

6 Diffusive Spin Transport

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6.1 Introduction

Classical information processing uses charge encoding where the bit values “0” and “1” are represented by a supplementary charge present or absent in a register. In the quantum limit, one eventually is led to consider a single elementary charge (electron or hole) in a quantum dot and hopes to realise quantum superpositions of “qubit” states $|0\rangle$ and $|1\rangle$ and entanglement between distinct qubits. But since they interact via long-range Coulomb forces, charge states suffer strongly from decoherence. Another discrete degree of freedom is spin. Spin $\frac{1}{2}$ states, typically noted $|\pm 1\rangle$ or $|\uparrow, \downarrow\rangle$, are *the* natural realisation of a qubit. But spin, and more generally information as such, needs a physical carrier. Candidates here are electrons or holes (massive particle of spin $s = \frac{1}{2}$) and photons (massless, spin $s = 1$). A new promising field therefore is “spint(r)onics”: spin-based information transport and processing with *electrons* and *photons*.

For these lectures, I chose to discuss the following model setting of diffusive spin transport (Fig. 6.1): spin-polarised particles are injected from the left with probability $p_{\uparrow}(0) = 1$ into a disordered sample and move diffusively towards the right, where a spin-sensitive detection reads out the final spin polarisation $p_{\uparrow}(L)$ that we should calculate.

The leitmotiv of this lecture was as follows: Spin is a geometrical quantity, and one should be able to use irreducible representations of the rotation group

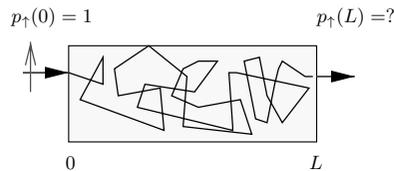


Fig. 6.1. Model setting of diffusive spin transport: spin-polarised particles are injected from the left with $p_{\uparrow}(0) = 1$ into a disordered sample and move diffusively towards the right, where a spin-sensitive detection reads out the spin-polarisation $p_{\uparrow}(L)$

in order to take advantage of symmetries. Since the participants of the school were not required to have been educated in group theory, I decided to give a rather complete introduction into representations of the rotation group with the hope that the sometimes intimidating jargon of group-theoretical arguments may become more familiar to everybody. Attending myself other lectures, I adopted a master-equation approach paralleling Klaus Hornberger’s lecture to which the present notes refer occasionally. During the lecture itself, only the first part on spin relaxation was delivered as presented in the following; in the second part on diffusion, I relied on arguments taken from diagrammatic perturbation theory that seemed to bewilder the audience more than anything else. The present notes remedy to this dissymmetry and treat also the diffusive part as momentum relaxation with a master equation. This parallel allows to combine both dynamics rather economically into a single, coherent picture of diffusive spin dynamics; it is my hope that this conceptual unity is appreciated by my readers.

These notes finish with a description of quantum corrections to diffusive spin transport including spin-flip effects. Other subjects covered during the school’s lecture were of a more anecdotic type and, although hopefully enjoyed by the audience, did not seem to fit into the present format; readers interested in spintronics properly speaking are referred to the recent review by Žutić, Fabian, and Das Sarma [1]. I have to admit that I made no attempt to cover systematically the vast literature on the subject of irreversible spin dynamics and quantum transport, which would have been a hopeless task in any case; my apologies to many colleagues whose excellent contributions may not be duly cited in the following.

6.2 Spin Relaxation

“Spin” is internal angular momentum [2, 3]. This was recognised by Uhlenbeck and Goudsmit [4] following Pauli [5] who postulated the existence of a fourth quantum number to explain fine-structure features of atomic spectra. The clearest experimental manifestation of quantised spin is arguably the Stern–Gerlach experiment [6], where silver atoms are deviated by an inhomogeneous magnetic field into two distinct spots on a detector screen.

Dirac discovered that bispinors (vectors of four components, a spin $\frac{1}{2}$ spinor and an anti-spinor) appear naturally when one looks for a Schrödinger-type wave equation in the relativistic framework of the four-dimensional Minkowski space. Wigner [7] showed that spin is one of the fundamental quantum numbers that permits to identify an elementary particle in the first place: it characterises the particle’s properties under rotations in its proper rest frame. Therefore, to understand spin is to understand rotations.

6.2.1 Spin – A Primer on Rotations

Rotation Group

Physical objects are described by coordinates $\mathbf{x} = (x_1, x_2, x_3) \in \mathbb{R}^3$ with respect to a reference frame in configuration space. Rotations (called “active” when the object is turned and “passive” when the reference frame is turned) are represented by 3×3 matrices: $\mathbf{x}' = R\mathbf{x}$. Proper rotations conserve the Euclidean scalar product $\mathbf{x} \cdot \mathbf{y} = \sum_i x_i y_i$ and the orientation of the frame. The rotation matrices are therefore members of $\text{SO}(3)$, the set of orthogonal matrices $RR^t = R^t R = \mathbb{1}_3$ of unit determinant $\det R = +1$. With the usual matrix multiplication as an internal composition law, these matrices form a *group*, satisfying the group axioms:

1. Internal composition: $\forall R_{1,2} \in \text{SO}(3) : R_{21} = R_2 R_1 \in \text{SO}(3)$;
2. Existence of the identity: $\exists E : RE = ER = R \forall R \in \text{SO}(3)$ with $E = \mathbb{1}_3$;
3. Existence of the inverse: $\forall R, \exists R^{-1} : RR^{-1} = R^{-1}R = E$.

The group is *non-Abelian* because the matrices do not commute: $R_2 R_1 \neq R_1 R_2$. An exception are rotations of the plane around one and the same axis, forming the Abelian group $\text{SO}(2)$.

A possible parametrisation of a rotation is the polar description $(\hat{\mathbf{n}}, \theta) =:$ θ with $\hat{\mathbf{n}}$ the unit vector along the rotation axis and $\theta \in [0, \pi]$ the rotation angle. The following two rotations of configuration space are identical:

$$R(\hat{\mathbf{n}}, \theta = \pi) = R(-\hat{\mathbf{n}}, \theta = \pi). \quad (6.1)$$

These opposite points must be identified such that there are closed parameter curves that cannot be contracted into a single point, see Fig. 6.2. This means that $\text{SO}(3)$ is a doubly connected manifold. Instead of studying this projective group, one may also turn to its *universal covering group* $\text{SU}(2)$, the group of all unitary 2×2 matrices over \mathbb{C} with unit determinant. $\text{SU}(2)$ is simply

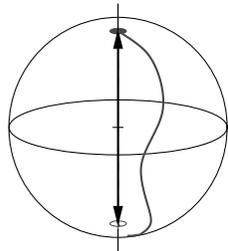


Fig. 6.2. The parameter space of the rotation group $\text{SO}(3)$, a filled sphere of radius π . Two identical rotations (see (6.1)) can be connected by a closed curve that is not reducible to a single point

connected, and there is a *homomorphism* (a mapping preserving the group structure) linking every element $U \in \text{SU}(2)$ to the rotation $R \in \text{SO}(3)$: the rotation $\mathbf{x}' = R(\theta)\mathbf{x}$ is described by

$$\mathbf{x}' \cdot \boldsymbol{\sigma} = U(\theta)\mathbf{x} \cdot \boldsymbol{\sigma}U(\theta)^\dagger. \quad (6.2)$$

Here, $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is a vector whose entries σ_i are the Pauli matrices such that

$$\mathbf{x} \cdot \boldsymbol{\sigma} = \begin{pmatrix} x_3 & x_1 - ix_2 \\ x_1 + ix_2 & -x_3 \end{pmatrix} \quad (6.3)$$

and the unitary rotation matrix acting from the left and from the right is given by

$$U(\theta) = \mathbb{1}_2 \cos \frac{\theta}{2} - i\hat{\mathbf{n}} \cdot \boldsymbol{\sigma} \sin \frac{\theta}{2} = \exp(-i\frac{\theta \cdot \boldsymbol{\sigma}}{2}). \quad (6.4)$$

Note that this mapping is two-to-one because U and $-U$ yield the same rotation, and that it takes a rotation by an angle of 4π to recover the identity transformation: $U(\theta = 2\pi) = -\mathbb{1}_2$, but $U(\theta = 4\pi) = +\mathbb{1}_2$. This is not a mysterious quantum property as is sometimes stated, but reflects the double-connectedness of $\text{SO}(3)$ -rotations in our everyday reference frame.¹ Dirac’s construction of a solid body connected by strings to a reference frame is supposed to convey an “experimental” idea of this property [3].

Representations

A group G can act in many different disguises that share the same abstract group structure, as defined by the multiplication law or group table. These different appearances are called (linear) *representations*. Mathematically, they are mappings $\mathcal{D}_i : G \rightarrow GL(V_i)$ from the group G to the general (linear) group of regular transformations $D : V_i \rightarrow V_i$ of a vector space V_i into itself.² Importantly, this mapping must be a *homomorphism* which means that the representation has the same group structure as G . Notably, for all elements $g_1, g_2 \in G$ (with the product $g_2 g_1 \in G$), the representing transformations verify $D(g_2 g_1) = D(g_2)D(g_1)$.

The dimension of the representation \mathcal{D}_i is given by $\dim V_i$. Finite-dimensional linear representations are given in terms of quadratic matrices of size $\dim V_i$. A representation is called *reducible* if there is a basis of $V = V_1 \oplus V_2$ such that all transformations $D \in \mathcal{D}$ are written

$$D = \begin{pmatrix} D_1 & * \\ 0 & D_2 \end{pmatrix}. \quad (6.5)$$

¹ Cartan developed half-integer spin representations as early as 1913 within the theory of projective groups [8].

² \mathcal{D} stands for the German word “Darstellung”; in anglo-saxon literature, often the symbol Γ is used.

In other words, the transformations $D_1 : V_1 \rightarrow V_1$ define already a representation \mathcal{D}_1 of its own. If the matrix is block-diagonal ($*$ = 0), the representation is *completely reducible*. If it is not reducible, it is called *irreducible*, meaning that one has achieved to work in the smallest possible subspace.

The rotation group $SU(2)$ is a manifold that depends on a continuous set of parameters $\boldsymbol{\theta} = (\theta_1, \theta_2, \theta_3)$ with respect to which it is infinitely differentiable. This structure is called a *Lie group*. The group multiplication law is completely determined by the commutation relation of its generators:

$$[J_j, J_k] := J_j J_k - J_k J_j = i\hbar \epsilon_{jkl} J_l. \quad (6.6)$$

Here, as in the following, the sum over repeated indices is understood. These generators are said to form a (representation of) the *Lie algebra* $\mathfrak{su}(2)$. In the so-called natural representation of $SU(2)$ by itself (see (6.4)), the generators are $\mathbf{J} = \hbar \boldsymbol{\sigma}$. Other representations will feature different generators, but all group representations share the same commutation relation! Finite rotations are generated by exponentiation: $U(\boldsymbol{\theta}) = \exp(-i\boldsymbol{\theta} \cdot \mathbf{J}/\hbar)$. Topologically speaking, $SU(2)$ is compact. According to a general theorem, all representations of a compact Lie group are completely reducible to finite-dimensional irreducible representations.

Functional Representation of $SO(3)$

As an example for an infinite-dimensional representation of the rotation group $SO(3)$ already useful in classical physics, consider the transformation of functions f describing the position of an object on the unit sphere. Saying that the object is rotated to $\mathbf{r}' = R\mathbf{r}$ implies that the function is transformed by

$$(Df)(\mathbf{r}) = f(R^{-1}\mathbf{r}). \quad (6.7)$$

The action of D in the (infinite-dimensional) functional space can be written $D = \exp\{-i\boldsymbol{\theta} \cdot \mathbf{T}\}$, where $\mathbf{T} = -i\mathbf{r} \times \boldsymbol{\nabla}$ is a differential operator, as can be verified by considering an infinitesimal rotation around $\boldsymbol{\theta} = \theta \hat{\mathbf{r}}$: to first order in θ , we have $f(R^{-1}\mathbf{r}) = f(\mathbf{r} - \boldsymbol{\theta} \times \mathbf{r}) = f(\mathbf{r}) - (\boldsymbol{\theta} \times \mathbf{r}) \cdot \boldsymbol{\nabla} f(\mathbf{r}) = [1 - \boldsymbol{\theta} \cdot (\mathbf{r} \times \boldsymbol{\nabla})]f(\mathbf{r})$.

The finite-dimensional irreducible representations to which this infinite-dimensional one can be reduced are obtained by decomposing f into surface harmonics Y_{Lm} : each subspace $L = 0, 1, \dots$ then admits an irreducible representation of dimension $2L+1$. Surface harmonics are a concept arising already with the multipole expansion of charge distributions in classical electrodynamics. But to cite Hermann Weyl [9]: “This reveals the true significance of surface harmonics; they are characterised by the fundamental symmetry properties here developed, and the solution of the potential equation in polar co-ordinates is merely an accidental approach to their theory.”

What Is Quantum About Spin?

Spin, and especially half-integer spin, is much less mysterious than sometimes suggested by standard textbook wisdom. Half-integer spin does not require the kinematic framework of special relativity, it arises already in Galilean relativity. Also, as mentioned at the end of Sect. 6.2.1, reference frames for solid bodies already introduce half-integer spin. However, there are genuine quantum features to be aware of:

1. In classical mechanics, Noether’s theorem assures that if the Lagrangian function is invariant under infinitesimal rotations, then the orbital angular momentum \mathbf{L} is a conserved quantity. However, \mathbf{L} a priori has nothing to do with the generator of rotations \mathbf{T} introduced in the previous section. In quantum mechanics, thanks to the appearance of \hbar , the generators can be *identified* with *observables* $\mathbf{J} = \hbar \mathbf{T}$ with dimension of angular momentum. If the Hamiltonian is invariant under all rotations $U(\boldsymbol{\theta})$, their generators itself are conserved quantities, and Noether’s theorem takes a very simple form:

$$H' = UHU^\dagger \Leftrightarrow [H, U] = 0 \Leftrightarrow [H, \mathbf{J}] = 0 \Leftrightarrow \dot{\mathbf{J}} = 0. \quad (6.8)$$

Separating the orbital part \mathbf{L} of angular momentum from the total angular momentum $\mathbf{J} = \mathbf{L} \otimes \mathbb{1}_S + \mathbb{1}_L \otimes \mathbf{S} =: \mathbf{L} + \mathbf{S}$, one identifies the rest-frame angular momentum or spin \mathbf{S} obeying the same fundamental commutation relations (6.6). In the remainder, we will only have to consider the spin part and let $\mathbf{L} = 0$.

