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Mesoscopic scattering of spin *s* particles

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Abstract

Quantum effects in weakly disordered systems are governed by the properties of the elementary interaction between propagating particles and impurities. Long-range mesoscopic effects due to multiple scattering are derived by iterating the single scattering vertex, which has to be appropriately diagonalized. In the present paper, we present a systematic and detailed diagonalization of the diffuson and cooperon vertices responsible for weak localization effects. We obtain general expressions for eigenvalues and projectors onto eigenmodes, for any spin and arbitrary elementary interaction with impurities. This description provides a common frame for a unified theory of mesoscopic spin physics for electrons, photons and other quantum particles. We treat in detail the case of spin-flip scattering of electrons by freely orientable magnetic impurities and briefly review the case of photon scattering from degenerate dipole transitions in cold atomic gases.

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1. Introduction

The physics of multiple scattering is governed by the iteration of elementary scattering events. The description of mesoscopic effects, due to phase-coherent multiple scattering of waves, therefore requires the elementary interaction to be in a form which is suitable for the iteration. The scattered particles in question may be electrons, photons, neutrons or cold atoms; the scatterers may be point-like impurities, spin-flip impurities interacting with the electron spin via an exchange interaction, spin–orbit impurities, atoms interacting with the photons via the dipolar interaction or classical dielectric light scatterers [1], to name a few.

On a classical level, multiple scattering is described by a Boltzmann-type transport equation, which in a microscopic description is generated by considering pairs of complex conjugate amplitudes co-propagating along the same scattering path. In a diagrammatic

representation, these amplitudes are depicted by the so-called ladder diagrams. The sum of these ladder diagrams constitutes the 'diffuson' which, in the long-distance limit, describes a diffusion process. Weak localization corrections to classical diffusive transport are described by the 'cooperon', the sum of so-called maximally crossed diagrams made of amplitudes that are counter-propagating along the same scattering path. If the wave scatters off structureless point scatterers, the maximally crossed diagrams can be disentangled by returning one amplitude and thus transform into a sum of ladder diagrams. Then, reciprocity [2] assures that the quantum correction due to this interference is maximal.

In the presence of scatterers with internal degrees of freedom, multiple scattering contains richer physics, since these internal degrees of freedom couple to the degrees of freedom of the propagating wave. The two subsystems, propagating wave and impurities, become entangled, and discarding all which-path information by tracing out the unobservable impurity degrees of freedom leads to an effective dephasing of coherent effects for the observed wave. In mesoscopic electronic samples, for example, the spin of a propagating electron couples to the spin of magnetic impurities, and in light-scattering atomic clouds the polarization of propagating photons interacts with the internal atomic angular momentum. In these cases, the elementary scattering vertex in the diffuson series is a tensor with 4 spin indices, connecting two incident spin states to two scattered spin states. A successful derivation of multiple scattering properties then requires that this elementary vertex be iterated. This problem has been studied and solved in several specific cases. For instance, in the case of spin–orbit coupling and scattering by magnetic impurities, Hikami, Larkin and Nagaoka [3] showed that the cooperon can be diagonalized in the singlet and triplet subspaces. Similar methods were employed for calculating conductance fluctuations [4]. In the context of light scattering by thermal atomic gases, the iteration structure of the photonic diffuson was completely determined by Barrat, Omont and others [5–7]. For the study of phase-coherent effects in cold atomic gases, the cooperon for the atom–photon problem was calculated exactly by two of us [8]. Its diagonal properties were used to describe coherent backscattering by cold atomic gases and weak localization phase coherence times [9]. In all these cases, the iteration of the elementary vertex properties was done by hand, finding the appropriate diagonal tensors and associated eigenvalues rather heuristically.

In the present contribution, we provide a thorough understanding of the diffuson and cooperon vertex diagonalization, of the different projectors and eigenvalues involved, of their spin and coupling dependence as well as of their precise relationships. In the next section, we start by recalling the example of the spin-flip scattering of spin $\frac{1}{2}$ particles. In section 3, we present a general diagonalization scheme for arbitrary ladder and crossed vertices. We derive in detail the isotropic projectors onto invariant subspaces for scalar vertices. Once the algebraic structure has thus been laid, in section 4 we calculate the corresponding eigenvalues from the microscopic scattering potential. Finally, we conclude this paper by indicating some possible extensions of the work. The appendix contains a brief review of photon scattering properties in the light of the present work.

2. A heuristic diagonalization of the electronic spin-flip vertex

2.1. Diffuson and cooperon

Let us first consider multiple scattering of a quantum particle by randomly distributed impurities without internal structure [1]. The disorder-averaged probability of a wave packet emanating at point $\boldsymbol{r}$ and time $t = 0$ with density matrix $\rho_0(\boldsymbol{r})$ to be detected at point $\boldsymbol{r}'$ and time $t > 0$ is given by $P(\boldsymbol{r}, \boldsymbol{r}', t) = \langle\langle \boldsymbol{r}'|U(t)\rho(\boldsymbol{r})U^\dagger(t)|\boldsymbol{r}'\rangle\rangle_{\rm av}$ where $\langle\cdots\rangle_{\rm av}$

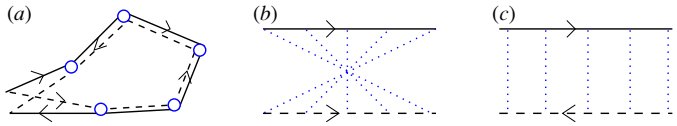


Figure 1. Three equivalent representations of the cooperon interference at five scatterers: (*a*) real-space representation of counter-propagating amplitudes; (*b*) momentum-space maximally crossed diagram with retarded propagator (upper full line) and advanced propagator (lower dashed line) connected by impurity scattering events (dotted lines) and (*c*) the same diagram with returned advanced propagator line exhibiting the ladder structure.

signifies a trace over the impurity configurations. For a quasimonochromatic wave packet of central energy ε and long evolution time, the Fourier transform of the detection probability is $P(\boldsymbol{r}, \boldsymbol{r}', \omega) = [2\pi\rho(\varepsilon)]^{-1}\langle G^{\mathrm{R}}(\boldsymbol{r}, \boldsymbol{r}', \varepsilon)G^{\mathrm{A}}(\boldsymbol{r}, \boldsymbol{r}', \varepsilon - \omega)\rangle_{\mathrm{av}}$ in terms of the retarded and advanced Green functions $G^{\mathrm{R,A}}(E)$ and the average density of states $\rho(\varepsilon)$.

This average probability satisfies an integral equation of the Bethe–Salpeter type generating a multiple scattering sequence. In weakly disordered samples, the interference of amplitudes propagating along different scattering paths will be washed out by the disorder average. Therefore, the dominant contribution will come from co-propagating amplitudes along identical scattering paths, thus discarding interference effects and recovering a classical propagation picture. This propagation is described by the so-called diffuson, the propagation kernel of the multiple scattering sequences defined in operator form by $D = L + L\mathsf{G}D$ where L describes the elementary scattering by a single impurity and the four-point operator $\mathsf{G} = \langle G^{\mathrm{A}}\rangle_{\mathrm{av}}\langle G^{\mathrm{R}}\rangle_{\mathrm{av}}$ is the intensity propagator (of Boltzmann–Drude type with factorized averages) between scattering events. In diagrammatic representations, this series has a ladder structure and can formally be summed as a geometric series, $D = L/(1 - \mathsf{G}L)$. Going to the diffusion approximation (Kubo limit of large distances and long times) permits one to derive the effective diffusion constant of this classical diffusion process as a function of the microscopic parameters, in a spirit similar to the kinetic equation in the Boltzmann–Lorentz model of classical particles colliding with fixed impurities. In the case of electrons, the Einstein relation between the diffusion constant and the conductivity then allows one to recover the classical Drude conductivity.

Quantum corrections generated by the interference of amplitudes propagating along different scattering paths can be incorporated by considering more general scattering processes. A particular interference that survives the disorder average is the weak localization correction of the classical diffusion constant due to amplitudes counter-propagating along identical scattering paths [10], depicted in figure 1(*a*). In a diagrammatic representation, this interference is given by maximally crossed diagrams (figure 1(*b*)) that can be unfolded to a ladder structure (figure 1(*c*)) and summed to $C = X/(1 - \mathsf{G}X)$ where X is the single scattering vertex for the returned advanced amplitude line. For simple impurities without internal structure, one has $X = L$. Weak localization then enhances the classical return probability of a particle by a factor of 2 and reduces the diffusion constant. Experimentally, this effect can be measured for instance in the electronic negative magnetoresistance where an external magnetic field suppresses the weak localization corrections and thus leads to a larger conductance. In optics, the interferential enhancement of backscattered intensity is called coherent backscattering and has been observed in a large variety of samples. The case of impurities with internal structure acting on the spin degrees of freedom of the propagating particle is more involved as should become apparent in the following example of electronic spin-flip scattering.

