{equation}
\mathcal{D}_i \equiv V_i + 2T_{ij}, \quad \mathcal{D}_i \equiv V_i + 2T_{ij}.
\end{equation}
This assumption is not obvious since e.g. \( \rho(x) \) might be very anisotropic, and then induce a nontrivial diffusion tensor. Typical configurations of dislocations are, however, assumed to be translationally and rotationally invariant on a long scale. Technically, Eqs. (4.2) and (4.4) will be maintained, and supplemented by a conveniently chosen ensemble for \( \rho(x) \).

The ensemble is taken to be Gaussian with zero mean, and homogeneous and isotropic second moments, i.e., in terms of Fourier transforms, \( \tilde{\rho}(q) = 0 \), \( \tilde{\rho}(q)\tilde{\rho}(p) = \eta(q^2\delta(q + p)) \). We also assume that screening effects of the topological charges have contributed during the stage of preparation of the sample. They will imply charge neutrality of a dislocation cluster when its linear size considerably exceeds a screening length \( 1/m \). Thus, for most configurations, \( \tilde{\rho}(0) = 0 \), which in the ensemble leads us to assume \( \eta(q^2) \approx q^2 \) for \( q^2 \ll m^2 \). On the other hand, on a scale small compared to the screening length, the dislocations will be randomly distributed, so that \( \eta(q^2) \approx \text{const} \) for \( q^2 \gg m^2 \). As a model we eventually take for \( \eta(q^2) \) a simple Padé approximation matching the two behaviours, and thus supplement (4.4) by

\[
\tilde{\rho}(q) = \frac{1}{q^2}, \quad \tilde{\rho}(q)\tilde{\rho}(p) = \frac{\eta(q^2)}{q^2 + m^2}(2\pi)^2\delta(q + p). \tag{4.5}
\]

In conclusion we have mapped, in space dimension two, the problem of diffusion in a random array of dislocations into a random-drift problem. The latter is given by the Fokker-Planck equation

\[
\partial_t P(x,t) = \partial_i \left[ -V^i(x) + D \delta^{ij} \partial_j \right] P(x,t) \tag{4.6}
\]

where the \( V^i(x) \) are Gaussian distributed with zero mean, and the variance

\[
\langle V^i(x) V^j(x') \rangle = D \delta^{ij}\frac{1}{q^2 + m^2}(2\pi)^2\delta(q + p). \tag{4.7}
\]

Since (4.6) is linear in \( V^i(x) \), the ensemble average in (3.11) can explicitly be performed, with the result

\[
J[P,Q] = \int dt \int d^dx \frac{1}{q^2 + m^2} \partial_i \left[ D \partial_i \tilde{\rho}(x) \right] \partial_j \tilde{\rho}(x) \tag{4.8}
\]

\[
-\frac{1}{2} \int d^dx d^dy \left[ \partial_i \tilde{\rho}(x) \tilde{\rho}(y) V^i(x)V^j(y) \right] \left[ \partial_j \tilde{\rho}(y) \right] \tilde{\rho}(x) \tilde{\rho}(y) \tag{4.9}
\]

generalized to space dimension \( d \).

Random-drift models of the type (4.8) have repeatedly been discussed in the literature by means of renormalization-group methods [6]. In the limit \( q^2/m^2 \rightarrow 0 \) the model (4.8) reduces to one considered by Kratsov, Lederer, and Yudson [5]. They found that \( d_c = 2 \) just is the upper critical dimension of the system in which the dimensionless coupling constant \( \nu = \gamma/(4\pi m^4) \) is not renormalized. This is a rigorous result and means that in a flow diagram of coupling constants the \( \nu \)-axis constitutes a line of fixed points. Via (3.13) this gives rise to the nonuniversal subdiffusional behaviour

\[
\langle x^2 \rangle(t) \sim t^{1+\nu/2}\gamma m^d. \tag{4.9}
\]

The opposite limit \( m^2/q^2 \rightarrow 0 \) in (4.7) leads to a model with the upper critical dimension \( d_c = 4 \). Its properties in dimension \( d = 4 \) have been studied by Bouchaud, Comtet, Georges, and La Doussal [6]. They especially have considered the behaviour of the coupling constant \( \nu = \gamma/(4\pi m^4) \) under renormalization where \( \mu \) is an inverse scaling length. To all orders of an expansion in powers of \( \nu \) they found the simple scaling behaviour \( \mu \langle \nu \rangle = -\lambda \nu \).