2. The observables \mathbf{S} generate irreducible representations $\mathcal{D}^{(s)}$ of dimension $d_s = 2s + 1$ with $s = 0, \frac{1}{2}, \dots$ and discrete magnetic quantum numbers $m = -s, -s + 1, \dots, s$. Pure states are noted $|sm\rangle$. The *Casimir operator* S^2 specifies the irreducible representation, $S^2|sm\rangle = \hbar^2 s(s + 1)|sm\rangle$, whereas the magnetic quantum number gives the projection of the spin onto the quantisation axis (usually called the z -axis): $S_z|sm\rangle = \hbar m|sm\rangle$.
3. States can be classified regarding their transformation properties, but here with a more general importance than in classical mechanics due to the superposition principle. An atomic s -orbital, for instance, may be seen as a “coherent superposition of all possible Kepler orbits” and is invariant under all rotations. In Sect. 6.2.3, we will introduce the irreducible components of mixed quantum states, also known as *state multipoles*.

6.2.2 Master Equation Approach to Spin Relaxation

As a simple model for spin dynamics, we shall study the Hamiltonian

$$H = -\boldsymbol{\mu} \mathbf{S} \cdot \mathbf{B}. \quad (6.9)$$

It describes the coupling of the magnetic moment $\boldsymbol{\mu} = \mu \mathbf{S}$ to a magnetic field \mathbf{B} . For electrons, $\mu = -g\mu_B$ in terms of the Bohr magneton $\mu_B =$

$|e|\hbar/(2m_e c)$ and the gyromagnetic ratio $g = 2.003\dots$ in vacuum. The spin operator has been chosen dimensionless such that its action in the irreducible representation $\mathcal{D}^{(s)}$ will be $S_z|sm\rangle = m|sm\rangle$ and $S^2|sm\rangle = s(s+1)|sm\rangle$ for the remainder of the lecture. The density matrix or statistical operator ρ of a spin S is a positive linear operator of trace unity on the state Hilbert space $\mathcal{H}_s = \mathbb{C}^{d_s}$ of dimension $d_s := \dim \mathcal{H}_s = 2s + 1$ that determines the expectation values of arbitrary observables O as $\langle O \rangle = \text{tr}\{\rho O\}$.

Unitary Spin Dynamics

According to one of the fundamental axioms of quantum theory, any closed quantum system evolves unitarily according to the Liouville–von Neumann equation

$$i\hbar\partial_t\rho = [H, \rho]. \quad (6.10)$$

This equation of motion is formally solved as $\rho(t_2) = U(t_2, t_1)\rho(t_1)U(t_2, t_1)^\dagger$ by applying the time evolution operator for a time-dependent Hamiltonian,

$$U(t_2, t_1) = \text{T exp} \left\{ -\frac{i}{\hbar} \int_{t_1}^{t_2} H(t') dt' \right\}, \quad (6.11)$$

where $\text{T}[H(t_1)H(t_2)\dots H(t_n)] = H(t_i)H(t_j)\dots H(t_k)$ for $t_i > t_j > \dots > t_k$ is Dyson's time-ordering operation.

Non-unitary Spin Dynamics: A Classical Model Derivation

Phenomena like “relaxation, damping, dephasing, decoherence,…” have in common irreversible dynamics with an “arrow of time” [10] due to the irrevocable loss of energy and/or information into inobservable degrees of freedom, which are usually called “bath” or “environment”.

As an introductory model, we consider the Hamiltonian $H = -\mu\mathbf{S} \cdot \mathbf{B}(t)$ with a randomly fluctuating magnetic field $\mathbf{B}(t)$. Predictions about the spin will involve an average over the field fluctuations, which we describe as a *classical* stochastic process [11]. This approach is typical for the physics of nuclear magnetic resonance; a regular driving magnetic field can of course be included in the treatment, but here we concentrate on the effect of random fluctuations.

To obtain the effective dynamics, we develop the time-propagated density matrix $\rho(t + \Delta t) = U(t + \Delta t, t)\rho(t)U(t + \Delta t, t)^\dagger$ to second order in the interaction Hamiltonian,

$$\begin{aligned} \rho(t + \Delta t) = & \rho(t) - \frac{i}{\hbar} \int_t^{t+\Delta t} [H(t_1), \rho(t)] dt_1 + \frac{1}{\hbar^2} \iint_t^{t+\Delta t} H(t_1)\rho(t)H(t_2) dt_1 dt_2 \\ & - \frac{1}{2\hbar^2} \iint_t^{t+\Delta t} \text{T}(H(t_1)H(t_2)\rho(t) + \rho(t)H(t_1)H(t_2)) dt_1 dt_2, \end{aligned} \quad (6.12)$$

and perform an average over all possible realisations of the fluctuating magnetic field $\mathbf{B}(t)$. As a stochastic process [11], it is completely specified by its correlation functions

$$C_{i_1 i_2 \dots i_n}(t_1, t_2, \dots, t_n) := \overline{B_{i_1}(t_1)B_{i_2}(t_2)\dots B_{i_n}(t_n)}, \quad (6.13)$$

the overline indicating an ensemble average over the field distribution. This distribution is taken to be centred Gaussian hence all correlation functions factorise into products of pair correlations. Therefore, only the first two moments need to be specified: $\overline{B_i(t)} = 0$ (zero mean) and

$$\overline{B_i(t_1)B_j(t_2)} =: B^2 c_{ij}(t_1, t_2). \quad (6.14)$$

We assume a stationary process that depends only on the time difference $t_1 - t_2$ and has a very short internal correlation time τ_c such that $c_{ij}(t) = c_{ij}\tau_c\delta(t)$. This last assumption of “white noise” (the power spectrum $\tilde{c}_{ij}(\omega) = cst$. contains all frequencies with equal weight) is valid if the noise correlation time τ_c is much shorter than the relevant timescale of the spin dynamics that is still to be determined. Lastly, we assume that the fluctuations are *isotropic*, $c_{ij} = \frac{1}{3}\delta_{ij}$.

Now we average the time-propagated density matrix (6.12) over the field fluctuations and use the *Born assumption* that there are no further correlations between the fields appearing explicitly and the average density matrix. Then, the ensemble average applies to the fields only. The term linear in H disappears because $\overline{B_i} = 0$. In the second-order terms, one of the time integrations is contracted by the $\delta(t_1 - t_2)$ -distribution of the correlation function; the remaining integrand is time independent such that the integral gives just a factor Δt . The average time-evolved density matrix then becomes

$$\rho(t + \Delta t) = (1 - \gamma_s \Delta t)\rho(t) + \gamma_s \Delta t \sum_i \hat{S}_i \rho(t) \hat{S}_i + O((\gamma_s \Delta t)^2), \quad (6.15)$$

where $\hat{S}_i := S_i/\sqrt{s(s+1)}$ is the “normalised spin operator” with $\sum_i \hat{S}_i^2 = \mathbb{1}$. The spin relaxation rate $\gamma_s := s(s+1)\omega_0^2\tau_c$ is given in terms of the squared effective Larmor frequency $\omega_0^2 = \mu^2 B^2/(3\hbar^2)$. The relevant timescale of evolution turns out to be $\tau_s := 1/\gamma_s$. The effective time evolution (6.15) is then valid for a small time step $\Delta t \ll \tau_s$ such that indeed $\gamma_s \Delta t \ll 1$.

Exercise 1 (Non-unitary spin dynamics: quantum derivation)

Consider the time-independent model Hamiltonian $H = -\hbar J \mathbf{S} \cdot \boldsymbol{\tau}$, where our spin \mathbf{S} is coupled to a freely orientable magnetic impurity, here modelled as a spin $\frac{1}{2}$ with Pauli matrices $\boldsymbol{\tau}$. The effective spin dynamics of \mathbf{S} is described by its reduced density matrix $\rho(t) = \text{tr}_\tau\{\rho_{S\tau}(t)\}$ obtained by tracing out the uncontrolled impurity spin. Develop the time-evolved complete density matrix $\rho_{S\tau}(t)$ to second order in J as in Sect. 6.2.2 and take the trace over the impurity with initial statistical mixture $\rho_\tau(0) = \frac{1}{2}\mathbb{1}_2$ (it is

helpful to use the identities $\text{tr}_\tau\{\tau_i\} = 0$ and $\text{tr}_\tau\{\tau_i\tau_j\} = 2\delta_{ij}$). Show that one finds exactly the evolution (6.15) with a relaxation rate $\gamma_s = s(s+1)J^2\Delta t$ up to higher-order terms that become negligible in the formal limit $\Delta t \rightarrow 0$ together with $J \rightarrow \infty$ taken at constant γ_s .³

The Quantum Channel and Its Operator Sum Representation

In the language of quantum information, the time evolution (6.15) up to order Δt defines a *quantum channel* $\rho = \rho(t) \mapsto \rho' = \rho(t + \Delta t)$ and is here given in the so-called *operator sum representation* (see [12] Sect. 8.2.3.)

$$\rho' = \sum_{i=0}^3 W_i \rho W_i^\dagger \quad (6.16)$$

with

$$W_0 := \sqrt{1 - \gamma_s \Delta t} \mathbb{1}, \quad W_i := \sqrt{\gamma_s \Delta t} \hat{S}_i, \quad i = 1, 2, 3. \quad (6.17)$$

It is easy to verify that $\sum_{i=0}^3 W_i^\dagger W_i = \mathbb{1}$, which guarantees the trace conservation $\text{tr}\rho' = \text{tr}\rho$. Kraus has proved that a channel of this form assures that the final density matrix is again completely positive. Therefore, it is also known as the *Kraus representation*, and the W_i are commonly referred to as *Kraus operators*, cf. Sect. 5.3.1. In contrast to the unitary evolution $\rho' = U\rho U^\dagger$ of (6.10), the appearance of several independent terms in the sum (6.16) signals non-unitary dynamics.

For a spin $\frac{1}{2}$ with $\hat{S}_i = \sigma_i/\sqrt{3}$, this quantum channel is the *qubit depolarising channel* (see [12] Sect. 8.3.4.):

$$\rho' = (1 - p_1)\rho + \frac{p_1}{3} \sum_i \sigma_i \rho \sigma_i, \quad p_1 = \gamma_s \Delta t. \quad (6.18)$$

With equal probability $p_1/3$, the qubit is affected by the action of one of the Pauli matrices σ_i , and with probability $1 - p_1$, it remains untouched. Since for spin $\frac{1}{2}$ one may write $\sum_i \sigma_i \rho \sigma_i = 2\mathbb{1}_2 - \rho$, the channel also takes the suggestive form

$$\rho' = (1 - p_2)\rho + \frac{p_2}{2} \mathbb{1}_2. \quad (6.19)$$

This means that with probability $p_2 = 4p_1/3$ (remember $p_1 \ll 1$ such that also $p_2 \ll 1$), the density matrix is taken to a complete statistical mixture and remains identical with probability $(1 - p_2)$.

³ But attention: at finite coupling J , the dynamics of our spin shows *recurrence* on a timescale given by the so-called Poincaré time $t_{\text{rec}} \propto 1/J$. One could obtain a truly irreversible dynamics only by supposing that the single impurity spin is reset rapidly enough in order to dispose the coherence. Alternatively, one may imagine the setting treated in Sect. 6.4.1: our spin is moving and encounters different impurity spins such that in the thermodynamic limit, the Poincaré recurrence time goes to infinity and true irreversibility sets in.

By convention, the “depolarising channel” for higher spin $S \geq 1$ (i.e., $d_s \times d_s$ density matrices with $d_s = 2s + 1 \geq 3$) is still defined via the relation (6.19) with the statistical mixture $\frac{1}{d_s} \mathbb{1}_{d_s}$ on the right-hand side. This channel is also called “SU(n) channel” with $n = d_s$ because the corresponding Kraus operators are the $n^2 - 1$ generators of the Lie algebra $\text{su}(n)$ [13]. Note that our physical model of an arbitrary spin S coupled to a fluctuating magnetic field does *not* lead to this specific Lie algebra channel: obviously, the operator-sum representation (6.16) contains only the three generators of $\text{su}(2)$, albeit in a representation of dimension $d_s = 2s + 1$. We will see in the following that this makes the spin dynamics richer and its description more involved. Group-theoretical methods will be introduced that are well adapted to cope with this complexity.

The Liouvillian

The linear operators on the state Hilbert space \mathcal{H}_s are themselves elements of a linear vector space (we can add operators and multiply them by complex numbers). This vector space is called *Liouville space* $L(\mathcal{H}_s)$ and is spanned, for example, by the basis of *dyadics* induced by basis vectors $|n\rangle$ of \mathcal{H}_s :

$$|m\rangle\langle n| =: |mn\rangle, \quad n, m = 1, \dots, d_s. \quad (6.20)$$

The Liouville–von Neumann equation of motion $i\partial_t \rho = \mathcal{L}\rho$ for a closed quantum system defines the *Liouvillian*

$$\mathcal{L} = \frac{1}{\hbar} [H, \cdot], \quad (6.21)$$

whose matrix elements in the dyadic basis are

$$(mn|\mathcal{L}|m'n') = \mathcal{L}_{mn,m'n'} = H_{mm'}\delta_{nn'} - H_{n'n}\delta_{mm'}. \quad (6.22)$$

Exercise 2 (Liouvillian eigenvalues)

Show that the eigenvalues of the Liouvillian in the basis $\{|mn\rangle\}$ induced by the energy basis $H|m\rangle = \varepsilon_m|m\rangle$ are the possible transition frequencies $\omega_{mn} = (\varepsilon_m - \varepsilon_n)/\hbar$. These are experimentally accessible quantities, in contrast to the absolute energy eigenvalues of the Hamiltonian H .