2.2. Definition of the spin-flip vertex

We consider now a particle of spin $\boldsymbol{S}$ propagating in a disordered sample with spin $\boldsymbol{J}$ magnetic impurities. The particle spin states are written as eigenstates $|s\alpha\rangle$ of $\boldsymbol{S}^2$ and S^z. For electrons, $s = \frac{1}{2}$ and $\alpha = \pm\frac{1}{2}$. The spin operator then is $\boldsymbol{S} = \boldsymbol{\sigma}/2$ (in natural units $\hbar = 1$) where the components of $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ are the usual Pauli matrices. The interaction with a given magnetic impurity is described by the Hermitian operator $V_m = g\boldsymbol{J}\cdot\boldsymbol{S}$ with coupling strength g. The Born scattering amplitude for the spin-flip process $|s\alpha\rangle \mapsto |s\gamma\rangle$ is

$$\langle s\gamma|V_m|s\alpha\rangle = g\boldsymbol{J}\cdot\langle s\gamma|\boldsymbol{S}|s\alpha\rangle = g\boldsymbol{J}\cdot\boldsymbol{S}_{\gamma\alpha}. \tag{1}$$

The effective scattering intensity of this process is described by the four-point vertex (the overline indicates complex conjugation)

$$\mathcal{L}_{\alpha\beta,\gamma\delta} = \quad \alpha\,\gamma\ /\ \beta\,\delta \quad = \langle\langle s\gamma|V_m|s\alpha\rangle\overline{\langle s\delta|V_m|s\beta\rangle}\rangle_{\mathrm{av}} = \frac{|g|^2 J(J+1)}{3}\boldsymbol{S}_{\gamma\alpha}\cdot\boldsymbol{S}_{\beta\delta} \tag{2}$$

where $\langle\cdots\rangle_{\mathrm{av}}$ denotes a trace over the impurity configurations, here an isotropic average $\langle J_i J_j\rangle_{\mathrm{av}} = \delta_{ij}J(J+1)/3$ over all possible orientations of the freely orientable magnetic impurity. This average is the fundamental reason for the non-deterministic dephasing of the multiple scattering process. We choose to normalize the spin-flip scattering strength g such that the intensity vertex is written as

$$\mathcal{L}_{\alpha\beta,\gamma\delta} = \frac{\boldsymbol{S}_{\gamma\alpha}\cdot\boldsymbol{S}_{\beta\delta}}{s(s+1)}. \tag{3}$$

This normalization choice endows the vertex with the convenient trace-preserving property $\mathcal{L}_{\alpha\alpha,\gamma\delta} = \delta_{\gamma\delta}$; here as in the following, summation over repeated spin indices is understood.

Weak localization corrections to transport are embodied in the so-called cooperon and are generated by maximally crossed diagrams. These diagrams can be 'unfolded' to a ladder structure such that the intensity vertex (3) is replaced by the crossed vertex

$$X_{\alpha\beta,\gamma\delta} = \mathcal{L}_{\alpha\delta,\gamma\beta} = \quad \alpha\,\gamma\ \times\ \beta\,\delta \quad = \langle s\gamma s\delta|X|s\alpha s\beta\rangle = \frac{\boldsymbol{S}_{\gamma\alpha}\cdot\boldsymbol{S}_{\delta\beta}}{s(s+1)}. \tag{4}$$

For reasons that will become clear later, the crossed vertex X is denoted by a roman letter, whereas the vertex $\mathcal{L}$ is held in curly script.

2.3. Elementary diagonalization

The natural coupling scheme for the vertices (3) and (4) is the 'vertical' combination $(\alpha\gamma) \leftrightarrow (\beta\delta)$ between the elementary scattering amplitudes. However, in multiple scattering diagrams, the above intensity vertices have to be chained 'horizontally' in the direction $(\alpha\beta) \leftrightarrow (\gamma\delta)$ according to the following product rule of four-point vertices:

$$(\mathsf{G}\mathcal{L})_{\alpha\beta,\gamma\delta} = \mathcal{L}_{\alpha\beta,\mu\nu}\mathsf{G}_{\mu\nu,\gamma\delta}. \tag{5}$$

In the product definition, the order of operators is inverted since operators are conventionally applied to their arguments from the left, but their vertex symbols are usually added to a diagram on the right. The rank-four tensor $\mathsf{G}_{\alpha\beta,\gamma\delta} = \langle G^{\mathrm{R}}_{\alpha\gamma}\rangle_{\mathrm{av}}\langle G^{\mathrm{A}}_{\beta\delta}\rangle_{\mathrm{av}}$ describes the average propagation between scattering events. By virtue of rotational invariance, the average propagators $\langle G_{\alpha\gamma}\rangle_{\mathrm{av}} = \langle G\rangle_{\mathrm{av}}\delta_{\alpha\gamma}$ are proportional to the identity in spin space such that $\mathsf{G}_{\alpha\beta,\gamma\delta} = \langle G^{\mathrm{R}}\rangle_{\mathrm{av}}\langle G^{\mathrm{A}}\rangle_{\mathrm{av}}\delta_{\alpha\gamma}\delta_{\beta\delta}$ is proportional to the 'horizontal' identity. (Note that for photons, however, transversality implies that $\mathsf{G}_{\alpha\beta,\gamma\delta}$ is not proportional to the identity which leads to the more complicated scenario described in the appendix, featuring nonetheless the

general properties discussed in the present section.) But in order to calculate the summed diffuson $\mathcal{D} = \mathcal{L}/(\mathbb{1} - \mathsf{G}\mathcal{L})$ and the cooperon $C = X/(\mathbb{1} - \mathsf{G}X)$, the vertices $\mathcal{L}_{\alpha\beta,\gamma\delta}$ and $X_{\alpha\beta,\gamma\delta}$ have to be diagonalized with respect to the horizontal direction $(\alpha\beta) \leftrightarrow (\gamma\delta)$. For electrons with $s = \frac{1}{2}$, this amounts to diagonalizing 4×4 matrices [1]. It turns out that the diffuson and cooperon vertices can be cast in the form

$$\mathcal{L}_{\alpha\beta,\gamma\delta} = \lambda_0 \mathcal{T}^{(0)}_{\alpha\beta,\gamma\delta} + \lambda_1 \mathcal{T}^{(1)}_{\alpha\beta,\gamma\delta}, \tag{6}$$

$$X_{\alpha\beta,\gamma\delta} = \chi_0 T^{(0)}_{\alpha\beta,\gamma\delta} + \chi_1 T^{(1)}_{\alpha\beta,\gamma\delta}. \tag{7}$$

Here, the diffuson vertex tensors

$$\mathcal{T}^{(0)}_{\alpha\beta,\gamma\delta} = \tfrac{1}{2}\delta_{\beta\alpha}\delta_{\gamma\delta}, \tag{8}$$

$$\mathcal{T}^{(1)}_{\alpha\beta,\gamma\delta} = \tfrac{1}{2}\boldsymbol{\sigma}_{\beta\alpha} \cdot \boldsymbol{\sigma}_{\gamma\delta} = \delta_{\gamma\alpha}\delta_{\beta\delta} - \tfrac{1}{2}\delta_{\beta\alpha}\delta_{\gamma\delta} \tag{9}$$

are orthogonal projectors with respect to the horizontal product rule (5):

$$\mathcal{T}^{(K)}_{\alpha\beta,\mu\nu}\mathcal{T}^{(K')}_{\mu\nu,\gamma\delta} = \delta_{KK'}\mathcal{T}^{(K)}_{\alpha\beta,\gamma\delta}. \tag{10}$$

Likewise, the cooperon vertex tensors

$$T^{(0)}_{\alpha\beta,\gamma\delta} = \tfrac{1}{2}(\delta_{\gamma\alpha}\delta_{\delta\beta} - \delta_{\delta\alpha}\delta_{\gamma\beta}), \tag{11}$$

$$T^{(1)}_{\alpha\beta,\gamma\delta} = \tfrac{1}{2}(\delta_{\gamma\alpha}\delta_{\delta\beta} + \delta_{\delta\alpha}\delta_{\gamma\beta}) \tag{12}$$

are orthogonal projectors such that $T^{(K)}_{\alpha\beta,\mu\nu}T^{(K')}_{\mu\nu,\gamma\delta} = \delta_{KK'}T^{(K)}_{\alpha\beta,\gamma\delta}$. Both sets of projectors sum up to the identity $\delta_{\gamma\alpha}\delta_{\beta\delta}$ for the horizontal product rule (5). Obviously, the diffuson projectors (8) and (9) are different from the cooperon projectors (11) and (12). This is in sharp contrast to the case of photon scattering ($s = 1$) by atoms with degenerate dipole transitions, where the *same* set of orthogonal projectors can be used for both vertex types [8] (see the appendix for details).

In the diagonal decomposition (6), the eigenvalues of the diffuson vertex are found to be $\lambda_0 = 1$ (non-degenerate) and $\lambda_1 = -\frac{1}{3}$ (three-fold degenerate). The eigenvalues of the normalized crossed vertex are $\chi_0 = -1$ (non-degenerate) and $\chi_1 = \frac{1}{3}$ (three-fold degenerate). It has been noted that the cooperon spin vertex eigenvalues χ_K correspond to the singlet channel $K = 0$ and the triplet channel $K = 1$, respectively, which accounts for the degeneracies [3]. Remarkably, the eigenvalues λ_K and χ_K are equal in magnitude but opposite in sign, which is not properly explained on this level of heuristic diagonalization.

Prompted by these observations, we wish to answer the following questions:

(i) Given diffuson and cooperon vertices for arbitrary spin s, which are the orthogonal projectors that assure a least redundant diagonalization?
(ii) How do the diffuson and cooperon eigenvalues depend on the microscopic spin scattering mechanism?