Thus the system is, in the infrared limit, driven into a strong-coupling regime where perturbation theory breaks down. The authors now argue that in this regime the Brownian particle is trapped for long periods of time by the potential \( U \), introduced in (4.2). They estimate an escape rate \( 1/\tau \sim \exp(-\mu U) \) which is the equilibrium solution of the Fokker-Planck equation (4.6). Since \( U \sim \sqrt{m \mu^{-1/2}} \) for \( \mu \rightarrow 0 \), one finds \( \mu^{-1/2} \sim (\ln t)^{d_c/2 \nu} \). This suggests a Sinai-type diffusion behaviour [7] which for \( d \rightarrow 2 \) reads

\[
\langle x^2 \rangle(t) \sim (\ln t)^{d_c/2}. \tag{4.10}
\]

In the context of Brownian motion in topologically disordered crystals the result (4.10) is of a more theoretical interest. Since on a long scale screening effects will eventually come into play, the already unusual behaviour (4.9) probably is nearer to physics. This applies even more to the situation described in the next chapter.

5. The case of screw dislocations

In the following we consider a three-dimensional crystal which in the continuum limit and in the absence of defects is described by the isotropic elastic constants

\[
C_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}). \tag{5.1}
\]

We now want to determine the distortion of the crystal caused by a single straight screw-dislocation line along the \( x^3 \)-axis. The corresponding defect density \( \eta(x) \) has the only component

\[
\eta_{x3}(x) = b \delta(x^3) \delta(x^1) \tag{5.2}
\]

where \( b \) is the magnitude of the Burgers vector. One easily verifies that Eqs. (2.10) and (2.11) are solved by the distortion tensor \( \beta_i(x) \) with the nonzero components [2]

\[
\beta_3^3 = -\partial_2, \quad \beta_2^3 = \partial_1 U \tag{5.3}
\]

if \( U = b \Phi \), again with the two-dimensional Coulomb potential \( \Phi(x^1, x^2) \).

In (5.3) the indices have been placed in their original positions which is important in forming the nonlinear combinations (2.3) with the help of (2.9). The results for (2.3), inserted into (3.3), yield \( g = 1 \), \( V = 0 \), and the anisotropic diffusion tensor

\[
\partial_t P(x,t) = D \partial_i \left[ \partial_i \partial_j \tilde{\rho}(x) \right] \tilde{\rho}(x) \tag{5.4}
\]

With the notation \( \partial \equiv \partial_1 \partial_2 \partial_3 \), \( \partial_\alpha \equiv \partial_\alpha \), \( \beta_\alpha \equiv \partial_\alpha \), the Fokker-Planck equation (3.4) thus reduces to

\[
\partial_t P(x,t) = D \left[ \partial_1 \partial_2 \partial_3 \right] \tilde{\rho}(x) \tag{5.5}
\]

\[
+ D \left[ 2 \partial_1 (\partial_2 \tilde{\rho}(x)) \partial_2 \partial_3 \right] \tilde{\rho}(x) \tag{5.5}
\]

\[
+ \partial_3 \tilde{\rho}(x) (\partial_2 \tilde{\rho}(x)) \partial_2 \partial_3 \tilde{\rho}(x) \right] P(x,t). \tag{5.5}
\]

where from now on \( i,j = 1,2 \).
It is instructive to evaluate the terms in (5.5), involving $U(x)$, in cylindrical coordinates which then leads to the form
\begin{equation}
\dot{\rho}_i P = D \Delta P + \frac{b_i}{\pi^{i/2}} \left[ \delta_0 \dot{\rho}_i \epsilon_i + \frac{b_i}{4\pi^2} \dot{\rho}_i^2 \right] P
\end{equation}
(5.6)
of the diffusion equation. According to (5.6) one effect due to the screw dislocation is an enhancement $\sim 1/r^2$ of the mobility of the particle in the $z$-direction. A second effect is a coupling $\sim 1/r^2$ of the particle motion in the $\phi$- and $z$-direction which reflects the spiral-staircase structure of the screw dislocation.