As an operator between operators, the Liouvillian $\mathcal{L} : L(\mathcal{H}_s) \rightarrow L(\mathcal{H}_s)$ is called a *superoperator* [14–17]. The superoperator formalism is a convenient starting point for projection operator techniques in statistical dynamics [15], effective dynamics of open quantum systems [18] and time-dependent perturbation theory [19].

The Lindbladian

The effective dynamics of our spin coupled to a randomly fluctuating field can also be formulated in terms of a superoperator. Taking the formal limit $\lim_{\Delta t \rightarrow 0} \frac{\rho(t+\Delta t) - \rho(t)}{\Delta t} =: \partial_t \rho(t)$ in (6.15) leads to the *master equation*

$$\partial_t \rho(t) = \bar{\mathcal{L}}\rho(t), \quad (6.23)$$

a linear equation of motion for the effective density operator, whose effective generator of time evolution is the *Lindbladian* [17]

$$\bar{\mathcal{L}}\rho(t) = -\frac{\gamma_s}{2} \sum_i [\hat{S}_i, [\hat{S}_i, \rho(t)]] = \frac{\gamma_s}{2} \sum_i \left(2\hat{S}_i \rho(t) \hat{S}_i - \hat{S}_i \hat{S}_i \rho(t) - \rho(t) \hat{S}_i \hat{S}_i \right). \quad (6.24)$$

This is a pure relaxation superoperator in the Lindblad form, which assures the complete positivity of the time-evolved density matrix (see Sect. 5.3.2). The symbolic limit $\Delta t \rightarrow 0$ really means $\Delta t \gamma_s \ll 1$ but is still assumed to be “coarse-grained” compared to the field correlations, $\Delta t \gg \tau_c$. In this limit, the master equation (6.23) is a linear equation for the density matrix $\rho(t)$ local in time t and thus describes Markovian dynamics without any memory effects.

Exercise 3 (Lindbladian matrix elements)

Show that the superoperator matrix elements of the Lindbladian (6.24) are given by

$$\bar{\mathcal{L}}_{mn,m'n'} = \gamma_s \left(\hat{S}_{mm'} \cdot \hat{S}_{n'n} - \delta_{mm'} \delta_{nn'} \right), \quad (6.25)$$

and verify the trace-preserving property $\sum_m \bar{\mathcal{L}}_{mm,m'n'} = 0$ from this expression.

6.2.3 Irreducible Scalar Spin Relaxation Rates

Formally, the solution of the master equation (6.23) is very simple:

$$\rho(t) = \exp[\bar{\mathcal{L}}t]\rho(0). \quad (6.26)$$

The dynamics induced by the Lindbladian is called a “quantum dynamic semigroup”, cf. Sect. 5.3.1. Indeed, the time evolution superoperator satisfies $\exp[\bar{\mathcal{L}}(t_2 + t_1)] = \exp[\bar{\mathcal{L}}t_2] \exp[\bar{\mathcal{L}}t_1]$ and $\exp[\bar{\mathcal{L}}0] = \mathbb{1}$, which indicates a group structure. “Semigroup” means that the inverse to each element does not need to exist, and indeed here it does not since the non-unitary dynamics obtained by tracing out the environment has induced an arrow of time. The Kraus representation (6.16) and the Lindblad form (6.24) guarantee the complete positivity of the final density matrix if the initial one is completely positive, but the inverse is not true: the Lindbladian is not invertible (see [17] Sect. 3.4.1). We will indeed see in Sect. 6.2.3 that $\bar{\mathcal{L}}$ has one vanishing eigenvalue.

In Liouville space, the master equation is a matrix equation $\partial_t |\rho\rangle = \bar{\mathcal{L}}|\rho\rangle$ of dimension $d_s^2 \times d_s^2$. As always when dealing with matrix equations, we have to diagonalise the Lindbladian in Liouville space in order to be able to use the formal solution (6.26). For spin $\frac{1}{2}$ and $d_s = 2$, diagonalising a 4×4 matrix is elementary and can be done by hand, but already for spin 1 with $d_s^2 = 9$,

this becomes cumbersome. For higher spin, one definitely needs to resort to an efficient strategy to find the eigenstructure of the Lindbladian. In the following, we show how to take maximal advantage of rotational symmetries by using group-theoretical methods that lead to a very simple and physically transparent description for the effective spin dynamics.

Scalar Relaxation Process: What Results We Should Expect

The Lindbladian was obtained by an isotropic average and is thus a *scalar* object, i.e., invariant under rotations. A rather high-brow way of expressing this simple property is to say “it transforms under the trivial representation $\mathcal{D}^{(0)}$ ”. We may anticipate that the statistical operator can be decomposed into parts that transform under the irreducible representations $\mathcal{D}^{(K)}$ of the rotation group, $\rho = \sum_K \rho^{(K)}$. The Lindbladian as a scalar object can only connect subspaces of equal rank K . Furthermore, inside each subspace, it cannot distinguish between different orientations. Thus, in an adapted basis of Liouville space, it can be written as a purely diagonal matrix

$$\bar{\mathcal{L}} = \begin{pmatrix} \lambda_0 & 0 & \dots & 0 \\ 0 & \lambda_1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \lambda_{d_s^2} \end{pmatrix}. \quad (6.27)$$

How many *different* eigenvalues may we expect? The total number is the dimension of the Liouville space, d_s^2 . Each subspace of rank K will have dimension $d_K = 2K + 1$. Therefore, we will have to find only $2s + 1$ different eigenvalues λ_K , each of which has degeneracy $2K + 1$:

particle	s	d_s	d_s^2	eigenvalues	degeneracy
electron	$\frac{1}{2}$	2	4	λ_0, λ_1	1, 3
photon	1	3	9	$\lambda_0, \lambda_1, \lambda_2$	1, 3, 5

Can some of the eigenvalues be identical which would imply an even larger degeneracy? A trivial example for this would be any operator proportional to the identity. But we will see below that this is not the case for the Lindbladian (6.24): the eigenvalues pertaining to different subspaces $K \neq K'$ are indeed different, $\lambda_K \neq \lambda_{K'}$. We are therefore sure to have reduced the problem to the simplest possible formulation.

Irreducible Tensor Operators

Before we can define irreducible superoperators, we first had better understand the simpler concept of ordinary irreducible operators. An irreducible tensor operator of rank K is, by definition, a set of $2K + 1$ components T_Q^K ,

$Q = -K, -K + 1, \dots, K$, that transform under irreducible representations of rank K (i.e., whose transformation does not mix different K):

$$(T_Q^K)' = UT_Q^K U^\dagger = \sum_{Q'=-K}^K D_{QQ'}^{(K)} T_{Q'}^K. \quad (6.28)$$

Equivalently, one specifies the infinitesimal rotation properties by requiring

$$[J_\pm, T_Q^K] = \hbar \sqrt{K(K+1) - Q(Q \pm 1)} T_{Q \pm 1}^K, \quad (6.29)$$

$$[J_0, T_Q^K] = \hbar Q T_Q^K. \quad (6.30)$$

Here, the angular momentum raising and lowering operators are $J_\pm = J_x \pm iJ_y$. The simplest examples for irreducible tensor operators we need to know for the following are

- $K = 0$ or scalar operator T_0^0 , a single operator that commutes with all components of the total angular momentum \mathbf{J} . For instance S^2 , the Casimir operator indexing the irreducible representations $\mathcal{D}^{(s)}$.
- $K = 1$ or vector operator with Euclidean components $\mathbf{A} = (A_1, A_1, A_3)$ satisfying

$$[J_j, A_k] = i\hbar \epsilon_{jkl} A_l, \quad (6.31)$$

and spherical components $A_0 = A_3$ and $A_{\pm 1} = \mp \frac{1}{\sqrt{2}}(A_1 \pm iA_2)$.

Exercise 4 (Irreducible or Not?)

Is the Hamiltonian $H = \frac{p^2}{2m} - \mu \mathbf{S} \cdot \mathbf{B}$ of a free massive particle coupled to an external magnetic field \mathbf{B} via the magnetic moment $\boldsymbol{\mu} = \mu \mathbf{S}$ of its spin \mathbf{S} a scalar? An irreducible tensor operator?

State Multipoles

In the usual Hilbert space basis, the statistical operator reads

$$\rho = \sum_{m, m'} \rho_{mm'} |sm\rangle \langle sm'|. \quad (6.32)$$

Here, the ket $|sm\rangle$ transforms under the irreducible representation $\mathcal{D}^{(s)}$, whereas the bra $\langle sm'|$, as its complex conjugate, transforms under $(\mathcal{D}^{(s)})^*$, the contragredient representation. The ket-bra $|sm\rangle \langle sm'|$ transforms under the direct product $\mathcal{D}^{(s)} \otimes (\mathcal{D}^{(s)})^*$, which is reducible. One introduces therefore an ensemble of elements that do transform under the irreducible representation $\mathcal{D}^{(K)}$,

$$T_Q^K := T_Q^K(s, s) := \sum_{m, m'} (-)^{s-m} \langle ssm' - m | KQ \rangle |sm'\rangle \langle sm| \quad (6.33)$$

with $K = 0, 1, \dots, 2s$ and $Q = -K, -K + 1, \dots, K$. The Clebsch–Gordan coefficients $\langle s_1 s_2 m_1 m_2 | KQ \rangle$ are the coefficients of the unitary basis change from the direct product $\mathcal{H}_{s_1} \otimes \mathcal{H}_{s_2}$ towards the Hilbert subspace \mathcal{H}_K of spin K that should be familiar from the addition of two spins. The CG coefficients are non-zero only if two selection rules are satisfied: (i) the two magnetic quantum numbers on the left add up to the one on the right, $m_1 + m_2 = Q$; (ii) the angular momentum on the right satisfies the triangle inequality $|s_1 - s_2| \leq K \leq s_1 + s_2$.

In our case, we do not couple two spins, but a spin and its complex conjugate. Since there is a contragredient representation in the game, the CG coefficients in (6.33) feature a characteristic minus sign in front of $-m$. The triangle selection rule implies for us $0 \leq K \leq 2s$.

The irreducible tensor operators $T_Q^K := |KQ\rangle$ form a basis of Liouville space that is properly orthonormal with respect to the trace scalar product of matrices:

$$(KQ|K'Q') := \text{tr}\{(T_Q^K)^\dagger T_{Q'}^{K'}\} = \delta_{KK'} \delta_{QQ'}. \quad (6.34)$$

The Hermitian conjugate is $(T_Q^K)^\dagger = (-)^Q T_{-Q}^K$. Any linear operator A can be decomposed in this basis,

$$A = \sum_{KQ} A_{KQ} T_Q^K \quad \text{with} \quad A_{KQ} := (KQ|A) = \text{tr}\{(T_Q^K)^\dagger A\}. \quad (6.35)$$

The irreducible components

$$\rho_{KQ} = \text{tr}\{(T_Q^K)^\dagger \rho\} = \langle (T_Q^K)^\dagger \rangle \quad (6.36)$$

of the density matrix are called *state multipoles* or statistical tensors, and have been introduced already in the 1950s by Fano and Racah [20–22].

Exercise 5 (Irreducible Tensor Operators)

(0) Show that all T_Q^K except T_0^0 have zero trace and calculate the state monopole moment ρ_{00} (use $\sqrt{2s+1} \langle ssm' - m | 00 \rangle = (-)^{s-m} \delta_{mm'}$).

(1) Show that the irreducible vector operator is proportional to the spin operator, $T_Q^1 = c_s^{-1/2} S_Q$. Hint: consider the action of T_0^1 ($\sqrt{c_s} \langle ssm - m | 10 \rangle = (-)^{s-m} m$), argue with rotational invariance and fix the proportionality constant $c_s = s(s+1)d_s/3$ by computing $\text{tr}[(T^1)^2]$.

Irreducible Spin Superoperators

By inserting the decomposition (6.35) on the left and right side of an arbitrary superoperator acting like $\mathcal{L}A$, one obtains

$$\mathcal{L}A = \sum_{KQK'Q'} |K'Q'\rangle \langle K'Q'| \mathcal{L} |KQ\rangle \langle KQ| A, \quad (6.37)$$

such that with the notation $\mathcal{L}_{K'Q',KQ} := (K'Q'|\mathcal{L}|KQ)$ the superoperator reads

$$\mathcal{L} = \sum_{KQK'Q'} \mathcal{L}_{K'Q',KQ} |K'Q'\rangle\langle KQ|, \quad (6.38)$$

where the Liouville-space dyadics on the right-hand side transform under $\mathcal{D}^{(K')} \otimes (\mathcal{D}^{(K)})^*$, in an analogous manner to (6.32). Following the same strategy as previously, we recouple the elements again using the appropriate CG-coefficients to get irreducible superoperators [23]

$$\mathcal{T}_M^L(K, K') := \sum_{Q,Q'} (-)^{K-Q} \langle K'KQ' - Q | LM \rangle |K'Q'\rangle\langle KQ|. \quad (6.39)$$

Finally, any superoperator in completely decomposed form reads

$$\mathcal{L} = \sum_{LM} \sum_{K,K'} \mathcal{L}_{LM}(K, K') \mathcal{T}_M^L(K, K') \quad (6.40)$$

with coefficients $\mathcal{L}_{LM}(K, K') = \sum_{Q,Q'} (-)^{K-Q} \langle K'KQ' - Q | LM \rangle \mathcal{L}_{K'Q',KQ}$. This decomposition is completely general and applies to arbitrary superoperators. It is only worth the effort, however, if the superoperator has rotational symmetries. The greatest gain in computational speed and conceptual clarity is obtained if the superoperator is a scalar such that its only non-zero component is $L = 0, M = 0$. In that case, which applies to our Lindbladian (6.24), one finds by virtue of the triangle rule that $K = K'$: as promised, \mathcal{L} indeed connects subspaces of equal rank. We can choose the decomposition

$$\mathcal{L} = \sum_{K=0}^{2s} \lambda_K \mathcal{T}^{(K)}, \quad (6.41)$$

where the $\mathcal{T}^{(K)}$ are orthogonal projectors onto the subspaces $L(\mathcal{H}_s)^{(K)}$ of irreducible tensor operators of rank K :

$$\mathcal{T}^{(K)} = \sqrt{2K+1} \mathcal{T}_0^0(K, K) = \sum_Q |KQ\rangle\langle KQ|. \quad (6.42)$$

They are indeed orthogonal, $\mathcal{T}^{(K)}\mathcal{T}^{(K')} = \delta_{KK'}\mathcal{T}^{(K)}$, by virtue of (6.34), and resolve the identity in Liouville space, $\sum_K \mathcal{T}^{(K)} = 1$, by virtue of a completeness relation of CG coefficients.