2.4. First answers

2.4.1. General idea. In essence, the intensity vertices map two incident spins s onto two final spins. Furthermore, they are scalar objects since they are obtained by an isotropic average over microscopic degrees of freedom. The invariance under rotations is then responsible for the eigenvalue degeneracies. The key idea is to decompose the argument and image spaces into

irreducible subspaces with respect to the rotation group. The relevant subspaces are labelled by the effective recoupled spin $K = 0, \ldots, 2s$. A generic scalar vertex A can only connect irreducible subspaces with equal K, and its eigenvalues are degenerate in each subspace. In the appropriate recoupled basis, a scalar vertex takes the diagonal form

$$A = \begin{pmatrix} a_0 \mathbb{1}_0 & 0 & \ldots & 0 \\ 0 & a_1 \mathbb{1}_1 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & a_{2s} \mathbb{1}_{2s} \end{pmatrix} = \sum_{K=0}^{2s} a_K T^{(K)}. \tag{13}$$

The projectors $T^{(K)}$ are simply projectors onto the irreducible subspaces. Therefore, rotational symmetry alone dictates that there are at most $(2s+1)$ different eigenvalues, each $(2K+1)$-fold degenerate. This decomposition is optimal if the scalarity is the only information available and holds for arbitrary spin.

2.4.2. Recoupling schemes. Clearly, the natural coupling between spin indices in the ladder and crossed vertices (2) and (4) is the 'vertical' coupling scheme $(\alpha\gamma) \leftrightarrow (\beta\delta)$ that is inherited from the scattering amplitude (1). Unfortunately, this coupling is not suited for an iteration with the product (5). For the diagonalization, we therefore have to recouple the spin indices into the 'horizontal' coupling scheme $(\alpha\beta) \leftrightarrow (\gamma\delta)$ for the ladder vertex, and the 'diagonal' coupling scheme $(\alpha\delta) \leftrightarrow (\beta\delta)$ for the crossed vertex. Consequently, all vertex eigenvalues we derive will feature $6j$-symbols that describe the recoupling of 4 spins in angular momentum theory.

By exchanging the indices $\delta \leftrightarrow \beta$ in the crossed vertex, we are actually able to recover formally the ladder structure, but there is a price to be paid. Taking seriously the disposition of kets and bras, we see that the two vertices have different rotational structure: the crossed vertex defines a linear mapping between product states

$$X: \quad |s\alpha\rangle|s\beta\rangle \mapsto |s\gamma\rangle|s\delta\rangle,$$

whereas the diffuson vertex is a mapping not between states, but between operators:

$$\mathcal{L}: \quad |s\alpha\rangle\langle s\beta| \mapsto |s\gamma\rangle\langle s\delta|.$$

This difference, due to the exchange $\langle s\beta| \leftrightarrow |s\delta\rangle$ and subsequent relabelling $\beta \leftrightarrow \delta$ in the unfolding procedure of the crossed to the ladder series, leads eventually to two distinct sets of projectors. We will therefore diagonalize the diffuson vertex as a *superoperator*, but treat the cooperon vertex as an ordinary operator.

2.4.3. Projectors. In section 3, we will explicitly construct the diffuson projectors onto irreducible subspaces. For spin $\frac{1}{2}$, this reduces indeed to the electronic projectors (8) and (9). The cooperon vertex projectors (11) and (12) will be shown to be given by

$$T^{(0)}_{\alpha\beta,\gamma\delta} = -\tfrac{1}{2}\mathcal{T}^{(0)}_{\alpha\delta,\gamma\beta} + \tfrac{1}{2}\mathcal{T}^{(1)}_{\alpha\delta,\gamma\beta}, \tag{14}$$

$$T^{(1)}_{\alpha\beta,\gamma\delta} = \tfrac{3}{2}\mathcal{T}^{(0)}_{\alpha\delta,\gamma\beta} + \tfrac{1}{2}\mathcal{T}^{(1)}_{\alpha\delta,\gamma\beta}. \tag{15}$$

This is in fact the spin $\frac{1}{2}$ version of the more general relation

$$T^{(K)}_{\alpha\beta,\gamma\delta} = \sum_{K'} R_s(K, K')\mathcal{T}^{(K')}_{\alpha\delta,\gamma\beta} \tag{16}$$

between the cooperon and diffuson projectors, valid for arbitrary spin, to be derived in section 3.6. Here, our notation

$$R_s(K, K') = (2K+1) \begin{Bmatrix} s & s & K \\ s & s & K' \end{Bmatrix} \tag{17}$$

is a $6j$-symbol from standard angular momentum theory [11, 12]. Thanks to the $6j$-symbol orthogonality [12, (35c)][5]

$$\sum_{K'} R_s(K, K') R_s(K', K'') = \delta_{K,K''}, \tag{18}$$

the inverse relation to (16) is equally simple:

$$\mathcal{T}^{(K)}_{\alpha\beta,\gamma\delta} = \sum_{K'} R_s(K, K') T^{(K')}_{\alpha\delta,\gamma\beta}. \tag{19}$$

2.4.4. Eigenvalues. We will show in section 4 that the eigenvalues of the normalized spin-flip vertices (3) and (4) are given by

$$\lambda_K = 1 - \frac{K(K+1)}{2s(s+1)} = -\chi_K. \tag{20}$$

The eigenvalues for an arbitrary microscopic spin scattering potential will be derived below in full generality. In all cases, the eigenvalues of a scalar scattering vertex are linked by the recoupling relations

$$\lambda_K = \sum_{K'} R_s(K', K) \chi_{K'}, \qquad \chi_K = \sum_{K''} R_s(K'', K) \lambda_{K''}. \tag{21}$$

These relations between eigenvalues take the form of a contravariant transformation of coordinates associated with the respective covariant transformation (16) and (19) of the projectors.

These results should motivate our readers to consider with interest the following, more involved derivations. In section 3, we lay the algebraic foundations of the decomposition by deriving the orthogonal projectors, before turning to the eigenvalues in section 4.

3. Diagonalization of intensity vertices

Let us now consider a general spin interaction defined by its matrix elements $\langle s\gamma|V|s\alpha\rangle$ for arbitrary spin s. The corresponding diffuson and cooperon vertices are given by

$$\mathcal{L}_{\alpha\beta,\gamma\delta} = \langle\langle s\gamma|V|s\alpha\rangle\langle s\beta|V^\dagger|s\delta\rangle\rangle_{\mathrm{av}}, \tag{22}$$

$$X_{\alpha\beta,\gamma\delta} = \mathcal{L}_{\alpha\delta,\gamma\beta} = \langle\langle s\gamma|V|s\alpha\rangle\langle s\delta|V^\dagger|s\beta\rangle\rangle_{\mathrm{av}}. \tag{23}$$

3.1. The diffuson vertex as a spin superoperator

Spin states $|s\alpha\rangle$ are vectors in the Hilbert space $H_s = \mathbb{C}^{d_s}$ with dimension $d_s = 2s+1$. The diffuson vertex $\mathcal{L}$ is a linear mapping $|s\alpha\rangle\langle s\gamma| \mapsto |s\delta\rangle\langle s\beta|$ between spin operators. Its argument space therefore is the space of linear operators acting on H_s, the so-called Liouville space $L(H_s)$ with dimension d_s^2 [13]. Any linear operator $A \in L(H_s)$ is simply a $d_s \times d_s$

[5] Instead of compiling a large appendix, we will refer to standard definitions and sum rules by citing the exact location in appendix C of Messiah's book, e.g., his equation (35a) by writing [12, (35a)].

matrix. The trace-preserving vertex $\mathcal{L}: L(H_s) \to L(H_s)$ then is a *superoperator* (thus the notation with a curly script), mapping a matrix A onto another matrix $A' = \mathcal{L}A$. Its action in the basis of spin projectors $\{|s\alpha\rangle\langle s\beta|\}$ reads $A'_{\gamma\delta} = \mathcal{L}_{\alpha\beta,\gamma\delta}A_{\alpha\beta}$ in terms of the matrix elements

$$\mathcal{L}_{\alpha\beta,\gamma\delta} = \mathrm{tr}\{(|s\delta\rangle\langle s\gamma|)\mathcal{L}(|s\alpha\rangle\langle s\beta|)\}. \tag{24}$$

Here, $\mathrm{tr}\{\cdot\} = \sum_\alpha \langle s\alpha|\cdot|s\alpha\rangle$ is the trace over H_s. In superoperator notation, the diffuson vertex reads

$$\mathcal{L} = \sum_{\alpha\beta\gamma\delta} (|s\gamma\rangle\langle s\delta|)\mathcal{L}_{\alpha\beta,\gamma\delta}\,\mathrm{tr}\,\{(|s\beta\rangle\langle s\alpha|)\cdot\}\,. \tag{25}$$

With this notation, the resemblance with the Liouvillian $\mathcal{L} = -\frac{\mathrm{i}}{\hbar}[H,\cdot]$, the generator of time evolution, becomes apparent. We define the trace of $\mathcal{L}$ as a linear operator in the Liouville space as

$$\mathrm{Tr}_\mathrm{L}\,\mathcal{L} = \sum_{\alpha,\beta} \mathcal{L}_{\alpha\beta,\alpha\beta}. \tag{26}$$

In the extensive literature on Liouville space formalism [14–17], one often views the spin operators as vectors in $L(H_s)$ and defines corresponding kets by $|s\beta\rangle\langle s\alpha| = |\alpha\beta\rangle\rangle$. Using this notation, the diffuson vertex matrix elements are given by $\mathcal{L}_{\alpha\beta,\gamma\delta} = \langle\langle\gamma\delta|\mathcal{L}|\alpha\beta\rangle\rangle$, and the superoperator takes the very simple form $\mathcal{L} = \sum_{\alpha\beta\gamma\delta}\mathcal{L}_{\alpha\beta,\gamma\delta}|\gamma\delta\rangle\rangle\langle\langle\alpha\beta|$. In this notation, the parallel with the cooperon vertex operator (see (44) below) is especially clear. However, we deliberately choose to use the superoperator formulation in the following because it allows us in section 3.3.2 to derive the ladder vertex projectors in terms of spin operators (which is needed to get expression (9)). Moreover, to answer completely question (i) raised in section 2.3, we have to explain the *difference* between the diffuson and cooperon eigenstructures rather than their similarity. This difference reflects the different behaviour under rotations of spin states $|s\alpha\rangle$ and their conjugates $\langle s\alpha|$ that are explicitly featured in the superoperator notation (25).