Our interest now is in an array of screw-dislocation lines which all are parallel to the $z$-axis and intersect the $\xi^1, x^2$-plane at random positions $X_\nu$. The magnitudes $b_\nu$ of the Burgers vectors, including their signs, also are assumed to be random. It is then convenient to introduce, by analogy with (4.3), a two-dimensional topological-charge density
\begin{equation}
\rho(x) = \sum_\nu b_\nu \delta(x - X_\nu).
\end{equation}
(5.7)
For well-behaved defect densities the linear theory remains valid and leads to the relation (4.4) between $\rho(x)$ and the potential $U(x)$. We furthermore adopt from the disclination case the $\rho$-ensemble so that eq. (4.5) is also maintained. One only should observe that due to the different topological charges $\Omega_\nu$ and $b_\nu$, the parameter $\gamma$ in (4.5) has the dimension of $m^2$ for disclinations but is dimensionless in the present case.

To summarize, our model can be described by the diffusion equation (5.5) where $U(x)$ is Gaussian distributed with zero mean and the variance
\begin{equation}
\bar{U}(q)U(p) = \frac{1}{q^2 + m^2} \delta(q + p).
\end{equation}
(5.8)
The functional representation (3.11) of the model reads
\begin{equation}
\text{exp} \{ -J[P, Q] \} = \int D[U] \exp \{ -K[P, Q, U] \}
\end{equation}
(5.9)
with the new action
\begin{equation}
K[P, Q, U] = \int dt dz d^2x \{ Q(\dot{Q} - D(\dot{Q}^2 + \dot{Q}^2))P \}
+ D Q(2\dot{Q}^2 \dot{Q} \dot{\rho} + \dot{Q}^2 \dot{Q} \dot{\rho}^2)
+ \frac{1}{2\gamma}(\dot{Q}^2 + m^2) U(q).
\end{equation}
(5.10)

On the basis of (5.9), (5.10) the Green function (3.12) can now be calculated by perturbation theory. In view of Dyson's equation we first represent the Fourier transform of $G(x, z, t)$ in space and time as
\begin{equation}
\tilde{G}(q, k, \omega) = \frac{1}{-i \omega + D(q^2 + k^2) - 2(q, k, \omega)}
\end{equation}
(5.11)

For the self energy $\Sigma$ we then establish a diagram expansion. According to (5.10) the elements of such an expansion are
\begin{equation}
\left( \frac{1}{i \omega D(q^2 + k^2) - 2(q, k, \omega)} \right) \equiv \bullet
\end{equation}
(5.12)
and
\begin{equation}
\left( \frac{1}{p^2 + m^2} \right) \equiv \bullet
\end{equation}
(5.13)

The arrows denote connections to $\Sigma$-fields, and all wave vectors are directed towards the vertices.

By causality the diffusion propagator (5.12) cannot form closed loops in any diagram. Any contribution to $\Sigma$ therefore consists of a single open string of such propagators where the vertices are connected by the disorder propagator (5.13) in all possible ways leading to an irreducible diagram. Since the related integrals only are over the two-dimensional $q$-variables in (5.12), the variable $b$ (as well as $a$) runs freely through the diagram. Therefore, in the expansion
\begin{equation}
\dot{\Sigma}(q, k, \omega) = \sum_{a,b} \sigma_{ab}(q) q^2 b^2
\end{equation}
(5.16)
only a finite number of the vertices (5.14), (5.15) appears in each contribution to the coefficients $\sigma_{ab}(q)$. As a consequence of this, the same statement is true for the cumulants of the particle position,
\begin{equation}
\langle x^a x^b \rangle(t) = \left[ \frac{\omega}{2\pi} e^{-i\omega t} \tilde{G}(q, k, \omega) \right]_{q = k = 0}.
\end{equation}
(5.17)