Scalar Relaxation Rates

Once the invariant subspaces are known, the eigenvalues are obtained by projecting the superoperator onto an arbitrary basis element:

$$\lambda_K = (KQ|\bar{\mathcal{L}}|KQ) = \text{tr} \{ (T_Q^K)^\dagger \bar{\mathcal{L}} T_Q^K \}. \quad (6.43)$$

For the spin relaxation Lindbladian (6.24), one must calculate commutators of the form $[S_i, [S_i, T_Q^K]]$. In order to use the defining commutation relations (6.29) and (6.30) for irreducible tensor operators, one writes the scalar product of spin operators in terms of the spherical components $S_0 = S_z$, $S_{\pm 1} = \mp \frac{1}{\sqrt{2}}(S_x \pm iS_y)$,

$$\sum_i S_i S_i = \sum_{p=0,\pm 1} (S_p)^\dagger S_p = \sum_{p=0,\pm 1} (-)^p S_p S_{-p}, \quad (6.44)$$

such that

$$\lambda_K = -\frac{\gamma_s}{2s(s+1)} \sum_{p=0,\pm 1} (-)^p \text{tr} \{ (T_Q^K)^\dagger [S_{-p}, [S_p, T_Q^K]] \}. \quad (6.45)$$

It is now a simple exercise to show with the help of (6.29) and (6.30) (by paying attention to the supplementary factor $\sqrt{2\hbar}S_{\pm 1}$ in the definition of the raising/lowering components $J_{\pm} = \sqrt{2\hbar}S_{\pm 1}$) that the double commutator gives back the tensor operator itself, $[S_{-p}, [S_p, T_Q^K]] = c(p, Q, K) T_Q^K$. Summing all three terms gives remarkably simple eigenvalues,

$$\lambda_K = -\gamma_s \frac{K(K+1)}{2s(s+1)}, \quad K = 0, 1, \dots, 2s. \quad (6.46)$$

These real, negative eigenvalues describe a pure relaxation process as expected from the definition of the Lindbladian (6.24). They are scalar objects, also known as *rotational invariants*, and can be expressed in terms of 6j-coefficients that are constructed out of the irreducible representations $\mathcal{D}^{(K)}$ for the state multipole, $\mathcal{D}^{(s)}$ for the spin \mathbf{S} itself and $\mathcal{D}^{(1)}$ for its coupling to the vector field \mathbf{B} [3, 23]. This type of consideration is of considerable importance in many different fields of physics involving angular momentum or spin; for example, relaxation coefficients very similar to (6.46) characterise spatial correlations in certain ground states of quantum spin chains [24].

Isotropic Spin Relaxation

The master equation $\partial_t \rho(t) = \bar{\mathcal{L}}\rho(t)$ separates into uncoupled equations for each invariant subspace:

$$\partial_t \rho(t) = \sum_{KQ} \partial_t \rho_{KQ}(t) T_Q^K = \sum_{KQ} \rho_{KQ}(t) \bar{\mathcal{L}} T_Q^K = \sum_{KQ} \rho_{KQ}(t) \lambda_K T_Q^K. \quad (6.47)$$

The resulting differential equation $\partial_t \rho_{KQ}(t) = \lambda_K \rho_{KQ}(t)$ for the state multipoles is easily solved to yield a simple exponential decay

$$\rho_{KQ}(t) = e^{-\gamma_K t} \rho_{KQ}(0) \quad (6.48)$$

with relaxation rates $\gamma_K = |\lambda_K|$. This is a particular example for a state multipole relaxation as described by Blum in Chap. 8 of [20]. The first two

values deserve a special discussion. The scalar mode relaxation rate $\gamma_0 = 0$ assures the trace preservation of $\rho(t)$. At the same time, this vanishing eigenvalue is responsible for the fact that the Lindbladian is not invertible. The vector mode relaxation rate $\gamma_1 = \gamma_s/[s(s+1)] =: 1/\tau_1$ describes the relaxation of the *orientation* or average spin vector:

$$\langle \mathbf{S}(t) \rangle = \text{tr}\{\rho(t)\mathbf{S}\} = e^{-t/\tau_1} \langle \mathbf{S}(0) \rangle \quad (6.49)$$

since $\text{tr}\{T_Q^K S_Q\}$ projects onto $K = 1$ (remember exercise 5(1) and the orthogonality relation (6.34)).

For a qubit spin $\frac{1}{2}$, this is all that needs to be calculated since any 2×2 -density matrix can be parameterised as $\rho_2(t) = \frac{1}{2} \mathbb{1}_2 + \langle \mathbf{S}(t) \rangle \cdot \boldsymbol{\sigma}$ and thus

$$\rho_2(t) = e^{-t/\tau_1} \rho(0) + (1 - e^{-t/\tau_1}) \frac{1}{2} \mathbb{1}_2. \quad (6.50)$$

This isotropic spin $\frac{1}{2}$ relaxation therefore is for all times given by the depolarising channel (6.19) with $p_2(t) = 1 - e^{-t/\tau_1}$. The Kraus operators for the operator sum representation (6.16), valid for *all* times, follow by using $p_1(t) = \frac{3}{4} p_2(t)$:

$$W_0(t) = \frac{\sqrt{1+3e^{-t/\tau_1}}}{2} \mathbb{1}_2, \quad W_i(t) = \frac{\sqrt{1-e^{-t/\tau_1}}}{2} \sigma_i, \quad i = 1, 2, 3. \quad (6.51)$$

Naturally, by developing these expressions to first order in $t/\tau_1 = \frac{4}{3}\gamma_s t$, one finds the Kraus operators for an infinitesimal time step derived in Sect. 6.2.2. In general, it is easy to show by derivation that to each quantum dynamical semigroup described by an exponential superoperator $\exp[\mathcal{L}t]$ corresponds a Lindblad-type master equation [25], cf. Sect. 5.3.2. However, as always, the inverse operation of integrating the infinitesimal time evolution to finite times is much harder. Deriving a set of Kraus operators for an arbitrary quantum channel in general requires the complete diagonalisation of the microscopic Hamiltonian. Luckily, for spin $\frac{1}{2}$ everything is so simple that the complete calculation is possible.

Naturally, one thus wonders whether the full-fledged angular momentum formalism is necessary at all to describe isotropic spin relaxation. A simple calculation shows that in the “depolarising channel” defined by (6.19), all non-scalar eigenvalues $\lambda_1, \lambda_2, \dots$ are identical, such that again the Kraus operators are the generators of the $\text{su}(n)$ Lie algebra. For that channel, one does not need to employ angular momentum theory, and the Kraus operators are the generators of the $\text{su}(n)$ Lie algebra [13]. But please be aware that this is *not* the case for our arbitrary spin coupled to a freely fluctuating impurity spin where all higher state multipoles $K \geq 1$ come with their own different decay rates (6.46). For this channel, the author has not been able to determine the Kraus operators for finite times (but would certainly be happy to receive any valuable information on that point by his readers). In this case, there

seems to be no easier way to describe the spin relaxation than in terms of the irreducible components:

$$\rho(t) = \sum_{KQ} e^{-\gamma_K t} \rho_{KQ}(0) T_Q^K. \quad (6.52)$$

This implies the simple exponential decay

$$A_{KQ}(t) = e^{-\gamma_K t} A_{KQ}(0) \quad (6.53)$$

for the irreducible components (6.35) of any observable A .

6.3 Diffusion

6.3.1 Transport

We may call “transport” a movement from a point \mathbf{r} to a point \mathbf{r}' that is induced by an external cause. In free space, propagation is *ballistic*: the average square of the distance covered after a time t scales like $\langle r^2 \rangle \sim v^2 t^2$, where v is the particle’s velocity. A disordered medium contains *impurities* that interrupt the ballistic movement. So-called “quenched” disorder is fixed for each realisation of an experiment, but varies from experiment to experiment when samples are changed. Predictions about observables will involve an average $\langle \dots \rangle$ by integrating over a classical disorder distribution or by tracing out uncontrolled quantum degrees of freedom. Generically, the averaged expectation value behaves as a diffusive quantity: $\langle r^2 \rangle \sim 2Dt$ with D the *diffusion constant*.

In a hydrodynamic description, diffusion is a direct consequence of two very basic hypotheses:

- (i) a local conservation law $\partial_t n + \nabla \cdot \mathbf{j} = 0$, also known as the continuity equation, linking the local density $n(\mathbf{r}, t)$ and the local current density $\mathbf{j}(\mathbf{r}, t)$, and
- (ii) a linear response relation $\mathbf{j} = -D\nabla n$, known as Fourier’s law in the context of heat transport and Fick’s law in the context of particle diffusion.

By inserting the second relation into the first, one finds immediately the diffusion equation $(\partial_t - D\nabla^2)n = 0$. The hydrodynamic description is only valid for times and distances large compared to the scales on which microscopic scattering takes place. The linear response coefficient D has to be determined microscopically. In essence, the simplest physical process leading to diffusion is a random walk or repeated elastic scattering. A kinetic description where point particles collide with obstacles permits to derive the diffusion constant D associated with this process as function of microscopic scattering parameters. In this section, we will derive the appropriate kinetic equation for elastic momentum scattering from first principles using a master equation approach

and determine the relevant diffusion constant. A largely equivalent presentation with more details can be found in Chap. 4 of the recommendable book “Quantum Transport Theory” by J. Rammer [26].

6.3.2 Momentum – a Primer on Translations

If spin is to be understood by considering rotations, then momentum is understood by considering translations.

Let a particle be prepared at a point $\mathbf{r}_0 = 0$ with a spreading described by a function $f(\mathbf{r})$. After translation of the entire preparation apparatus by a vector $\mathbf{a} \in \mathbb{R}^d$, the new position is described by the function

$$[T_{\mathbf{a}}f](\mathbf{r}) := f(\mathbf{r} - \mathbf{a}) \quad (6.54)$$

such that the particle is indeed centred around $\mathbf{r}'_0 = \mathbf{a}$. In this so-called “active” formulation of translations, relation (6.54) defines the action of the translation operator $T_{\mathbf{a}}$ in a functional space of, say, probability distributions, in exact analogy to the case of rotations treated in Sect. 6.2.1. Here, it is an infinite-dimensional representation of the group $(\mathbb{R}, +)$ of real numbers with the addition “+” as a group law; to be precise, in d dimensions it is the d -fold direct product of such representations. Translations have the identity element $E = T_0$ and inverse $T_{\mathbf{a}}^{-1} = T_{-\mathbf{a}}$. This group is Abelian because different translations commute: $T_{\mathbf{a}}T_{\mathbf{b}} = T_{\mathbf{a}+\mathbf{b}} = T_{\mathbf{b}+\mathbf{a}} = T_{\mathbf{b}}T_{\mathbf{a}}$. Furthermore, this group is a simply connected Lie group, and all translations can be generated by exponentiation $T_{\mathbf{a}} = \exp\{-i\mathbf{a} \cdot \mathbf{T}\}$ of $i = 1, \dots, d$ generators T_i that form a Lie algebra.⁴

In the functional representation (6.54), all translations $T_{\mathbf{a}} = \exp\{-i\mathbf{a} \cdot \mathbf{T}\}$ are generated by $\mathbf{T} = -i\nabla$, the derivative with respect to the position coordinate, which becomes apparent through a Taylor series expansion

$$f(\mathbf{r} - \mathbf{a}) = f(\mathbf{r}) - \mathbf{a} \cdot \nabla f(\mathbf{r}) + \dots = \exp\{-\mathbf{a} \cdot \nabla\} f(\mathbf{r}). \quad (6.55)$$

In quantum physics, the fundamental commutation relation between position and momentum, $[\hat{r}_i, \hat{p}_j] = i\hbar\delta_{ij}$, implies that the momentum observable $\hat{\mathbf{p}} = \hbar\mathbf{T}$ is the translation generator $\hat{\mathbf{p}} = -i\hbar\nabla$ in position representation. Translations are implemented by the unitary operator

⁴ If, however, the possible positions lie on a lattice, only discrete translations by lattice vectors are allowed, and translations are a representation of $(\mathbb{Z}, +)$, the additive group of integer numbers. In an infinite volume, the translation group is not compact because it is not bounded such that its representation theory is quite different from the compact rotation groups $SU(n)$. Notably, it has no finite-dimensional irreducible representations. An exception is the discrete translations on a lattice with periodic boundary conditions, often used for classification of crystalline lattices. This group is the cyclic group, and its irreducible representations are labelled by the admissible wave vectors of the reciprocal lattice [27]. Physicists are taught to know this under the epithet of Bloch’s theorem.

$$U(\mathbf{a}) = \exp\{-i\mathbf{a} \cdot \hat{\mathbf{p}}/\hbar\}, \quad (6.56)$$

such that the particle’s position operator $\hat{\mathbf{r}}$ transforms as

$$\hat{\mathbf{r}}' = U(\mathbf{a})\hat{\mathbf{r}}U(\mathbf{a})^\dagger = \hat{\mathbf{r}} - \mathbf{a}, \quad (6.57)$$

quite similarly to the corresponding identity (6.2) for rotations. In contrast to the angular momentum commutation relations (6.6), the simpler version $[\hat{p}_i, \hat{p}_j] = 0$ for the translation generators reflects their Abelian structure.