3.2. Decomposition into irreducible superoperators

An incident state $|s\alpha\rangle$ in scattering amplitudes like (1) is a spinor, i.e., a vector in H_s that transforms under the irreducible representation $D^{(s)}$ of the rotation group SU(2): $|s\alpha\rangle \mapsto U|s\alpha\rangle = \sum_\mu |s\mu\rangle\langle s\mu|U|s\alpha\rangle = \sum_\mu U_{\mu\alpha}|s\mu\rangle$ with an appropriate unitary and unimodular matrix $UU^\dagger = \mathbb{1}_{d_s}$, $\det U = +1$. A final state $\langle s\gamma|$, however, transforms contragradiently [18], i.e., under the complex conjugate representation $\overline{D^{(s)}}$, $\langle s\gamma| \mapsto \langle s\gamma|U^\dagger = \sum_\nu \overline{U}_{\nu\gamma}\langle s\nu|$. Under a rotation, the complete spin vertex is transformed as $\mathcal{L}_{\alpha\beta,\gamma\delta} \mapsto U_{\sigma\delta}(U^\dagger)_{\gamma\rho}\mathcal{L}_{\mu\nu,\rho\sigma}U_{\mu\alpha}(U^\dagger)_{\beta\nu}$. Clearly, this vertex is not a rank-four tensor (that would transform under the direct product $(\mathcal{D}^{(s)})^{\otimes 4}$), but rather a two-by-two mixed tensor that transforms under $(D^{(s)}\otimes\overline{D^{(s)}})^{\otimes 2}$. If the vertex is a scalar, it is invariant under this transformation.

In expressions (24) and (25), the operator arguments of $\mathcal{L}$ are decomposed over the decoupled product basis $\{|s\alpha\rangle\langle s\beta|\}$ of the Liouville space $L(H_s)$. But according to our diagonalization strategy, we want to use a basis adapted to irreducible representations of the rotation group. We first perform the Clebsch–Gordan (CG in short) decomposition of the argument and image representations $D^{(s)}\otimes\overline{D^{(s)}}$. These are then recoupled in turn to give the

complete CG-decomposition of $(D^{(s)} \otimes \overline{D^{(s)}})^{\otimes 2}$ which yields the irreducible components of the superoperator. The route thus taken may be traced in the following map:

$$\begin{array}{ccccc} (D^{(s)} \otimes \overline{D^{(s)}}) & & & & (D^{(s)} \otimes \overline{D^{(s)}}) \\ \searrow \quad \swarrow & & & & \searrow \quad \swarrow \\ D^{(K)} & & \otimes & & D^{(K')} \\ & \searrow & & \swarrow & \\ & & D^{(L)} & & \end{array} \quad . \tag{27}$$

Following standard procedures from angular momentum theory [18, 13], one can define a set of irreducible operators adapted to our purpose,

$$T_q^{(K)} = T_q^{(K)}(s, s) = \sum_{mm'} (-)^{s-m} \langle ssm' - m | Kq \rangle |sm'\rangle\langle sm| \tag{28}$$

with matrix elements

$$\langle sm'|T_q^{(K)}|sm\rangle = (-)^{s-m}\langle ssm' - m|Kq\rangle \tag{29}$$

where $\langle ssm' - m|Kq\rangle$ are the usual CG-coefficients. These types of tensors, called 'statistical tensors' or 'state multipoles' are irreducible components of the density matrix and have been developed by Fano and Racah in the 1950s [18]. Their construction is very similar to the coupling scheme of angular momentum eigenstates: one simply chooses a linear combination of spin projectors with suitable CG-coefficients. The definition (28) features a characteristic minus sign in front of the spin quantum number m that is reminiscent of the contragradient transformation of $\langle sm|$. Hermitian conjugation is defined by $T_q^{(K)\dagger} = (-)^q T_{-q}^{(K)}$.

The orthogonality of CG-coefficients assures that the operators (28) are orthonormalized with respect to the matrix scalar product $(A|B) = \mathrm{tr}\{A^\dagger B\}$,

$$\left(T_q^{(K)} \middle| T_{q'}^{(K')}\right) = \mathrm{tr}\left\{T_q^{(K)\dagger} T_{q'}^{(K')}\right\} = \delta_{KK'}\delta_{qq'}. \tag{30}$$

The set of irreducible tensor operators $T_q^{(K)}$ provides a natural basis that incorporates best the rotational symmetries. Any linear operator O can be developed in this basis according to $O = \sum_{Kq} O_{Kq} T_q^{(K)}$, with components

$$O_{Kq} = \left(T_q^{(K)} \middle| O\right) = \sum_{mm'} (-)^{s-m} \langle ssm' - m|Kq\rangle \langle sm'|O|sm\rangle. \tag{31}$$

Inserting $|sm'\rangle\langle sm| = \sum_{Kq} (-)^{s-m} \langle ssm' - m|Kq\rangle T_q^{(K)}$ in the vertex definition (25), the superoperator becomes

$$\mathcal{L} = \sum_{KqK'q'} T_{q'}^{(K')} \mathcal{L}_{q,K'q'}^{(K)} \left(T_q^{(K)} \middle| \cdot\right) \tag{32}$$

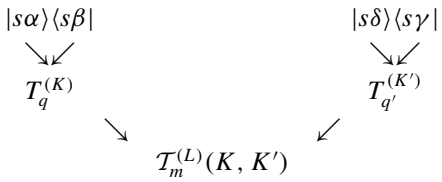
where its left–right irreducible components are $\mathcal{L}_{q,K'q'}^{(K)} = \left(T_{q'}^{(K')} \middle| \mathcal{L} T_q^{(K)}\right)$ or

$$\mathcal{L}_{q,K'q'}^{(K)} = \sum_{\alpha\beta\gamma\delta} (-)^{s-\beta} \langle ss\alpha - \beta|Kq\rangle \mathcal{L}_{\alpha\beta,\gamma\delta} (-)^{s-\delta} \langle ss\delta - \gamma|K' - q'\rangle. \tag{33}$$

Now we recouple the irreducible argument and image representations to get the complete CG-decomposition (last line in (27)). We define a basis of irreducible superoperators $\mathcal{T}_m^{(L)}(K, K')$ of rank L with components $m = -L, \ldots, L$:

$$\mathcal{T}_m^{(L)}(K, K') = \sum_{qq'} (-)^{K-q} \langle K'Kq' - q|Lm\rangle T_{q'}^{(K')} \left(T_q^{(K)} \middle| \cdot\right). \tag{34}$$

The recoupled objects can be precisely located on the decomposition map (27):



(35)

The vertex in irreducible superoperator notation is then

$$\mathcal{L} = \sum_{KK'} \sum_{Lm} \mathcal{L}_{Lm}(K, K') \mathcal{T}_m^{(L)}(K, K') \tag{36}$$

with components $\mathcal{L}_{Lm}(K, K') = \sum_{qq'} (-)^{K-q} \langle K' K q' - q | Lm \rangle \mathcal{L}^{(K)}_{q,K'q'}$.

3.3. Scalar diffuson vertex

The above basis set construction and decomposition into irreducible superoperators apply to arbitrary superoperators. This basis change is especially profitable when the diffuson vertex under consideration is a scalar with respect to rotations. In this case, its only non-vanishing irreducible component is $\mathcal{L}_{00}(K, K')$ for $L = 0, m = 0$. The usual selection rules of CG-coefficients then require in (36) that $K = K'$ and $q = q'$: scalar superoperators indeed connect irreducible subspaces $L(H_s)^{(K)}$ with equal rank K. Each of these subspaces has dimension $(2K + 1)$ and the total dimension is of course preserved, $\sum_{K=0}^{2s}(2K + 1) = d_s^2 = (2s + 1)^2$. As found heuristically in section 2.3, $\mathcal{L}$ then takes the form

$$\mathcal{L} = \sum_{K=0}^{2s} \mathcal{L}_{00}(K, K) \mathcal{T}_0^{(0)}(K, K) = \sum_{K=0}^{2s} \lambda_K \mathcal{T}^{(K)} \tag{37}$$

with $\lambda_K = \mathcal{L}_{00}(K, K)/\sqrt{2K + 1}$ and $\mathcal{T}^{(K)} = \sqrt{2K + 1}\, \mathcal{T}_0^{(0)}(K, K)$. The calculation of eigenvalues will be treated in detail in section 4. We now complete the algebraic characterization of the projectors.