Graphically the lowest-order coefficients are given by
\begin{equation}
\sigma_{01} = \tilde{G}(q, k, \omega)|_{q = k = 0},
\end{equation}
(5.18)
\begin{equation}
\sigma_{11}(q) = \tilde{G}(q, k, \omega)|_{q = k = 0},
\end{equation}
(5.19)
\begin{equation}
\sigma_{02}(q) = \frac{1}{2} \tilde{G}(q, k, \omega)|_{q = k = 0},
\end{equation}
(5.20)
and generally $\sigma_{aa} = 0$. The contribution (5.18) and the leading terms of (5.19) and (5.20) in the limit $\omega \to 0$ are calculated in Appendix B. There we also present the calculations for the corresponding cumulants, with the results
\begin{equation}
\langle x^2 \rangle(t) = 4Dt, \quad \langle x^4 \rangle(t) = 0,
\end{equation}
(5.21)
\begin{equation}
\langle x^2 x^2 \rangle(t) = 2D \left[ 1 + \frac{y}{2\pi} \ln \sqrt{\lambda^2/m^2 + 1} \right] t,
\end{equation}
(5.22)
\begin{equation}
\langle x x^2 \rangle(t) = 8D \frac{y}{2\pi} \ln t + O(t),
\end{equation}
(5.23)
\begin{equation}
\langle x^4 \rangle(t) = 12D \left[ \frac{y}{2\pi} \right]^2 \frac{1}{m^2} \ln t + O(t).
\end{equation}
(5.24)
In (5.22) A is a wave-number cutoff of the order of the inverse lattice constant which also occurs in the subleading terms of (5.23) and (5.24). Due to the discussed simplifying properties of the model (5.10) the result (5.21), (5.22), and the amplitudes of the leading terms in (5.23), (5.24) are exact to all orders of the perturbation expansion.

Equation (5.21) shows that the diffusion process in the transverse directions is unaffected by the disorder, reflecting the almost ideal crystalline structure in the x\(^3\), x\(^2\),-planes. According to (5.22) the mobility of a Brownian particle is enhanced in the longitudinal direction which has already been ascribed to the spiral-staircase structure of the screw dislocations. The influence of this structure is not strong enough to generate an (at least logarithmic) superdiffusional correction in the longitudinal direction. However, anomalies do show up in the fourth-order cumulants (5.23) and (5.24). These results demonstrate that topological disorder can give rise to a non-Gaussian behaviour. The appearance of the cutoff A in (5.22) is not surprising since the normal diffusion behaviour also holds on a short time scale. Contrary to that, the leading terms in (5.23), (5.24) only apply to the asymptotic regime t \(\to\) \(\infty\), and accordingly are cutoff independent. It is our hope that the behaviour (5.21)-(5.24) can be seen experimentally or in a simulation.

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Appendix A

It has already been argued that the expressions (3.5) for the drift velocity and the diffusion tensor lead to the covariant form (3.8) of the Fokker-Planck equation (3.4). We here want to show that only the Stratonovich interpretation of the Langevin equation (3.3) leads to the results (3.5).

Generally, (3.3) yields (3.4) with the formal definitions [11]

\[ V^i = \lim_{\tau \to 0} \frac{\langle \Delta x^i(\tau) \rangle}{\tau}, \]  
\[ D^{ij} = \lim_{\tau \to 0} \frac{\langle \Delta x^i(\tau) \Delta x^j(\tau) \rangle}{\tau} \]  
where \( \Delta x^i(\tau) \equiv x^i(\tau) - x(0) \). According to (3.3) one finds

\[ \Delta x^i(\tau) = \int_0^\tau B^i_j(x(t')) dw^j(t') \]  
with

\[ w^j(t) = \int_0^t dt' A^j(t'), \]  
and by iteration of (A.3)

\[ \Delta x^i(\tau) = B^i_j w^j(\tau) + (\partial_j B^i_j) B^j_k \int_0^\tau w^k(t') dw^i(t') + O(w^3). \]  

Equations (A.4), (A.5) imply

\[ \langle \Delta x^i(\tau) \rangle = B^i_j \partial_j B^k_l \int_0^\tau w^l(t') dw^k(t') + O(\tau^2), \]  
\[ \langle \Delta x^i(\tau) \Delta x^j(\tau) \rangle = B^i_j B^k_l \langle w^l(t') w^k(t') \rangle + O(\tau^3). \]  

Since due to (3.2)

\[ \langle w^l(t') w^k(t') \rangle = 2D \delta^{lk} \min(t, t'), \]
(A.6)

(A.2), and (A.7) directly lead to the result (3.5) for the diffusion tensor.