The momentum operator is diagonal in the basis of momentum eigenstates, $\hat{\mathbf{p}}|\mathbf{p}\rangle = \mathbf{p}|\mathbf{p}\rangle$. Any operator O is translation invariant if and only if it commutes with the momentum operator, $[O, \hat{\mathbf{p}}] = 0$. Therefore, it is diagonal in the momentum representation, $\langle \mathbf{p}'|O|\mathbf{p}\rangle = \delta_{\mathbf{p}'\mathbf{p}}O_{\mathbf{p}}$. Notably, in absence of any external perturbation, the Hamiltonian H_0 should be translation invariant, $H_0|\mathbf{p}\rangle = \varepsilon_{\mathbf{p}}|\mathbf{p}\rangle$, a property sometimes referred to by the expression “the p_i s are good quantum numbers”. Henceforth, we will choose units such that $\hbar = 1$ and thus drop the distinction between momentum and wave vectors: $\mathbf{p} = \hbar\mathbf{k} = \mathbf{k}$.

The spatial form of the wave functions $\psi_{\mathbf{p}}(\mathbf{r}) = \langle \mathbf{r}|\mathbf{p}\rangle$ is fixed by their translational properties: using (6.54) together with (6.56) yields $\langle \mathbf{r} - \mathbf{a}|\mathbf{p}\rangle = \langle \mathbf{r}|[U(\mathbf{a})|\mathbf{p}\rangle] = \exp\{-i\mathbf{a} \cdot \mathbf{p}\}\langle \mathbf{r}|\mathbf{p}\rangle$ such that $\langle \mathbf{r}|\mathbf{p}\rangle = C \exp\{i\mathbf{r} \cdot \mathbf{p}\}$ up to a normalisation factor. In a finite volume $\Omega = L^d$, these plane waves are square integrable and can be properly normalised. We choose to work in the limit $\Omega \rightarrow \infty$ and fix $C = 1$. The identity is resolved by

$$\mathbb{1} = \int d^d r |\mathbf{r}\rangle\langle \mathbf{r}| = \int \frac{d^d p}{(2\pi)^d} |\mathbf{p}\rangle\langle \mathbf{p}|. \quad (6.58)$$

Using the plane-wave expansion, Fourier transformation is written using the convention

$$f(\mathbf{x}) = \int \frac{d^d p}{(2\pi)^d} e^{i\mathbf{x} \cdot \mathbf{p}} f_{\mathbf{p}} \quad \text{with} \quad f_{\mathbf{p}} = \int d^d x e^{-i\mathbf{x} \cdot \mathbf{p}} f(\mathbf{x}). \quad (6.59)$$

This choice is convenient because factors of 2π are always associated with p -integrals which, if required, can be easily converted back to finite-volume sums, $\int \frac{d^d p}{(2\pi)^d} F(\mathbf{p}) = L^{-d} \sum_{\mathbf{p}} F(\mathbf{p})$.

6.3.3 Master Equation Approach to Diffusion

Hamiltonian

We will show that a microscopic quantum derivation of diffusive behaviour is possible starting from the single-particle Hamiltonian

$$H = H_0 + V. \quad (6.60)$$

Here the translation-invariant part H_0 describes free propagation in momentum eigenstates $|\mathbf{p}\rangle$ with eigenenergies $\varepsilon_p = p^2/2m$; the generalisation to more general dispersion relations is straightforward. The random impurity potential

$$V = \sum_i v(\hat{\mathbf{r}} - \mathbf{x}_i) = \sum_i e^{-i\hat{\mathbf{p}} \cdot \mathbf{x}_i} v(\hat{\mathbf{r}}) e^{i\hat{\mathbf{p}} \cdot \mathbf{x}_i} \quad (6.61)$$

describes momentum scattering by an arbitrary potential $v(\mathbf{r})$, typically quite short-ranged, centred on random classical positions $\{\mathbf{x}_i\}$. Deriving observable quantities will involve averages over all possible realisations of the disorder. The ensemble average of any quantity $O(\{\mathbf{x}_i\})$ is the integral

$$\bar{O} = \int \left(\prod_i d^d x_i \right) P(\{\mathbf{x}_i\}) O(\{\mathbf{x}_i\}) \quad (6.62)$$

over all impurity positions weighted by their distribution $P(\{\mathbf{x}_i\})$. The simplest distribution $P(\{\mathbf{x}_i\}) = \prod_i P(\mathbf{x}_i) = \prod_{i=1}^N \Omega^{-1}$ describes N uncorrelated impurities with average uniform density $n = N/\Omega$ in any finite volume Ω . This distribution will be used in the following, and we will go to the thermodynamic limit $N, \Omega \rightarrow \infty$ with fixed density n .

This description is valid if the mass M of scattering impurities is much larger than the mass m of scattered particles. This is the case for electrons scattered by lattice defects in solid-state devices or for photons scattered by cold atoms when recoil can be neglected. The impurities then have no internal dynamics and simply realise an external potential $v(\mathbf{r})$; this description can be obtained in the limit $m/M \rightarrow 0$ from the more general model, where also the dynamics of impurities is taken into account. Note that this limit is just the opposite of the usual picture used for quantum Brownian motion, cf. Sect. 5.4.3, where one tracks the movement of a large test particle bombarded frequently by smaller ones.

Derivation of the Master Equation

Here, we follow the standard derivation of a master equation for open quantum systems [18, 28] by adapting the Born–Markov or weak-coupling recipe to our case, cf. Sect. 5.4.1. The ensemble average (6.62) now plays the role of a trace over bath variables.

Starting from the Liouville–von Neumann equation $\partial_t \tilde{\rho}(t) = -i[\tilde{V}(t), \tilde{\rho}(t)]$ in the interaction representation $\tilde{A}(t) = U_0^\dagger(t) A U_0(t)$ and developing to second order in the interaction leads to the pre-master equation for the averaged density matrix $\bar{\rho}(\{\mathbf{x}_i\}, t) =: \bar{\rho}(t)$:

$$\partial_t \bar{\rho}(t) = -i[\bar{V}(t), \bar{\rho}(0)] - \int_0^t \left[\bar{V}(t), [\bar{V}(t-t'), \bar{\rho}(\{\mathbf{x}_i\}, t-t')] \right] dt'. \quad (6.63)$$

We may assume that the initial density matrix $\rho(0)$ does not depend on the disorder configuration – it may, for instance, represent an initial wave-packet

prepared far from impurities whose temporal evolution we wish to follow. Then, the first term $[\bar{V}(t), \rho(0)]$ vanishes because

$$\overline{\tilde{V}(t)} = \bar{V}(t) = \bar{V} \quad (6.64)$$

is a constant real number that shifts all energy levels ε_p of H_0 by a uniform amount and thus gives no contribution under the commutator.

The resulting equation is still exact, but not useful: it is not a closed equation for the ensemble-averaged $\bar{\rho}(t)$ since the density matrix inside the integral still depends on the disorder configuration. In order to cope with the integrand, one typically proceeds with the so-called *Born approximation*, replacing the exact density matrix inside the integral by its average:

$$\partial_t \bar{\rho}(t) = - \int_0^t \left[\bar{V}(t), [\bar{V}(t-t'), \bar{\rho}(t-t')] \right] dt'. \quad (6.65)$$

Now, we are left with an effective Gaussian model of disorder since everything depends on the pair correlations $\overline{V\bar{V}}$. Concerning the time dependence, we still face a difficult integro-differential equation for $\bar{\rho}(t)$. If the timescale of scattering is much smaller than the timescale of evolution we are interested in, we can perform the *Markov approximation* by replacing $\bar{\rho}(t-t') \mapsto \bar{\rho}(t)$ inside the integral and by letting the upper limit t of integration go to ∞ such that now we have a closed differential equation for $\bar{\rho}(t)$. Reverting to the Schrödinger representation we find the following master equation for scattering by fixed impurities:

$$\partial_t \bar{\rho}(t) = -i[H_0, \bar{\rho}(t)] + \mathcal{D}\bar{\rho}(t) \quad (6.66)$$

with a scattering superoperator \mathcal{D} defined by

$$\mathcal{D}\bar{\rho}(t) = \overline{V\bar{\rho}(t)W} + \overline{W\bar{\rho}(t)V} - \overline{VW}\bar{\rho}(t) - \bar{\rho}(t)\overline{WV}, \quad (6.67)$$

where

$$W := \int_0^\infty \tilde{V}(-t') dt' = \int_{-\infty}^0 U_0^\dagger(t') V U_0(t') dt' =: \sum_j e^{-i\hat{\mathbf{p}} \cdot \mathbf{x}_j} w(\hat{\mathbf{r}}) e^{i\hat{\mathbf{p}} \cdot \mathbf{x}_j}. \quad (6.68)$$

It will become apparent in Sect. 6.3.3 that the weak coupling or Born approximation discards genuine quantum corrections and entails purely classical dynamics. Instead of “approximation”, we had better speak of “simplification” because at this stage we have no means of knowing whether the resulting description is truly an approximation or perhaps qualitatively wrong. And really, in Sect. 6.4.2 we will see that quantum corrections need to be considered in phase-coherent samples.

Momentum Representation

In order to see what kind of evolution the master equation (6.66) describes, we evaluate it in the momentum representation in which the free Hamiltonian H_0 is diagonal. In the short-hand notation $|1\rangle = |\mathbf{p}_1\rangle$ and $\varepsilon_1 = \varepsilon_{\mathbf{p}_1}$, the first scattering contribution reads

$$\langle 1|\overline{V\bar{\rho}(t)\overline{W}}|4\rangle = \sum_{2,3} \sum_{i,j} \overline{\langle 1|e^{-i\hat{\mathbf{p}}\cdot\mathbf{x}_i}v(\hat{\mathbf{r}})e^{i\hat{\mathbf{p}}\cdot\mathbf{x}_i}|2\rangle\langle 3|e^{-i\hat{\mathbf{p}}\cdot\mathbf{x}_j}w(\hat{\mathbf{r}})e^{i\hat{\mathbf{p}}\cdot\mathbf{x}_j}|4\rangle\langle 2|\bar{\rho}(t)|3\rangle}. \quad (6.69)$$

The terms with $i \neq j$ are proportional to \overline{V}^2 and cancel with an equivalent contribution in (6.67) that comes with a minus sign (as before, the average \overline{V} gives no contribution thanks to the commutator structure of the equation of motion). In the terms $i = j$, we can take the translation operators outside the matrix elements and perform the ensemble average:

$$\begin{aligned} \sum_i \overline{e^{-i(\mathbf{p}_1-\mathbf{p}_2+\mathbf{p}_3-\mathbf{p}_4)\cdot\mathbf{x}_i}} &= \frac{N}{L^d} \int d^d x e^{-i(\mathbf{p}_1-\mathbf{p}_2+\mathbf{p}_3-\mathbf{p}_4)\cdot\mathbf{x}} \\ &= n(2\pi)^d \delta(\mathbf{p}_1 + \mathbf{p}_3 - \mathbf{p}_2 - \mathbf{p}_4). \end{aligned} \quad (6.70)$$

As expected, the average over a uniform distribution restores translational invariance which is equivalent to the conservation of total momentum expressed by $(2\pi)^d \delta(\mathbf{p}_1 + \mathbf{p}_3 - \mathbf{p}_2 - \mathbf{p}_4) =: \delta_{1+3,2+4}$.

Proceeding in the evaluation of (6.69), the first matrix element

$$\langle 1|v(\hat{\mathbf{r}})|2\rangle = \int d^d r e^{-i(\mathbf{p}_1-\mathbf{p}_2)\cdot\mathbf{x}} v(\mathbf{r}) = v_{\mathbf{p}_1-\mathbf{p}_2} =: v_{12} \quad (6.71)$$

is the Fourier transform of the scattering potential. In the second matrix element $\langle 3|w(\hat{\mathbf{r}})|4\rangle = \int_{-\infty}^0 \langle 3|U_0^\dagger(t')v(\hat{\mathbf{r}})U_0(t')|4\rangle dt'$, we can pull out the time integration

$$\int_{-\infty}^0 e^{i(\varepsilon_3-\varepsilon_4)t'} dt' = \frac{i}{\varepsilon_4 - \varepsilon_3 + i0} =: \Gamma_{34}. \quad (6.72)$$

Readers with a background in perturbation theory will recognise this as the matrix element $\Gamma_{34} = i\langle \mathbf{p}_3|G_0^R(\varepsilon_4)|\mathbf{p}_3\rangle$ of the free retarded resolvent operator $G_0^R(\omega) = (\omega - H_0 + i0)^{-1}$. This gives us a hint on the applicability of the Markov approximation: the rapid timescale here is the inverse energy difference $\varepsilon_3 - \varepsilon_4$ of incident and scattered state. The effective evolution on much longer timescales into a new state $|\mathbf{p}_3\rangle$ is constrained by (6.72) to the energy shell ε_4 of the incident state $|\mathbf{p}_4\rangle$. The imaginary contribution of Γ produces the *Lamb shift* that renormalises the original energy levels, cf. Sect. 5.4.1, whereas the real part yields the relaxation rates that render the dynamics irreversible.