3.3.1. Properties of the scalar projectors. The superoperators $\mathcal{T}^{(K)}$ which diagonalize a scalar vertex are projectors onto the Liouville subspaces $L(H_s)^{(K)}$ of irreducible operators of rank K:

$$\mathcal{T}^{(K)} = \sqrt{2K + 1}\, \mathcal{T}_0^{(0)}(K) = \sum_q T_q^{(K)} \big(T_q^{(K)} \big| \cdot \big) = \sum_q T_q^{(K)} \operatorname{tr} \big\{ T_q^{(K)\dagger} \cdot \big\}. \tag{38}$$

These operators are scalar objects themselves since $\sum_q T_q^{(K)} T_q^{(K)\dagger}$ generalizes the scalar product between vector operators ($K = 1$) to arbitrary rank K [12, (87)]. Thanks to the orthogonality (30) of the basis tensors, the $\mathcal{T}^{(K)}$'s are indeed orthogonal projectors,

$$\mathcal{T}^{(K)} \mathcal{T}^{(K')} = \sum_{qq'} T_q^{(K)} \underbrace{\big(T_q^{(K)} \big| T_{q'}^{(K')} \big)}_{\delta_{KK'}\delta_{qq'}} \big(T_{q'}^{(K')} \big| \cdot \big) = \delta_{KK'} \mathcal{T}^{(K)}. \tag{39}$$

Their matrix elements in the decoupled basis $\{|s\alpha\rangle\langle s\gamma|\}$ of spin projectors are found by inserting (38) into the superoperator definition (24),

$$\mathcal{T}^{(K)}_{\alpha\beta,\gamma\delta} = \operatorname{tr}\{(|\delta\rangle\langle\gamma|) \mathcal{T}^{(K)} (|\alpha\rangle\langle\beta|)\} = \sum_q \langle\gamma| T_q^{(K)} |\delta\rangle \langle\beta| T_q^{(K)\dagger} |\alpha\rangle. \tag{40}$$

Using the matrix elements (29) and the completeness relation of CG-coefficients [12, (14a)], it is straightforward to show that

$$\mathrm{Tr}_{\mathrm{L}}\, \mathcal{T}^{(K)} = \sum_{\alpha\beta} \mathcal{T}^{(K)}_{\alpha\beta,\alpha\beta} = 2K+1, \tag{41}$$

as expected for the identity in the subspace $L(H_s)^{(K)}$ of dimension $2K+1$. Furthermore, the projectors $\mathcal{T}^{(K)}$ sum up to the identity with respect to the horizontal product rule (5): $\sum_K \mathcal{T}^{(K)}_{\alpha\beta,\gamma\delta} = I_{\alpha\beta,\gamma\delta} = \delta_{\gamma\alpha}\delta_{\beta\delta}$.

3.3.2. Expression in terms of spin operators. The projector onto scalar operators is the 'trace-taker'

$$\mathcal{T}^{(0)} = \frac{1}{d_s}\mathbb{1}(\mathbb{1},\cdot) = \frac{1}{d_s}\mathbb{1}\,\mathrm{tr}\{\cdot\}, \tag{42}$$

with $\mathbb{1}$ the identity in H_s, which is all but a surprise considering that the scalar part of a matrix is its trace. In the decoupled basis, we have $\mathcal{T}^{(0)}_{\alpha\beta,\gamma\delta} = \frac{1}{d_s}\delta_{\alpha\beta}\delta_{\gamma\delta}$, justifying thereby the tensor (8) found by elementary diagonalization in the electron case. Now it is evident that a unit superoperator eigenvalue $\lambda_0 = 1$ is equivalent with trace preservation (and hence particle/energy conservation).

But already for the projector $\mathcal{T}^{(1)}$ onto vector operators, using (40) involves a sum over products of CG-coefficients, and it is advisable to look for a more transparent formulation. Equation (38) tells us that we need to find a contraction $\mathcal{T}^{(1)} = \sum_j O^j(O^j|\cdot)$ of components of a vector operator $\boldsymbol{O} = (O^1, O^2, O^3)$ that must be traceless, $\sum_\alpha O^j_{\alpha\alpha} = 0$, in order to be orthogonal to $\mathcal{T}^{(0)}$. The only available vector is the generator of rotations: the spin operator $\boldsymbol{S}$ itself. Its components have zero trace because they generate rotation matrices of unit determinant ($1 = \det U = \det\exp\{\mathrm{i}\theta S^j\} = \exp\{\mathrm{i}\theta\,\mathrm{tr}\,S^j\}$). Alternatively, one can use the Wigner–Eckart theorem [12, (85)] to show explicitly that $S_q = \sqrt{c_s}T^{(1)}_q$ up to a normalization constant such that

$$\mathcal{T}^{(1)} = \frac{1}{c_s}\sum_j S^j(S^j|\cdot). \tag{43}$$

The normalization constant c_s is fixed by requiring $\mathcal{T}^{(1)}\mathcal{T}^{(1)} = \mathcal{T}^{(1)}$: since $S^2 = s(s+1)\mathbb{1}_s$ is the Casimir operator of the irreducible representation $D^{(s)}$ of dimension $d_s = 2s+1$, we have $3\,\mathrm{tr}\{S^iS^j\} = s(s+1)(2s+1)\delta_{ij}$. The normalization factor therefore is $c_s = s(s+1)(2s+1)/3$. For electrons, $S^j = \sigma^j/2$ and $c_{1/2} = \frac{1}{2}$ such that $\mathcal{T}^{(1)} = \frac{1}{2}\sum_j \sigma^j(\sigma^j,\cdot)$. Its components in the decoupled basis are indeed those of (9).

This completes the derivation of projectors for the scalar electronic diffuson vertex. For larger spin, higher orders of K have to be considered which essentially involves a Gram–Schmidt procedure. In appendix A.2, this is done for the photon case $s = 1$.

3.4. The crossed vertex as an ordinary operator

We now turn to the diagonalization of the cooperon vertex X that maps an incident tensorial ket product $|s\alpha\rangle \otimes |s\beta\rangle$ onto the final tensorial ket product $|s\gamma\rangle \otimes |s\delta\rangle$. In operator form,

$$X = \sum_{\alpha\beta,\gamma\delta} |s\gamma s\delta\rangle X_{\alpha\beta,\gamma\delta}\langle s\alpha s\beta|. \tag{44}$$

Therefore, the crossed vertex $X : H_s \otimes H_s \to H_s \otimes H_s$ can be seen as an ordinary linear operator or $d_s^2 \times d_s^2$ matrix. In this respect, we define the trace for X as

$$\mathrm{Tr}_{\mathrm{C}}\, X = \sum_{\alpha\beta} X_{\alpha\beta,\alpha\beta}. \tag{45}$$

This trace definition is invariant under the exchange of spin indices (23), such that

$$\mathrm{Tr}_{\mathrm{L}}\,\mathcal{L} = \mathrm{Tr}_{\mathrm{C}}\,X. \tag{46}$$

In other words, the partial Liouville conjugation [19] $|s\beta\rangle\langle s\delta| \mapsto |s\delta\rangle\langle s\beta|$ that maps the diffuson onto the cooperon vertex preserves their trace, which in turn will permit us to derive useful sum rules between eigenvalues in section 4.3.

We wish to bring the vertex into a least redundant form for iteration by performing the usual Clebsch–Gordan decomposition of the argument and image spaces, i.e., a suitable basis change that transforms the direct product $D^{(s)} \otimes D^{(s)}$ of two irreducible representations acting on $H_s \otimes H_s$ into the direct sum $D^{(0)} \oplus D^{(1)} \oplus \cdots \oplus D^{(2s)}$ of irreducible representations $D^{(K)}$, $K = 0, 1, \ldots, 2s$. The appropriate recoupling route now can be mapped out as

$$\begin{array}{ccccc} (D^{(s)} \otimes D^{(s)}) & & & & (\overline{D^{(s)}} \otimes \overline{D^{(s)}}) \\ \searrow \quad \swarrow & & & & \searrow \quad \swarrow \\ D^{(K)} & & \otimes & & \overline{D^{(K')}} \\ & \searrow & & \swarrow & \\ & & D^{(L)} & & \end{array} \quad . \tag{47}$$

We first change to the spherical basis $|Kq\rangle = \sum_{\alpha\beta}\langle ss\alpha\beta|Kq\rangle|s\alpha s\beta\rangle$ of the irreducible subspace $H^{(K)}$. The corresponding vertex components are

$$X_{Kq,K'q'} = \sum_{\alpha\beta,\gamma\delta}\langle ss\alpha\beta|Kq\rangle X_{\alpha\beta,\gamma\delta}\langle ss\gamma\delta|K'q'\rangle \tag{48}$$

such that $X = \sum_{Kq,K'q'}|Kq\rangle X_{Kq,K'q'}\langle K'q'|$. Here, X is decomposed over the decoupled operator basis $|Kq\rangle\langle K'q'|$. We can therefore define recoupled irreducible operators, as in (28), but in the present context with rank L and their $(2L+1)$ components

$$T^{(L)}_m(K,K') = \sum_{qq'}(-)^{K'-q'}\langle KK'q-q'|Lm\rangle|Kq\rangle\langle K'q'|. \tag{49}$$

The objects thus used can be precisely located on the map (47)

$$\begin{array}{ccccc} |s\alpha\rangle|s\beta\rangle & & & & \langle s\delta|\langle s\gamma| \\ \searrow\swarrow & & & & \searrow\swarrow \\ |Kq\rangle & & & & \langle K'q'| \\ & \searrow & & \swarrow & \\ & & T^{(L)}_m(K,K') & & \end{array} \quad . \tag{50}$$

$T^{(L)}_m(K,K')$'s provide the most natural basis set for exploiting rotational symmetries in $H_s \otimes H_s$. Now the crossed vertex X can be decomposed over this basis set:

$$X = \sum_{KK'}\sum_{Lm} X_{Lm}(K,K')T^{(L)}_m(K,K') \tag{51}$$

where its irreducible components are

$$X_{Lm}(K,K') = \sum_{qq'}(-)^{K'-q'}\langle KK'q-q'|Lm\rangle X_{Kq,K'q'}. \tag{52}$$

3.5. Scalar crossed vertex: projectors

The decomposition into irreducible components is especially profitable for a scalar vertex since it has only a single non-vanishing component $X_{00}(K, K)$. The CG-coefficients in (49) and (52) then restrict the sum to $K = K'$. Therefore, the vertex connects irreducible subspaces $H^{(K)}$ of equal rank and can indeed be written as

$$X = \sum_{K=0}^{2s} \chi_K T^{(K)} \tag{53}$$

with eigenvalues $\chi_K = X_{00}(K)/\sqrt{2K+1}$ and associated tensors

$$T^{(K)} = \sqrt{2K+1}\, T_0^{(0)}(K) = \sum_q |Kq\rangle\langle Kq|. \tag{54}$$

These are indeed orthogonal projectors $T^{(K)}T^{(K')} = \delta_{KK'}T^{(K)}$ onto the irreducible subspaces $H^{(K)}$. Their matrix elements in the decoupled basis of $H_s \otimes H_s$ are

$$T^{(K)}_{\alpha\beta,\gamma\delta} = \sum_q \langle ss\alpha\beta|Kq\rangle\langle ss\gamma\delta|Kq\rangle, \tag{55}$$

Using [12, (14a)], one shows that

$$\mathrm{Tr_C} T^{(K)} = \sum_{\alpha\beta} T^{(K)}_{\alpha\beta,\alpha\beta} = 2K+1 \tag{56}$$

and that the projectors $T^{(K)}$ sum up to the identity, $\sum_K T^{(K)}_{\alpha\beta,\gamma\delta} = \delta_{\gamma\alpha}\delta_{\beta\delta}$.