In order to determine the drift velocity, we discretize the integral in (A.6) in the form [11]

\[ 0^{\eta}(\tau) = \sum_{n=0}^{N-1} \left[ (1-\theta) \omega^n(\tau_n) + \theta \omega^n(\tau_{n+1}) \right] \]  
\[ \left[ \omega^n(\tau_{n+1}) - \omega^n(\tau_n) \right] \]  
(A.5)

where \( 0 \leq \theta \leq 1 \), and \( 0 = \tau_0 < \cdots < \tau_N = \tau \) is a time lattice on the interval \([0, \tau]\). The choices \( \theta = 0 \) and \( \theta = 1 \) correspond to the i/o and to the Stratonovich interpretations, respectively [11]. Generally, from (A.1), (A.6), and (A.9) one obtains

\[ V^i = 2D B^i_j \partial_j 0^{\eta} \]

(A.11)

which for \( \theta = 1/2 \) agrees with (3.5).

The Fokker-Planck equation corresponding to (A.11) differs from (3.4) by a term \( F(\theta) \) which, by use of (3.7), can be written as

\[ F(\theta) = (2\theta - 1) D (\partial_i + \Gamma_{ik}) \gamma^{ik} \gamma_{jk} P. \]  

(A.11)

This fails to be the covariant divergence of a vector because the affine connection is no tensor. Consequently only with the choice \( \theta = 1/2 \) we arrive at a covariant Fokker-Planck equation.

Appendix B

In this appendix we sketch the derivation of the result (5.22)-(5.24). From (5.11), (5.16), (5.17) we first obtain

\[ \langle e^{ix^i} \rangle = 2 \int \frac{m^{-1} \omega \, m^{-1} \omega \, m^{-1} \omega}{2 \pi \iota \kappa - i \omega} \sigma_{11}(\omega), \]  
\[ \langle e^{ix^i} e^{ix^j} \rangle = 8 \int \frac{m^{-1} \omega \, m^{-1} \omega \, m^{-1} \omega}{2 \pi \iota \kappa - i \omega} \sigma_{11}(\omega), \]  
\[ \langle e^{ix^i} \rangle = 24 \int \frac{m^{-1} \omega \, m^{-1} \omega \, m^{-1} \omega}{2 \pi \iota \kappa - i \omega} \sigma_{12}(\omega), \]  
where according to (5.18)-(5.20)

\[ \sigma_{11}(\omega) = -D \gamma \int \frac{d^3 p}{(2\pi)^3} \frac{1}{p^2 + m^2}, \]  
\[ \sigma_{12}(\omega) = D^2 \gamma \int \frac{d^3 p}{(2\pi)^3} \frac{1}{m^2 + \omega^2 + D p^2 p^2 + m^2}, \]  

(B.4)

(B.5)
\[
\sigma_{11}(t) = \frac{\sigma_{11}(0)}{1 - \frac{1}{2} B t \left( \frac{\sigma_{11}(0)}{B t} \right)^{1/2}} + O(1)
\]
(6.7)

\[
\sigma_{11}(0) = \frac{1}{2} B t \left( \frac{\sigma_{11}(0)}{B t} \right)^{1/2} + O(1)
\]
(6.8)

(following from (6.5) and (6.6). By use of the identity

\[
\int \frac{1}{x^2} e^{-ax} dx = \frac{1}{a^2} \left[ - \frac{e^{-ax}}{a} \right] + C
\]

we eventually obtain from (6.2), (6.3), and (6.7), and (6.8), the results (5.23) and (5.24).

References


Note added in proof: After submission of the manuscript we received a paper by K. Kishihara, M. Araki, and K. Nakazato presented at the Yamada Conference IX on Dislocations in Solids, published by the University of Tokyo Press, 1985, etc. H. Suzuki, T. Nishida, K. Sumiya, and S. Takashita. In this work, eqs. (4.2) and (4.6) of our paper have already been derived.