Altogether, this first contribution to the collision functional reads

$$\langle 1|\overline{V\bar{\rho}(t)\overline{W}}|4\rangle = n \sum_{2,3} \delta_{1+3,2+4} v_{12} v_{34} \Gamma_{34} \langle 2|\bar{\rho}(t)|3\rangle. \quad (6.73)$$

Collecting all four contributions gives

$$\begin{aligned} \langle 1|\mathcal{D}\bar{\rho}(t)|4\rangle &= n \sum_{2,3} \left[\delta_{1+3,2+4} v_{12} v_{34} (\Gamma_{12} + \Gamma_{34}) \langle 2|\bar{\rho}(t)|3\rangle \right. \\ &\quad \left. - \delta_{2,3} (|v_{12}|^2 \Gamma_{21} + |v_{34}|^2 \Gamma_{43}) \langle 1|\bar{\rho}(t)|4\rangle \right]. \end{aligned} \quad (6.74)$$

We choose to use the parametrisation

$$\begin{aligned} \mathbf{p}_1 &= \mathbf{p} + \mathbf{q}/2, & \mathbf{p}_2 &= \mathbf{p}' + \mathbf{q}/2, \\ \mathbf{p}_4 &= \mathbf{p} - \mathbf{q}/2, & \mathbf{p}_3 &= \mathbf{p}' - \mathbf{q}/2, \end{aligned} \quad (6.75)$$

that complies with the conservation of total momentum (6.70). With this parametrisation, $v_{12} = v_{\mathbf{p}-\mathbf{p}'} = v_{34}^*$. Furthermore, energy differences become

$$\varepsilon_1 - \varepsilon_2 =: \varepsilon_p - \varepsilon_{p'} + \frac{(\mathbf{p} - \mathbf{p}') \cdot \mathbf{q}}{2m} \quad (6.76)$$

and $\varepsilon_1 - \varepsilon_4 = \mathbf{p} \cdot \mathbf{q}/m$, and we write the sum of matrix elements (6.72) in the form

$$\Gamma_{12} + \Gamma_{34} =: \Gamma_{\mathbf{p}\mathbf{p}'}(\mathbf{q}). \quad (6.77)$$

Finally, disposing of the overbar $\bar{\rho}(t) \mapsto \rho(t)$, the density matrix elements $\rho(\mathbf{p}, \mathbf{q}, t) := \langle \mathbf{p} + \frac{\mathbf{q}}{2} | \rho(t) | \mathbf{p} - \frac{\mathbf{q}}{2} \rangle$ obey the master equation

$$\partial_t \rho(\mathbf{p}, \mathbf{q}, t) = -i \frac{\mathbf{q} \cdot \mathbf{p}}{m} \rho(\mathbf{p}, \mathbf{q}, t) + \mathcal{D}[\rho(\mathbf{p}, \mathbf{q}, t)] \quad (6.78)$$

with the scattering functional

$$\mathcal{D}[\rho(\mathbf{p}, \mathbf{q}, t)] = n \int \frac{d^d p'}{(2\pi)^d} |v_{\mathbf{p}-\mathbf{p}'}|^2 [\Gamma_{\mathbf{p}\mathbf{p}'}(\mathbf{q}) \rho(\mathbf{p}', \mathbf{q}, t) - \Gamma_{\mathbf{p}'\mathbf{p}}(\mathbf{q}) \rho(\mathbf{p}, \mathbf{q}, t)]. \quad (6.79)$$

Trace Conservation and Continuity Equation

Clearly, the master equation (6.78) has the form of a kinetic balance equation where the scattering functional (6.79) contains transitions $\mathbf{p}' \rightarrow \mathbf{p}$ that increase the magnitude of $\rho(\mathbf{p}, \mathbf{q}, t)$ and also negative contributions of depleting transitions $\mathbf{p} \rightarrow \mathbf{p}'$. Since we have neither sinks nor external sources, the net effect must be zero which should be apparent in a conservation of the local probability density. And really, the master equation first of all preserves the trace, $\partial_t \text{tr}\{\rho(t)\} = \int \frac{d^d p}{(2\pi)^d} \partial_t \rho(\mathbf{p}, 0, t) = 0$, since the scattering functional is antisymmetric under the exchange $\mathbf{p} \leftrightarrow \mathbf{p}'$ and thus

$$\int \frac{d^d p}{(2\pi)^d} \mathcal{D}[\rho(\mathbf{p}, \mathbf{q}, t)] = 0. \quad (6.80)$$

This antisymmetry is inherited from the double-commutator structure of (6.65) and holds for all spatial Fourier momenta \mathbf{q} . Summing the \mathbf{q} -dependent master equation over \mathbf{p} thus leads to the *continuity equation*

$$\partial_t n_{\mathbf{q}}(t) + i\mathbf{q} \cdot \mathbf{j}_{\mathbf{q}}(t) = 0 \quad (6.81)$$

that links the Fourier transforms of the local density $n(\mathbf{r}, t)$ and local current density $\mathbf{j}(\mathbf{r}, t)$, given as the first two \mathbf{p} -moments of the density distribution:

$$n_{\mathbf{q}}(t) = \int d^d r e^{-i\mathbf{q} \cdot \mathbf{r}} n(\mathbf{r}, t) = \int \frac{d^d p}{(2\pi)^d} \rho(\mathbf{p}, \mathbf{q}, t), \quad (6.82a)$$

$$\mathbf{j}_{\mathbf{q}}(t) = \int d^d r e^{-i\mathbf{q} \cdot \mathbf{r}} \mathbf{j}(\mathbf{r}, t) = \int \frac{d^d p}{(2\pi)^d} \frac{\mathbf{p}}{m} \rho(\mathbf{p}, \mathbf{q}, t). \quad (6.82b)$$

The current vanishes by parity for isotropic distributions $\rho(p, \mathbf{q}, t)$.

Momentum Isotropisation

What kind of dynamics does the master equation describe? A first, simple answer is possible by considering the limit $\mathbf{q} = 0$ that describes spatially averaged quantities. The definitions (6.72), (6.76) and (6.77) imply $\Gamma_{\mathbf{p}\mathbf{p}'}(0) = 2\pi\delta(\varepsilon_p - \varepsilon_{p'})$, which assures the conservation of energy during elastic scattering. Since the isotropic energy ε_p fixes the modulus of $\mathbf{p}' = p\hat{\mathbf{n}}'$, the angular probability distribution $\rho(p\hat{\mathbf{n}}, 0, t) =: f_\varepsilon(\hat{\mathbf{n}}, t)$ at fixed energy satisfies

$$\partial_t f_\varepsilon(\hat{\mathbf{n}}, t) = 2\pi n \int \frac{d^d p'}{(2\pi)^d} \delta(\varepsilon - \varepsilon_{p'}) |v_{\mathbf{p}-\mathbf{p}'}|^2 [f_\varepsilon(\hat{\mathbf{n}}', t) - f_\varepsilon(\hat{\mathbf{n}}, t)]. \quad (6.83)$$

For an isotropic point-scatterer potential $v(\mathbf{r}) = v_0\delta(\mathbf{r})$ that has no dependence on momentum, the equation of motion takes the simple form

$$\partial_t f_\varepsilon(\hat{\mathbf{n}}, t) = -\gamma_{\text{el}}(\varepsilon) [f_\varepsilon(\hat{\mathbf{n}}, t) - \langle f_\varepsilon(t) \rangle], \quad (6.84)$$

where $\langle f_\varepsilon(t) \rangle := \int d\Omega'_d f_\varepsilon(\hat{\mathbf{n}}', t)$ is the angular average of the distribution, properly normalised: $d\Omega'_d$ is $d\theta'/2\pi$ in $d = 2$ dimensions and $d\phi'd(\cos\theta')/4\pi$ in $d = 3$. The elastic scattering rate

$$\gamma_{\text{el}}(\varepsilon) = 2\pi\nu(\varepsilon)nv_0^2 \quad (6.85)$$

is defined in terms of the density of states $\nu(\varepsilon) = \int \frac{d^d p'}{(2\pi)^d} \delta(\varepsilon - \varepsilon_{p'})$ and can equally well be obtained by Fermi's golden rule. Clearly, equation (6.83) describes a simple exponential decay of the initial angular distribution $f_\varepsilon(\hat{\mathbf{n}}, t = 0)$ towards a completely isotropic distribution $\langle f_\varepsilon(t) \rangle$. Thus, our model of elastic momentum scattering by fixed impurities leaves the kinetic energy conserved, but describes the isotropisation of the momentum distribution with a rate γ_{el} .

By the same token, a global net current $\mathbf{j}_0(t)$ initially different from zero decreases to zero exponentially fast. In other words, an initial wave packet launched with a definite velocity loses the memory of its initial direction on a timescale $\tau_{\text{el}} = 1/\gamma_{\text{el}}$.

Boltzmann–Lorentz Equation

In order to know on what spatial scale the momentum isotropisation occurs and how the average position of the wave packet evolves in time, we have to consider the master equation (6.78) at finite \mathbf{q} . We expect diffusive behaviour to appear on large spatial scales and thus make a Taylor expansion around $\mathbf{q} = 0$. Retaining only lowest-order terms in $q/p \ll 1$ (which corresponds to spatial scales much larger than the particle's wavelength), the equation of motion becomes

$$\partial_t \rho(\mathbf{p}, \mathbf{q}, t) + i\frac{\mathbf{q} \cdot \mathbf{p}}{m} \rho(\mathbf{p}, \mathbf{q}, t) = \mathcal{C}[\rho(\mathbf{p}, \mathbf{q}, t)] \quad (6.86)$$

with the purely *elastic* collision integral

$$\mathcal{C}[\rho(\mathbf{p}, \mathbf{q}, t)] = 2\pi n \int \frac{d^d p'}{(2\pi)^d} \delta(\varepsilon - \varepsilon_{p'}) |v_{\mathbf{p}-\mathbf{p}'}|^2 [\rho(\mathbf{p}', \mathbf{q}, t) - \rho(\mathbf{p}, \mathbf{q}, t)]. \quad (6.87)$$

The only explicit occurrence of \mathbf{q} in (6.86) is now in the ballistic term on the left-hand side that originates from the free evolution with H_0 .

The parametrisation (6.75) has the additional advantage that the density matrix elements $\rho(\mathbf{p}, \mathbf{q}, t)$ are the spatial Fourier transform of the Wigner distribution [29]

$$\begin{aligned} W(\mathbf{p}, \mathbf{r}, t) &= \frac{1}{(2\pi\hbar)^d} \int d^d r' \langle \mathbf{r} - \frac{\mathbf{r}'}{2} | \rho(t) | \mathbf{r} + \frac{\mathbf{r}'}{2} \rangle e^{i\mathbf{p} \cdot \mathbf{r}' / \hbar} \\ &= \frac{1}{(2\pi\hbar)^d} \int \frac{d^d q}{(2\pi)^d} e^{i\mathbf{q} \cdot \mathbf{r}} \rho(\mathbf{p}, \mathbf{q}, t) \end{aligned} \quad (6.88)$$

that represents the quantum density operator in a classical phase space, see also Sect. 4.6. Here, we have momentarily restored \hbar 's visibility. With this standard normalisation, the probability density $n(\mathbf{r}) = \langle \mathbf{r} | \rho | \mathbf{r} \rangle$ with normalisation $\int d^d r n(\mathbf{r}) = 1$ is given as the marginal $n(\mathbf{r}) = \int d^d p W(\mathbf{p}, \mathbf{r})$. Conversely, $w(\mathbf{p}) = \int d^d r W(\mathbf{p}, \mathbf{r}) = (2\pi\hbar)^{-d} \rho(\mathbf{p}, 0)$ is the momentum distribution, and $\int d^d r d^d p W(\mathbf{p}, \mathbf{r}) = 1$.

A Fourier transform with respect to \mathbf{q} now yields the kinetic equation

$$\partial_t W(\mathbf{p}, \mathbf{r}, t) + \frac{1}{m} \mathbf{p} \cdot \nabla_{\mathbf{r}} W(\mathbf{p}, \mathbf{r}, t) = \mathcal{C}[W(\mathbf{p}, \mathbf{r}, t)] \quad (6.89)$$

with the same elastic scattering integral (6.87). Remarkably, we have obtained precisely the linear Boltzmann–Lorentz equation for the classical phase-space density $W(\mathbf{p}, \mathbf{r}, t)$ under elastic scattering from fixed impurities [30]. For photons, this equation is known as the radiative transfer equation. Ex post, we can therefore conclude that the Born approximation (6.65) was the crucial step that discarded quantum corrections to propagation amplitudes and left us with a classical phase-space distribution. This interpretation transpires

also by analysing Feynman diagrams in perturbation theory and path-integral approaches (see Chap. 4 of [26] for details).

The *weak disorder limit* in which the Born approximation and Boltzmann transport theory are expected to be valid corresponds to the regime where disorder corrections to the free energy of the particle are small, $\gamma_{\text{el}}(\varepsilon) \ll \varepsilon$. The scattering time defines a typical length scale, the elastic scattering mean free path $\ell_{\text{el}} = v_0 \tau_{\text{el}}$ or average distance between successive scattering events. The weak disorder limit can also be stated as $1/(k\ell_{\text{el}}) \ll 1$ which requires that successive scatterers are placed in the scattering far field: the average distance ℓ_{el} must be larger than the wavelength $\lambda = 2\pi/k$. This is a low-density argument because $\ell_{\text{el}} = 1/(n\sigma_{\text{el}})$ in terms of the density n of scatterers and their total elastic scattering cross section σ_{el} .

It is allowed to neglect the explicit \mathbf{q} -dependence inside the collision integral (6.87), which contributes already a factor γ_{el} , on hydrodynamic scales $q\ell_{\text{el}} \ll 1$. Consistently, it is precisely in the hydrodynamic regime that we wish to determine the diffusion constant. We have already derived the continuity equation (6.81). Making step (ii) of the general argument presented in Sect. 6.3.1, we now turn to the calculation of the diffusion coefficient in the linear response regime.