Even the simplest projector $T^{(0)}$ on the singlet space $H^{(0)}$ has seemingly complicated matrix elements in the decoupled basis,

$$T^{(0)}_{\alpha\beta,\gamma\delta} = \frac{1}{d_s}(-)^{2s+\beta-\gamma}\delta_{-\beta,\alpha}\delta_{-\delta,\gamma}. \tag{57}$$

For electrons, one may check by hand that this is indeed equivalent to the much nicer formula (11). For spin 1 particles, the contractions $(-)^p\delta_{-p,q}$ of spherical basis components become δ_{ij} in the Cartesian basis, and one gets

$$T^{(0)}_{il,jk} = \tfrac{1}{3}\delta_{il}\delta_{jk} \tag{58}$$

as used in [8]. These heuristic writings in the decoupled basis are much less systematic than the exceedingly simple form (54) in the spherical basis. Moreover, the matrix elements of $T^{(1)}$ directly derived from (55) would be rather far from the simple form (12) we wish to justify. To that purpose, section 3.6 discusses a general way of deriving the crossed projectors $T^{(K)}$ from the ladder (super-)projectors $\mathcal{T}^{(K)}$ and vice versa.

3.6. Recoupling of projectors

The simple exchange rule $\mathcal{L}_{\alpha\beta,\gamma\delta} = X_{\alpha\delta,\gamma\beta}$ provides us with a convenient way of linking the diffuson and cooperon projectors. The two diagonalization procedures differ by the coupling scheme for the two pairs of spin indices and are related by a simple recoupling relation. Indeed, the matrix elements (40) of the diffuson projectors

$$\mathcal{T}^{(K)}_{\alpha\beta,\gamma\delta} = \sum_q (-)^{s-\delta}\langle ss\gamma-\delta|Kq\rangle(-)^{s-\beta}\langle ss\alpha-\beta|Kq\rangle \tag{59}$$

can be derived from the corresponding cooperon projectors (55) with exchanged spin indices $\beta \leftrightarrow \delta$, $T^{(K)}_{\alpha\delta,\gamma\beta} = \sum_q \langle ss\alpha\delta|Kq\rangle\langle ss\gamma\beta|Kq\rangle$, with the help of the appropriate recoupling relation [12, (34)]:

$$T^{(K)}_{\alpha\beta,\gamma\delta} = \sum_{K'} R_s(K,K')\mathcal{T}^{(K')}_{\alpha\delta,\gamma\beta}, \qquad \mathcal{T}^{(K)}_{\alpha\beta,\gamma\delta} = \sum_{K'} R_s(K,K')T^{(K')}_{\alpha\delta,\gamma\beta}. \tag{60}$$

These relations express a mapping between sets of projector matrix elements $\{\mathcal{T}^{(K)}_{\alpha\beta,\gamma\delta}\} \leftrightarrow \{T^{(K)}_{\alpha\delta,\gamma\beta}\}$ defined by a transformation matrix R_s with elements

$$R_s(K,K') = (2K+1)\begin{Bmatrix} s & s & K \\ s & s & K' \end{Bmatrix}. \tag{61}$$

General 6j-symbol symmetry properties and the orthogonality (18) imply that the matrix R_s is real and circular: $R_s = \overline{R_s} = R_s^{-1}$ such that $\det R_s = \pm 1$ with $\det R_{1/2} = \det R_1 = -1$. This transformation conserves the orthogonality of projectors: $\mathrm{Tr_L}\{\mathcal{T}^{(K)}\mathcal{T}^{(K')}\} = (2K+1)\delta_{KK'} = \mathrm{Tr_C}\{T^{(K)}T^{(K')}\}$.

Putting the transformations (60) to work, the scalar projector (57) on the singlet state $K = 0$ is predicted to be given by

$$T^{(0)}_{\alpha\beta,\gamma\delta} = \frac{(-)^{2s}}{d_s}\sum_{K'}(-)^{K'}\mathcal{T}^{(K')}_{\alpha\delta,\gamma\beta}. \tag{62}$$

Using the electron diffuson projectors (8) and (9), one obtains as expected the singlet cooperon projector in the form (11)

$$T^{(0)}_{\alpha\beta,\gamma\delta} = -\tfrac{1}{2}\big(\mathcal{T}^{(0)}_{\alpha\delta,\gamma\beta} - \mathcal{T}^{(1)}_{\alpha\delta,\gamma\beta}\big) = \tfrac{1}{2}(\delta_{\alpha\gamma}\delta_{\beta\delta} - \delta_{\alpha\delta}\delta_{\beta\gamma}). \tag{63}$$

Similarly, the projector (12) onto the triplet space is

$$T^{(1)}_{\alpha\beta,\gamma\delta} = 3\big(\tfrac{1}{2}\mathcal{T}^{(0)}_{\alpha\delta,\gamma\beta} + \tfrac{1}{6}\mathcal{T}^{(1)}_{\alpha\delta,\gamma\beta}\big) = \tfrac{1}{2}(\delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\beta\gamma}). \tag{64}$$

This completes the derivation of all projectors for the case of spin $\frac{1}{2}$. The photon case is discussed in the appendix. Now the stage is set for the calculation of eigenvalues.

4. Calculation of eigenvalues

4.1. Diffuson eigenvalues λ_K

The scalar spin superoperator eigenvalues λ_K defined through the general decomposition (37) are at least $(2K+1)$-fold degenerate[6]. They can be calculated either by projecting the vertex on an arbitrary component q of the respective subspace, $\lambda_K = \big(T^{(K)}_q\big|\mathcal{L}T^{(K)}_q\big)$ or directly from the vertex matrix elements $\mathcal{L}_{\alpha\beta,\gamma\delta}$ as

$$\lambda_K = \frac{\mathcal{L}_{00}(K,K)}{\sqrt{2K+1}} = \frac{1}{2K+1}\sum_q \mathcal{L}^{(K)}_{q,Kq} \tag{65}$$

$$= \frac{1}{2K+1}\sum_{q,\alpha\beta\gamma\delta}(-)^{s-\beta}\langle ss\alpha{-}\beta|Kq\rangle\mathcal{L}_{\alpha\beta,\gamma\delta}(-)^{s-\delta}\langle ss\delta{-}\gamma|K{-}q\rangle. \tag{66}$$

Useful information about the possible form of eigenvalues can be gained from this direct calculation. To that purpose, consider an arbitrary microscopic spin interaction with matrix

[6] Of course, larger degeneracies occur if the vertex possesses even higher symmetries; an elementary example is the identity $I_{\alpha\beta,\gamma\delta} = \delta_{\gamma\alpha}\delta_{\delta\beta}$ with its single d_s^2-fold degenerate eigenvalue $\lambda = 1$.

elements $V_{\gamma\alpha} = \langle s\gamma|V|s\alpha\rangle$. This interaction can itself be developed in the basis of irreducible operators (28), $V = \sum_{Kq} V_{Kq} T_q^{(K)}$. Its components

$$V_{Kq} = \left(T_q^{(K)}\middle|V\right) = \mathrm{tr}\left\{T_q^{(K)\dagger} V\right\} = \sum_{\alpha\gamma} (-)^{s-\alpha} \langle ss\gamma - \alpha|Kq\rangle V_{\gamma\alpha} \tag{67}$$

are the coupling amplitudes of scalar, vector, quadrupolar type, etc. These amplitudes may depend on microscopic degrees of freedom of the scattering object such as the orientation of a magnetic impurity. The scattering vertex $\mathcal{L}_{\alpha\beta,\gamma\delta} = \langle V_{\gamma\alpha}(V^\dagger)_{\beta\delta}\rangle_{\mathrm{av}}$ is the partial trace over these degrees of freedom,

$$\mathcal{L}_{\alpha\beta,\gamma\delta} = \sum_{KqK'q'} \langle V_{Kq}\overline{V_{K'q'}}\rangle_{\mathrm{av}} (-)^{2s-\alpha-\beta} \langle ss\gamma - \alpha|Kq\rangle \langle ss\beta - \delta|K' - q'\rangle. \tag{68}$$

As a scalar vertex has no angular dependence, it always takes the generic form

$$\langle V_{Kq}\overline{V_{K'q'}}\rangle_{\mathrm{av}} = \delta_{KK'}\delta_{qq'} s_K \tag{69}$$

where s_K is the vertex eigenvalue in the invariant subspace of rank K for the 'vertical' coupling scheme. The eigenvalue definition (66) then becomes a sum over products of four CG-coefficients that defines a $6j$-symbol [12, (32)] and finally yields

$$\lambda_K = (-)^{2s+K} \sum_{K'} (-)^{K'} R_s(K', K) s_{K'}. \tag{70}$$

Remarkably enough, the only information about the microscopic interaction is carried by the coupling constants s_K. The $6j$-symbol merely provides the recoupling from the 'vertical' form $(\alpha\gamma) \leftrightarrow (\beta\delta)$ of the initial product of amplitudes $\langle V_{\gamma\alpha}(V^\dagger)_{\beta\delta}\rangle_{\mathrm{av}}$ to the 'horizontal' form $(\alpha\beta) \leftrightarrow (\gamma\delta)$ necessary for the diagonalization with respect to the multiple scattering product rule (5).

The simplest possible example of a scalar diffuson vertex is of course given by isotropic scattering. The interaction is characterized by $V^{(0)}_{\gamma\alpha} = v_0\delta_{\gamma\alpha}$ with v_0 being a complex number. The only effective amplitude is then $s_0 = (2s+1)|v_0|^2$, and the eigenvalues are simply $\lambda_K = |v_0|^2$ for all K which is evident at once since this vertex is simply proportional to the identity.

The first non-trivial example is given by a vector coupling of the spin-flip form (2). Using the chosen normalization (3) and $S_q = \sqrt{s(s+1)d_s/3}\, T_q^{(1)}$ by virtue of the Wigner–Eckart theorem [12, (85)], one finds that the only non-zero coupling is the vector contribution $s_1 = d_s/3$. Using (17), the eigenvalues (66) are then

$$\lambda_K = (-)^{d_s+K} d_s \begin{Bmatrix} s & s & K \\ s & s & 1 \end{Bmatrix} = 1 - \frac{K(K+1)}{2s(s+1)}. \tag{71}$$

The scalar eigenvalue is identically $\lambda_0 = 1$, for any value of s, as required by trace preservation. For electrons $\left(s = \frac{1}{2}\right)$, we recover moreover the eigenvalue $\lambda_1 = -\frac{1}{3}$ of the vector mode $K = 1$ found heuristically in section 2.3.

4.2. Cooperon eigenvalues χ_K

From the vertex diagonalization (53), we find the eigenvalues

$$\chi_K = \frac{X_{00}(K)}{\sqrt{2K+1}} = \frac{1}{2K+1} \sum_q X_{Kq,Kq} \tag{72}$$

$$= \frac{1}{2K+1} \sum_{q,\alpha\beta\gamma\delta} \langle ss\alpha\beta|Kq\rangle X_{\alpha\beta,\gamma\delta} \langle ss\gamma\delta|Kq\rangle. \tag{73}$$

As a function of the elementary coupling coefficients s_K defined in (69), the eigenvalues are

$$\chi_K = (-)^{2s+K} \sum_{K'} R_s(K', K) s_{K'}. \tag{74}$$

Using (17), the eigenvalues of the normalized spin-flip crossed vertex (4) with the only non-zero coupling $s_1 = d_s/3$ are thus

$$\chi_K = (-)^{2s+K}(2s+1) \begin{Bmatrix} s & s & K \\ s & s & 1 \end{Bmatrix} = \frac{K(K+1)}{2s(s+1)} - 1. \tag{75}$$

In the electronic case ($s = \frac{1}{2}$), this yields indeed the previously found values $\chi_0 = -1$ in the singlet channel and $\chi_1 = \frac{1}{3}$ in the triplet channel.

4.3. Direct recoupling of eigenvalues

The precise relation between diffuson and cooperon eigenvalues can be understood by observing that both of them are obtained by a recoupling procedure from a 'vertical' coupling scheme of the initial scattering amplitudes towards the relevant direction of diagonalization, 'horizontal' for the diffuson vertex and 'diagonal' for the cooperon vertex. This implies that the different eigenvalues are linked by simple recoupling relations and useful sum rules.

Starting from a scalar intensity vertex V with no angular dependence, characterized by the product $\langle V_{Kq} \overline{V_{K'q'}} \rangle_{\mathrm{av}} = \delta_{KK'}\delta_{qq'}s_K$, the interaction vertices describing, respectively, the ladder and the crossed diagrams can be written in the form

$$\mathcal{L}_{\alpha\beta,\gamma\delta} = \sum_K s_K \mathcal{T}^{(K)}_{\delta\beta,\gamma\alpha}, \qquad X_{\alpha\beta,\gamma\delta} = \sum_K s_K \mathcal{T}^{(K)}_{\beta\delta,\gamma\alpha}. \tag{76}$$

Clearly, the coupling constants s_K appear as the vertex eigenvalues for the vertical coupling scheme. However, the projectors are not in a form suitable for iteration of the multiple scattering sequence with the horizontal product (5). Using the transformations

$$\mathcal{T}^{(K)}_{\delta\beta,\gamma\alpha} = (-)^K \sum_{K'} (-)^{2s+K'} R_s(K, K') \mathcal{T}^{(K')}_{\alpha\beta,\gamma\delta} \tag{77}$$

$$\mathcal{T}^{(K)}_{\beta\delta,\gamma\alpha} = \sum_{K'} (-)^{2s+K'} R_s(K, K') T^{(K')}_{\alpha\beta,\gamma\delta}, \tag{78}$$

the vertices can be brought into the suitable form

$$\mathcal{L}_{\alpha\beta,\gamma\delta} = \sum_K \lambda_K \mathcal{T}^{(K)}_{\alpha\beta,\gamma\delta} \qquad X_{\alpha\beta,\gamma\delta} = \sum_K \chi_K T^{(K)}_{\alpha\beta,\gamma\delta}. \tag{79}$$

Using the definitions (77) and (78), the eigenvalues λ_K and χ_K are then immediately derived as a function of the vertical eigenvalues s_K, given by expressions (70) and (74). But this in turn implies that the eigenvalues λ_K and χ_K are also directly linked to each other by a simple recoupling procedure. Inverting the relations (70) and (74) with the help of the orthogonality relation (18) for R_s, one obtains the vertical eigenvalues as

$$s_K = (-)^{2s+K} \sum_{K'} (-)^{K'} R_s(K', K) \lambda_K \tag{80}$$

$$= (-)^{2s+K} \sum_{K'} R_s(K', K) \chi_{K'}. \tag{81}$$

Injecting (80) into (70) and (81) into (74), we indeed find

$$\lambda_K = \sum_{K'} R_s(K', K) \chi_{K'}, \qquad \chi_K = \sum_{K'} R_s(K', K) \lambda_{K'}. \tag{82}$$

These relations had been derived previously in the case of photon scattering (formula (52) of [8], $s = 1$) and are here generalized to arbitrary spin. These recoupling relations replace the heuristic prescription $w_2 \leftrightarrow w_3$ for the exchange of contraction weights in the photonic case [20] to arbitrary spin.

Taking the trace (26) or (45) of the decompositions (79) and (76), we find the following useful sum rule:

$$\sum_K (2K+1)\chi_K = \sum_K (2K+1)\lambda_K = \sum_K (2K+1)\mathcal{T}^{(K)}_{\beta\beta,\alpha\alpha} = (2s+1)s_0. \quad (83)$$

The last equality is explained by the fact that the 'horizontal' trace over all modes K in (79) projects onto the scalar component $K = 0$ in (76). By symmetry of our recoupling relations, naturally also the inverse relation holds: taking the 'vertical' trace in (76) yields

$$\sum_K (2K+1)s_K = \mathcal{L}_{\alpha\alpha,\beta\beta} = (2s+1)\lambda_0. \quad (84)$$

Let us demonstrate the power of these relations by taking again the spin-flip vertex as a paradigmatic example. Its diffuson and cooperon eigenvalues (71) and (75) have turned out to be equal but of opposite sign, $\chi_K(s) = -\lambda_K(s)$ for any K and s. Indeed, comparing the eigenvalue expressions as a function of the elementary couplings s_K, (70) and (74), we can trace back this sign to the fact that the spin-flip vertex has only one finite component, the vector coupling $s_1 = d_s/3$. The relation (82) then reduces to an orthogonality of $6j$-symbols and yields immediately $\lambda_K(s) = -\chi_K(s)$. The trace (83) reduces to $\lambda_0 + 3\lambda_1 = 0$ (remember $s_0 = 0$) which immediately fixes the triplet eigenvalue to $\lambda_1 = -\frac{1}{3}$ once the trace-preserving eigenvalue $\lambda_0 = 1$ is known. By now it should be evident that these values are after all of purely geometrical origin.