6.3.4 Linear Response and Diffusion Constant

Any phase-space distribution $W_{\text{eq}}(p)$ that is homogeneous, independent of time and rotation invariant, i.e., depends only on the modulus of \mathbf{p} , is a solution of the Boltzmann–Lorentz equation (6.89) since each term vanishes separately. The corresponding density matrix elements are of the form $\rho_{\text{eq}}(\mathbf{p}, \mathbf{q}, t) = (2\pi)^d \delta(\mathbf{q}) \rho_{\text{eq}}(p)$. This type of solution is called a *global equilibrium*. The underlying statistics could be a Fermi–Dirac or Bose distribution, or their classical limit, the Boltzmann distribution.

By creating a small gradient of concentration, one can then induce a linear-response current that is proportional to the driving gradient; the coefficient of proportionality is the diffusion constant. Kinetic theory permits to calculate linear response coefficients. We will follow the linearisation method developed by Chapman and Enskog [30] in order to derive the diffusion constant, but in terms of the density matrix components $\rho(\mathbf{p}, \mathbf{q}, t)$ instead of the space-dependent Wigner distribution because it will prove useful to work with Fourier-transformed quantities.

Linearisation à la Chapman–Enskog

Suppose that initially, the distribution function $\rho(p, \mathbf{q}, 0)$ is a *local equilibrium* solution (i.e., isotropic in momentum) established by local scattering on a rapid timescale $\tau_{\text{el}} = 1/\gamma_{\text{el}}$. However, we assume a non-delta-like dependence on \mathbf{q} , i.e., a finite gradient in real space. It is therefore no longer a global

equilibrium solution of the Boltzmann–Lorentz equation. The time τ_{eq} it takes to reach global equilibrium is much longer than the local scattering time such that we have a small parameter $\tau_{\text{el}}/\tau_{\text{eq}} \ll 1$ (sometimes called the “Knudsen number”). The linearisation method of Chapman and Enskog works by expanding the distribution function formally in powers of this small parameter,

$$\rho(\mathbf{p}, \mathbf{q}, t) = \rho_0(\mathbf{p}, \mathbf{q}, t) + \tau_{\text{el}} \rho_1(\mathbf{p}, \mathbf{q}, t) + O(\tau_{\text{el}}^2). \quad (6.90)$$

For the linear response calculation, these first two terms will suffice. The collision integral effectively multiplies the distribution by $\gamma_{\text{el}} = 1/\tau_{\text{el}}$ such that $\mathcal{C}[\tau_{\text{el}}^n \rho_n] = O(\tau_{\text{el}}^{n-1})$. Identifying equal orders on both sides of the kinetic equation, we find to order τ_{el}^{-1} :

$$0 = \mathcal{C}[\rho_0], \quad (6.91)$$

which is satisfied if $\rho_0(p, \mathbf{q}, t)$ is *locally* isotropic. By parity, the current density (6.82b) then is entirely generated by the correction,

$$\mathbf{j}_{\mathbf{q}}(t) = \int \frac{d^d p}{(2\pi)^d} \frac{\mathbf{p}}{m} \tau_{\text{el}}(\varepsilon_p) \rho_1(\mathbf{p}, \mathbf{r}, t). \quad (6.92)$$

The continuity equation (6.81) then implies that to lowest order, the local density remains time independent: $\partial_t \rho_0(p, \mathbf{q}, t) = 0$. To this order $\tau_{\text{el}}^0 = 1$, the kinetic equation reduces to

$$i \frac{\mathbf{q} \cdot \mathbf{p}}{m} \rho_0(p, \mathbf{q}) = \mathcal{C}[\tau_{\text{el}} \rho_1(\mathbf{p}, \mathbf{q})]. \quad (6.93)$$

In order to calculate the current (6.92), we need to solve this equation for ρ_1 as function of ρ_0 . We content ourselves with the simple case of an isotropic point-scattering potential $v_{\mathbf{p}} = v_0$ treated in Sect. 6.3.3 (other cases can be treated by an expansion in angular eigenfunctions, see [31] for the case of a potential with scattering anisotropy). Then, using the right-hand side of (6.84), we find

$$\mathcal{C}[\tau_{\text{el}} \rho_1] = -\rho_1(\mathbf{p}, \mathbf{q}) \quad (6.94)$$

plus an isotropic term $\langle \rho_1 \rangle$ that does not contribute to the current (6.92) anyway and can be dropped such that altogether, the distribution takes the stationary form

$$\rho_1(\mathbf{p}, \mathbf{q}) = -i \frac{\mathbf{q} \cdot \mathbf{p}}{m} \rho_0(p, \mathbf{q}). \quad (6.95)$$

Diffusion Coefficient

Inserting (6.95) into (6.92), the resulting current reads

$$\mathbf{j}_{\mathbf{q}} = -\frac{i}{m^2} \int \frac{d^d p}{(2\pi)^d} \mathbf{p}(\mathbf{q} \cdot \mathbf{p}) \tau_{\text{el}}(\varepsilon_p) \rho_0(p, \mathbf{q}). \quad (6.96)$$

By isotropy, $\int d^d p p_i p_j f(p) = (\delta_{ij}/d) \int d^d p p^2 f(p)$, and the current is collinear with \mathbf{q} . To lowest order in q we find

$$\mathbf{j}_{\mathbf{q}} = -i\mathbf{q}D_0 n_{\mathbf{q}}, \quad (6.97)$$

the Fourier-transformed version of the linear response relation $\mathbf{j} = -D_0 \nabla n$. Kinetic theory has allowed us to calculate the diffusion coefficient

$$D_0 = \frac{\bar{v}_0^2 \bar{\tau}}{d} \quad (6.98)$$

as the product of an effective velocity and scattering time averaged over the momentum distribution,

$$\bar{v}_0^2 \bar{\tau} = \frac{1}{m^2} \int \frac{d^d p}{(2\pi)^d} p^2 \tau_{\text{el}}(\varepsilon_p) \rho_0(p). \quad (6.99)$$

Often, the distribution $\rho_0(p)$ is a sharply peaked function around a certain momentum p_0 (for instance, the Fermi momentum p_F for electrons), whereas $p^2 \tau_{\text{el}}(\varepsilon_p)$, according to (6.85), varies smoothly with the density of states such that $\bar{v}_0^2 \bar{\tau} = p_0^2 \tau_{\text{el}}(\varepsilon_{p_0})/m^2$. In terms of the scattering mean-free path ℓ_{el} , the diffusion constant for isotropic point scatterers can also be written

$$D_0 = \frac{\bar{v}_0 \ell_{\text{el}}}{d}. \quad (6.100)$$

For anisotropic scattering, one has to replace the scattering mean-free path ℓ_{el} by the transport mean-free path ℓ_{tr} [31].

Diffusion

Inserting the linear response current (6.97) in the continuity equation leaves us with a simple differential equation $\partial_t n_{\mathbf{q}}(t) = -D_0 q^2 n_{\mathbf{q}}(t)$ that is immediately integrated to give an exponential decay

$$n_{\mathbf{q}}(t) = e^{-D_0 q^2 t} n_{\mathbf{q}}(0) \quad (6.101)$$

for the Fourier components of the initial density fluctuation. Long-range fluctuations ($q \rightarrow 0$) take a very long characteristic time $\tau_q = 1/(D_0 q^2) \rightarrow \infty$ to relax because of the constraint imposed by local conservation. This diagonal decomposition into Fourier modes with their continuous momentum index \mathbf{q} is the analogue of the spin relaxation (6.53), where the discrete index K separates high- K irreducible modes with rather large relaxation rates γ_K from the isotropic component $K = 0$ or trace that is conserved.⁵

⁵ This analogy becomes even clearer if positions in a finite volume are restricted to a lattice of L^d sites, because the irreducible representations of the discrete translation group (which under periodic boundary conditions is the d -fold direct product of the cyclic group \mathbb{Z}_L) are precisely labelled by the different allowed \mathbf{q} -vectors of the reciprocal lattice [27].

The expectation value of the average radius squared,

$$\overline{\langle r^2 \rangle}(t) = \text{tr}\{r^2 \bar{\rho}(t)\} = -\nabla_{\mathbf{q}}^2 n_{\mathbf{q}}(t)|_{\mathbf{q}=0}, \quad (6.102)$$

for the diffuse density (6.101) reads:

$$\overline{\langle r^2 \rangle}(t) = \langle r^2 \rangle_0 + 2dD_0 t. \quad (6.103)$$

As expected, the long-time behaviour of the particle's displacement is indeed governed by the Boltzmann diffusion constant (6.100).

6.4 Diffusive Spin Transport

Having described in Sect. 6.2 the relaxation of a single motionless spin in a fluctuating field, and in Sect. 6.3 the diffusion of spin-less massive particles, we now combine these two pictures and consider a spin on a massive carrier particle that moves and encounters impurities. The Hamiltonian is still of the form $H = H_0 + V$, where H_0 describes ballistic propagation in momentum and spin eigenstates $|\mathbf{p}\sigma\rangle := |\mathbf{p}\rangle \otimes |\sigma\rangle$ with spin-independent eigenenergies $\varepsilon_{\mathbf{p}} = p^2/2m$ (spin quantum numbers will from now be called σ in order to avoid confusion with the particle's mass). The impurity potential V could describe momentum scattering, spin-flip scattering, spin-orbit coupling, and the like, by randomly distributed scatterers.

In the following, we will consider in detail the case of freely orientable magnetic impurities that induce *spin-flips*. Other mechanisms such as spin-orbit scattering can be treated along the same lines. Actual laboratory realisations include electronic spin-flip scattering, quite relevant even for very low impurity concentrations, and the randomisation of photon polarisation under the influence of scattering by atoms with degenerate dipole transitions in cold atomic clouds.

6.4.1 Master Equation Approach to Diffusive Spin Transport

Deriving the Master Equation

In addition to the elastic momentum scattering potential (6.61) that for clarity we now call V_{el} , consider then a spin-flip interaction potential

$$V_{\text{sf}} = \sum_j v_{\text{sf}}(\hat{\mathbf{r}} - \mathbf{x}_j) \mathbf{S} \cdot \boldsymbol{\tau}_j \quad (6.104)$$

between the spin \mathbf{S} and a collection of freely orientable magnetic impurities modelled as spin $\frac{1}{2}$ with Pauli matrices $\boldsymbol{\tau}_j$ centred at sites \mathbf{x}_j . The magnitude of spin-spin coupling has been included in the short-ranged potential $v_{\text{sf}}(\mathbf{r})$

whose spatial dependence induces momentum scattering. The ensemble average now contains the usual average (6.62) over random sites as well as a trace $\text{tr}_{\{\tau\}}(\rho_{\{\tau\}})$ over impurity spins. We will assume that these impurities are distributed independently and isotropically, $\rho_{\{\tau\}} = \bigotimes_j \rho_j$ with $\rho_j = \frac{1}{2} \mathbb{1}_2$.

It is now a simple task to derive a spin-diffusion master equation for the density matrix $\rho(t)$ that operates on the combined Hilbert space $\mathcal{H} = \mathcal{H}_s \otimes \mathcal{H}_p$ of spin and momentum by retracing exactly the steps of Sect. 6.3.3 with the new potential $V = V_{\text{el}} + V_{\text{sf}}$ instead of just V_{el} . Within the Born approximation second order in V , mixed terms $\overline{V_{\text{sf}} V_{\text{el}}} = \overline{V_{\text{sf}}} \overline{V_{\text{el}}}$ give no contribution (just as the product of averages before), and we can consider the impact of V_{sf} separately. A typical term arising in the new spin-flip part is the counterpart of (6.69), $\langle 1 | \overline{V_{\text{sf}} \rho(t) W_{\text{sf}}} | 4 \rangle$. Together with the momentum-scattering factors appearing already in (6.73), we find now an additional sum over spin indices that defines the action of a spin-flip superoperator

$$\begin{aligned} \langle \sigma_1 | \mathcal{V} \rho | \sigma_4 \rangle &= \sum_{\sigma_2, \sigma_3} \overline{\langle \sigma_1 | \mathbf{S} \cdot \boldsymbol{\tau} | \sigma_2 \rangle \langle \sigma_3 | \mathbf{S} \cdot \boldsymbol{\tau} | \sigma_4 \rangle \langle \sigma_2 | \rho | \sigma_3 \rangle} \\ &= \sum_{\sigma_2, \sigma_3} \mathbf{S}_{\sigma_1 \sigma_2} \cdot \mathbf{S}_{\sigma_3 \sigma_4} \langle \sigma_2 | \rho | \sigma_3 \rangle, \end{aligned} \quad (6.105)$$

where the isotropic average over the impurity spin leads to the scalar contraction $\frac{1}{2} \text{tr}_{\tau} \{ \tau_i \tau_j \} = \delta_{ij}$ (cf. Exercise 1).

Collecting all terms then gives the master equation that describes elastic and spin-flip scattering in the small- \mathbf{q} limit:

$$\partial_t \rho(\mathbf{p}, \mathbf{q}, t) + i \frac{\mathbf{q} \cdot \mathbf{p}}{m} \rho(\mathbf{p}, \mathbf{q}, t) = \mathcal{C}[\rho] + \mathcal{L}[\rho]. \quad (6.106)$$

Here, the elastic collision integral

$$\mathcal{C}[\rho] = \frac{\gamma}{\nu(\varepsilon)} \int \frac{d^d p'}{(2\pi)^d} \delta(\varepsilon - \varepsilon_{p'}) [\rho(\mathbf{p}', \mathbf{q}, t) - \rho(\mathbf{p}, \mathbf{q}, t)] \quad (6.107)$$

describes momentum isotropisation with a total scattering rate

$$\gamma = \gamma_{\text{el}} + \gamma_{\text{sf}} \quad (6.108)$$

that includes the spin-flip contribution $\gamma_{\text{sf}} = s(s+1)2\pi\nu(\varepsilon)v_{\text{sf}}^2 n_{\text{sf}}$. Summing the rates, a prescription known as ‘‘Mathiessen’s rule’’ [32], is permitted if the scattering mechanisms do not interfere with each other, which is the case in the low-density Born approximation considered here. Note that the collision integral (6.107) acts solely on the momentum degrees of freedom, but is the identity in spin space. Genuine spin-flips are generated by

$$\mathcal{L}[\rho] = \frac{1}{\nu(\varepsilon)} \int \frac{d^d p'}{(2\pi)^d} \delta(\varepsilon - \varepsilon_{p'}) \overline{\mathcal{L}} \rho(\mathbf{p}', \mathbf{q}, t), \quad (6.109)$$

where $\overline{\mathcal{L}} = \gamma_{\text{sf}} \hat{\mathcal{L}}$ is precisely the spin relaxation Lindbladian (6.24) derived in Sect. 6.2.2, now with the spin-flip relaxation rate γ_{sf} .

Diffusive Spin Relaxation

Solving the spin-flip master equation (6.106) in the linear response regime is now exceedingly simple by projecting it onto irreducible spin components $\rho^{(K)} = \sum_Q \rho_{KQ} T_Q^K$ since the spin relaxation Lindbladian is diagonal in that basis, $\overline{\mathcal{L}} \rho^{(K)} = \lambda_K \rho^{(K)}$, with eigenvalues λ_K given by (6.46).

Summing the master equation for the K th spin sector over \mathbf{p} gives the continuity equation

$$\partial_t n_{\mathbf{q}}^{(K)}(t) + i \mathbf{q} \cdot \mathbf{j}_{\mathbf{q}}^{(K)}(t) = -\gamma_K n_{\mathbf{q}}^{(K)}(t) \quad (6.110)$$

for the density $n_{\mathbf{q}}^{(K)} = \int \frac{d^d p}{(2\pi)^d} \rho^{(K)}(\mathbf{p}, \mathbf{q})$ and associated current density $\mathbf{j}_{\mathbf{q}}^{(K)}$. The spin-flip Lindbladian is responsible for the appearance of a source term on the right-hand side, or rather a sink with spin relaxation rate

$$\gamma_K = |\lambda_K| = \gamma_{\text{sf}} \frac{K(K+1)}{2s(s+1)}. \quad (6.111)$$

In the limit $\mathbf{q} \rightarrow 0$, we recover exactly the global spin relaxation (6.48) of Sect. 6.2.3. In particular, the total trace is conserved since the spin trace is the $K=0$ sector with vanishing eigenvalue $\lambda_0 = 0$.

In the linear response regime, the Chapman–Enskog method of Sect. 6.3.4 carries through in each spin sector K . A difference occurs for the time derivative of the locally isotropic component $\rho_0^{(K)}(p, \mathbf{q}, t)$. The master equation (6.106) implies

$$\partial_t \rho_0^{(K)}(p, \mathbf{q}, t) = -\gamma_K \rho_0^{(K)}(p, \mathbf{q}, t), \quad (6.112)$$

which is solved by $\rho_0^{(K)}(p, \mathbf{q}, t) = e^{-\gamma_K t} \rho_0^{(K)}(p, \mathbf{q}, 0)$ instead of just being constant as in Sect. 6.3.4. Finally, the spin-sector density components show diffusive as well as spin-relaxation dynamics

$$n_{\mathbf{q}}^{(K)}(t) = e^{-D_0 q^2 t} e^{-\gamma_K t} n_{\mathbf{q}}^{(K)}(0), \quad (6.113)$$

where the Boltzmann diffusion constant D_0 is evaluated with the total momentum relaxation time $\tau = 1/\gamma$ from (6.108).

Now we can answer the question that was the starting point of the lecture (cf. Fig. 6.1): Imagine that we can inject spin-polarised particles $|\uparrow\rangle := |s, \sigma = +s\rangle$ with probability $p_{\uparrow}(0) = \langle \uparrow | \rho_0 | \uparrow \rangle = 1$ on one end of a diffusive medium of length L . What is the probability $p_{\uparrow}(L)$ of retaining the spin polarisation at the other end, assuming that we have spin-sensitive detection?

By taking the matrix elements $\langle \uparrow | \rho^{(K)}(t) | \uparrow \rangle$ of each irreducible spin component, we find that the probability relaxes during the transmission time $t = L^2/2D_0$ as

$$\begin{aligned} p_{\uparrow}(t) &= \frac{1}{2s+1} + \frac{3s^2}{s(s+1)(2s+1)} e^{-t/\tau_1} + \dots \\ &= \frac{1}{2} (1 + e^{-t/\tau_1}) \end{aligned} \quad (6.114)$$

with the last line valid for electrons for which $1/\tau_1 = 4\gamma_{sf}/3$. Equivalently, the *degree of spin polarisation*

$$\pi(t) = \frac{p_\uparrow(t) - p_\downarrow(t)}{p_\uparrow(t) + p_\downarrow(t)} = e^{-t/\tau_1} \quad (6.115)$$

simply relaxes from unity to zero. Naturally, for long enough times, the distribution relaxes towards its equilibrium value $p_{eq} = \frac{1}{2s+1}$ to have any magnetic quantum number $\sigma = -s, \dots, s$.

In terms of length scales, the spin relaxation time permits to define the spin relaxation length $\lambda_{sf} = \sqrt{2D_0\tau_{sf}}$. In solid-state devices, the density of magnetic impurities can be controlled such that $\gamma_{sf} \ll \gamma_{el}$ which means that spin coherence can be maintained quite efficiently, even on scales $L \gg \ell_{el}$ where the momentum dynamics is no longer ballistic, but already diffusive.

6.4.2 Quantum Corrections

In the Boltzmann transport theory developed in Sect. 6.3, one propagates effectively classical probabilities. However, in an environment that preserves the phase coherence of the wave, one must propagate probability *amplitudes* that, by the superposition principle, allow for interference phenomena. Elastic impurity scattering does preserve the phase coherence of the propagating wave which means that we have to expect quantum corrections to the Boltzmann transport theory whenever external phase-breaking mechanism are so rare that the corresponding dephasing time τ_ϕ is much longer than the elastic scattering time τ_{el} .

Weak Localisation

A prominent example for such a quantum correction is weak localisation (WL): the resistance of weakly disordered metallic samples shows a negative magnetoresistance $\partial\rho/\partial B > 0$ at small fields if spin-orbit scattering is absent [33, 34]. This contradicts the classical Boltzmann–Drude picture that predicts that the resistance should increase with a magnetic field. The reason can be understood by considering the quantum return probability to a point which includes the constructive interference of counter-propagating amplitudes and is therefore larger than the classical probability, see Fig. 6.3. The interference effect is masked by a large enough magnetic field since loops of different sizes pick up different Aharonov–Bohm phases.

Without any dephasing mechanism nor an external magnetic field, the interference correction $D = D_0 + \Delta D$ to the classical diffusion constant D_0 is given by summing the contributions of all closed diffusive paths,

$$\frac{\Delta D}{D_0} = -\frac{1}{\pi\hbar\nu(\epsilon)} \int \frac{d^d q}{(2\pi)^d} \int_0^\infty dt e^{-D_0 q^2 t} \propto \int \frac{d^d q}{(2\pi)^d} \frac{1}{D_0 q^2}. \quad (6.116)$$

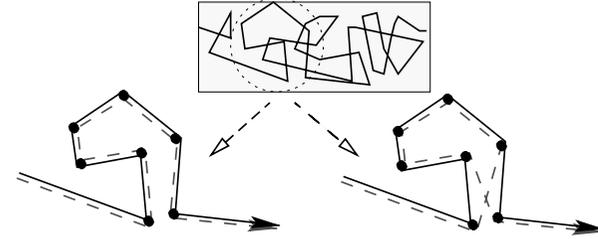


Fig. 6.3. Diffusive path (*above*) with the classical Boltzmann contribution of co-propagating amplitudes (*left*) and the corresponding counter-propagating amplitudes (*right*) that lead to weak localisation corrections

In low dimensions $d = 1, 2$, this q -integral diverges for small q which indicates that WL corrections become very important whenever the interfering amplitudes can explore large length scales. The formal divergence is cured by a cutoff that can be either the system size itself or a finite phase-coherence length $L_\phi = \sqrt{D_0\tau_\phi}$ due to dephasing mechanisms on a timescale τ_ϕ .⁶

Dephasing of Weak Localisation by Spin-Flip Scattering

Including spin-flip scattering into the weak-localisation picture can be done by diagonalising the spin-flip vertex appropriately [23]. The irreducible subspaces turn out to be the usual singlet and triplet state subspaces spanned by the Hilbert-space vectors $|KQ\rangle$.⁷ To sketch the result, the WL correction is written

$$\frac{\Delta D}{D_0} = -\frac{1}{\pi\hbar\nu(\epsilon)} \int \frac{d^d q}{(2\pi)^d} \sum_{K=0}^{2s} \frac{w_K}{D_0 q^2 + \tau_c(K)^{-1}}, \quad (6.117)$$

where each spin channel comes with a weight $w_K = (-)^{2s+K}(2K+1)/(2s+1)$. For electrons, $w_0 = -\frac{1}{2}$ and $w_1 = \frac{3}{2}$. More importantly, each spin channel is damped with its coherence time $\tau_c(K)$. They are given in terms of the spin relaxation rates (6.46) by a recoupling relation that reduces to

$$\frac{1}{\tau_c(K)} = \frac{2}{\tau_{sf}} + \lambda_K = \frac{2}{\tau_{sf}} \left(1 - \frac{K(K+1)}{4s(s+1)} \right) \quad (6.118)$$

such that for electrons $\tau_c(0) = \tau_{sf}/2$ and $\tau_c(1) = 3\tau_{sf}/2$.

⁶ The ultraviolet divergence for large q is cut off by the shortest scale of scattering, ℓ_{el} , and irrelevant for the present considerations.

⁷ Not operators $|KQ\rangle$ in Liouville space as for the propagated intensity: the difference is due to the fact that the two amplitudes in weak localisation loops propagate in opposite directions such that two states have to be recoupled instead of a state and its complex conjugate.

Clearly, the interference in all spin channels is dephased rather efficiently with a rate given essentially by the spin-flip rate, the numerical prefactor being entirely fixed by geometry. This effect is visible even in quite pure samples as admirably shown by F. Pierre and coworkers [35], see Fig. 6.4. The complete theory needed for linking the experimental data to impurity concentrations requires to take into account the interaction between electronic excitations near the magnetic impurity (Kondo physics) as well as the temperature-dependent dynamics of impurity spins (Korringa physics) that have both been neglected within the present lecture; for details, see [35].

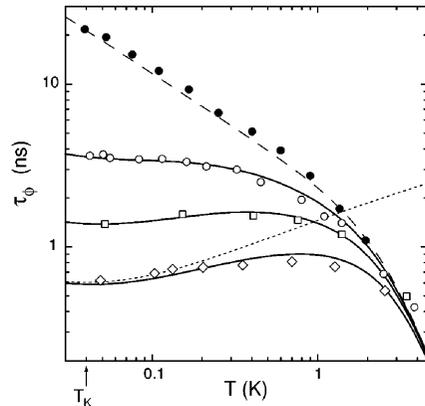


FIG. 5. Phase coherence time as function of temperature in several silver wires. Sample Ag(6N)c (●) is made of the purest silver source. Samples Ag(5N)b (○), Ag(5N) $c_{Mn0.3}$ (□), and Ag(5N) d_{Mn1} (◇) were evaporated simultaneously using our 5N silver source. Afterward, 0.3 ppm and 1 ppm of manganese were added by ion implantation respectively in samples Ag(5N) $c_{Mn0.3}$ and Ag(5N) d_{Mn1} . The presence of very dilute manganese atoms, a magnetic impurity of Kondo temperature $T_K=40$ mK, reduces τ_ϕ leading to an apparent “saturation” at low temperature. Continuous lines are fits of $\tau_\phi(T)$ taking into account the contributions of electron–electron and electron–phonon interactions (dashed line) and spin–flip collisions using the concentration c_{mag} of magnetic impurity as a fit parameter (dotted line is τ_{sf} for $c_{mag}=1$ ppm). Best fits are obtained using $c_{mag}=0.13$, 0.39, and 0.96 ppm, respectively, for samples Ag(5N)b, Ag(5N) $c_{Mn0.3}$, and Ag(5N) d_{Mn1} , in close agreement with the concentrations implanted and consistent with the source material purity used.

Fig. 6.4. This “set of experiments suggests that the frequently observed ‘saturation’ of τ_ϕ in weakly disordered metallic thin films can be attributed to spin-flip scattering from extremely dilute magnetic impurities, at a level undetectable by other means”; reprinted with permission from F. Pierre et al. [35]. Copyright (2003) by the American Physical Society

Multiple coherent scattering of photons in clouds of laser-cooled atoms is also subject to spin-flip physics: the so-called coherent backscattering effect (an interference enhancement of backscattered intensity) is severely reduced when photons are scattered by dipole transitions with a Zeeman degeneracy [36]. The analytical theory for multiple coherent scattering of polarised photons by degenerate dipole transitions employs the concepts of irreducible decompositions exposed in Sect. 6.2. Compared to electrons, the theory appears much simpler because at low light intensity, photons do not interact. However, the treatment of photon propagation is more involved because the field transversality adds another source of polarisation relaxation that needs to be taken into account [37].

Thus, magnetic impurities are a very efficient source of dephasing for interference of spin-carrying particles: the large ground-state degeneracy implied by the random orientations of freely orientable impurity spins permits dephasing even at zero temperature – when other decoherence processes like electron–phonon or electron–electron scattering are suppressed – because no energy exchange is involved and stocking which-path information comes for free. In return, whenever the impurity degrees of freedom can be constrained by other means, then perfect coherence is restored. This has been shown in Aharonov–Bohm interference experiments with electronic samples subject to a strong external magnetic field that aligns the impurity spins [38, 39]. Similarly, in atomic clouds, an external magnetic field that lifts the internal atomic Zeeman degeneracy can be used to enhance the effective phase coherence length of diffusing photons [40].

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