4.4. Reciprocity

Quite generally, the diffuson vertex of some microscopic spin interaction V is $\mathcal{L}_{\alpha\beta,\gamma\delta} = \langle V_{\gamma\alpha}\overline{V_{\delta\beta}}\rangle_{\rm av} = \langle V_{\gamma\alpha}(V^\dagger)_{\beta\delta}\rangle_{\rm av}$ while the corresponding crossed vertex is $X_{\alpha\beta,\gamma\delta} = \mathcal{L}_{\alpha\delta,\gamma\beta} = \langle V_{\gamma\alpha}(V^\dagger)_{\delta\beta}\rangle_{\rm av} = \langle V_{\gamma\alpha}([V^{\rm t}]^\dagger)_{\beta\delta}\rangle_{\rm av}$. Clearly, these vertices are identical if the microscopic interaction is *symmetric*, $V = V^{\rm t}$. This complies with the general rule that the reciprocity theorem assures perfect equality of ladder and crossed contributions if the system's S-matrix is symmetric [2]. In terms of the irreducible amplitudes V_{Kq} defined in (67), symmetry of the microscopic interaction is equivalently stated as

$$V = V^{\rm t} \quad \Leftrightarrow \quad V_{Kq} = (-)^q V_{K-q}. \quad (85)$$

This is to be contrasted with the Hermiticity condition

$$V = V^\dagger \quad \Leftrightarrow \quad \overline{V_{Kq}} = (-)^q V_{K-q}. \quad (86)$$

For example, a simple scalar interaction $V^{(0)} = v_0\mathbb{1}$ is Hermitian if v_0 is real. Non-Hermitian interaction would describe absorption or gain which is known to preserve equality between ladder and crossed contributions [2]. Indeed, $V^{(0)}$ is always symmetric since $V^{(0)}_{Kq} = \delta_{K0}\delta_{q0}\sqrt{2s+1}v_0$ fulfils (85).

Less trivially, the spin-flip vector coupling $V^{(1)} = g\boldsymbol{J}\cdot\boldsymbol{S}$ has irreducible components

$$V^{(1)}_{Kq} = \delta_{K1}\frac{g}{\sqrt{c_s}}(-)^q J_{-q}. \quad (87)$$

Of course, the interaction is Hermitian for a real g. But it is not symmetric in general because (87) is different from $(-)^q V^{(1)}_{K-q}$ as soon as $J_q \neq (-)^q J_{-q}$, i.e., if the impurities are not all aligned. This is at the origin of the fact that spin-flip scattering suppresses the diffusive

pole of the cooperon (the 'unitary case' in magnetoresistance [3]). Furthermore, it explains the observation that it is precisely the antisymmetric part $t_{ij}^{(1)}$ of the atomic photon scattering tensor (i.e., the vector coupling component) that breaks the equivalence of ladder and crossed vertices [20]. If, however, one can align all vectorial scatterers, for example with an external magnetic field, one can choose the quantization axis in this direction such that $J_q = \delta_{q0} J_0$, and equality of ladder and crossed terms is re-established. This effect has been observed with electronic transport in metal samples containing magnetic impurities and subject to a strong magnetic field [21]. There, weak localization corrections to transport are suppressed by spin-flip processes at low fields, but are restored at high fields because all magnetic impurities are then aligned with the field. A similar argument is at the origin of the observed magnetic field enhancement of coherent backscattering of light by a resonant sample of ultracold atoms [22] whose ground-state degeneracies are lifted by a magnetic field.

Having at hand the diffuson and cooperon eigenvalues (70) and (74) as functions of the elementary coupling coefficients s_K, we see immediately that a difference between eigenvalues is generated only by coupling amplitudes s_K with odd $K = 1, 3, \ldots$ (for electrons and photons, only $K = 1$ is possible). A simple inspection of the microscopic interaction vertex of a particular physical impurity type permits to decide whether this coupling is of vectorial rank $K = 1$, therefore breaks the equivalence of ladder and crossed structures and eventually leads to an effective dephasing of weak localization effects, or whether it is of scalar or symmetric type $K = 0, 2$ and then does not affect localization effects.

5. Consequences for relevant transport quantities

5.1. Diffuson spin transport

The formalism of irreducible spin representations greatly simplifies the expression of spin transport quantities that are of interest in the growing number of 'spintronics' applications. The probability of quantum diffusion, defined in subsection 2.1, with spin degrees of freedom can be decomposed into its irreducible components:

$$P_{\alpha\beta,\gamma\delta}(\boldsymbol{q},\omega) = \frac{1}{2\pi\rho}\left\langle G^{\mathrm{R}}_{\alpha\gamma} G^{\mathrm{A}}_{\beta\delta}\right\rangle = \sum_{K=0}^{2s} P_K(\boldsymbol{q},\omega)\mathcal{T}^{(K)}_{\alpha\beta,\gamma\delta}. \tag{88}$$

The probability $P_K(\boldsymbol{q},\omega)$ with spatial and temporal Fourier variables $\boldsymbol{q}$ and ω can be computed independently in each spin sector K if the elementary scattering vertex as well as the average propagation between scatterers has been diagonalized appropriately. For the summed ladder series $\mathcal{D} = \mathcal{L}/(1 - \mathsf{G}\mathcal{L})$, each diffuson mode up to an overall normalization reads

$$P^{(d)}_K(\boldsymbol{q},\omega) = \frac{\lambda_K}{1 - \lambda_K(1 + \mathrm{i}\omega\tau - Dq^2\tau)} \tag{89}$$

where the diffusion approximation for the intensity propagation in the Kubo limit $\omega\tau, q\ell \ll 1$ has been made; the diffusion constant in d dimensions is $D = \ell^2/\tau d$ in terms of the scattering mean-free path ℓ and the mean-free time $\tau = \ell/v = 1/(2\pi\rho\lambda_0)$ (evaluated from the self-energy in the Born approximation with $\lambda_0 = \sum_\gamma \mathcal{L}_{\alpha\alpha,\gamma\gamma} = 1$ in our normalization). The probability time dependence for each irreducible sector therefore is of the form $P_K(\boldsymbol{q},t) \sim \exp[-Dq^2 t - t/\tau_d(K)]$ with a diffuson spin decay time

$$\tau_d(K) = \tau\frac{\lambda_K}{1 - \lambda_K} \tag{90}$$

given directly as a function of the vertex eigenvalue λ_K. The time-dependent diffuson probability of classical scattering behaves as

$$P^{(d)}_{\alpha\beta,\gamma\delta}(\boldsymbol{q},t)=\sum_{K=0}^{2s}\mathrm{e}^{-Dq^2t-t/\tau_d(K)}\mathcal{T}^{(K)}_{\alpha\beta,\gamma\delta}. \tag{91}$$

After injection of a certain spin state $|s\alpha\rangle$ at $\boldsymbol{r}$, the total classical probability for final states with arbitrary spin γ at arbitrary position $\boldsymbol{r}'$ should be normalized to unity, $\sum_\gamma P_{\alpha\alpha,\gamma\gamma}(\boldsymbol{q}=0,t)=1$. Indeed, the trace over the final spin index γ in (91) projects onto the scalar component $K=0$, such that the conservation of probability requires $1/\tau_d(0)=0$ which is indeed the case for a unit scalar eigenvalue $\lambda_0=1$.

The overall probability of retaining the initial spin state, say $\alpha=+\frac{1}{2}=:+$, is $P_{++,++}(t)=\left(\mathcal{T}^{(0)}_{++,++}\right)+\mathrm{e}^{-t/\tau_1}\left(\mathcal{T}^{(1)}_{++,++}\right)=\frac{1}{2}(1+\mathrm{e}^{-t/\tau_d(1)})$ which deviates only for short times from the equidistribution value $\frac{1}{2}$. The degree of spin polarization $\pi(t)=P_{++,++}(t)-P_{++,--}(t)$ relaxes on the time scale $\tau_d(1)$ as $\pi(t)=\mathrm{e}^{-t/\tau_d(1)}$.

Consider for the sake of concreteness the case of multiple electronic spin-flip scattering with the vertex (2). This vertex has a negative eigenvalue $\lambda_1=-\frac{1}{3}$ such that formally the decay time $\tau_d(1)$ becomes negative, which renders the above predictions unacceptable. In fact, in a disordered electronic sample, there are scalar defects responsible for elastic scattering and momentum relaxation, say with a rate $\gamma_e=n_e v_0^2$ depending on the density n_e of defects and their interaction strength v_0. In spin space, these vertices have unit eigenvalues both for ladder and crossed vertices. In addition there are magnetic impurities, each with a scattering vertex (2), centred at random positions $\boldsymbol{r}_m$ with density n_m and corresponding momentum scattering rate $\gamma_m=n_m g^2\frac{1}{3}J(J+1)s(s+1)$. The inverse of the total scattering rate $\gamma=\gamma_e+\gamma_m$ is the mean-free time $\tau=1/\gamma$. The effective average spin-flip scattering vertex then has the normalized ladder eigenvalues

$$\lambda_K^{\mathrm{eff}}=\frac{\gamma_e+\gamma_m\lambda_K}{\gamma}=1-\frac{\gamma_m}{\gamma}(1-\lambda_K) \tag{92}$$

which for the spin-flip case are $\lambda_0^{\mathrm{eff}}=1$ and $\lambda_1^{\mathrm{eff}}=1-4\gamma_m/3\gamma$. The characteristic spin polarization decay rate reads

$$\frac{1}{\tau_d(1)}=\frac{1-\lambda_1^{\mathrm{eff}}}{\tau\lambda_1^{\mathrm{eff}}}=\frac{1-\lambda_1}{\tau_m}+O\left(\frac{\gamma_m}{\gamma}\right)\approx\frac{4}{3\tau_m}. \tag{93}$$

5.2. *Cooperon dephasing*

The cooperon is the sum of all maximally crossed diagrams which, strictly speaking, starts with the second-order scattering term because the single scattering event is already counted in the diffuson: $C=X\mathsf{G}X/(1-\mathsf{G}X)$. Here, X is the crossed vertex associated with the diffuson vertex for scattering with a total rate $\gamma=1/\tau$ and normalized to a unit diffuson eigenvalue $\lambda_0=1$. Summing the geometric series with the returned advanced propagator line (see figure 1(*c*)) gives the decomposition

$$C_{\alpha\beta,\gamma\delta}(\boldsymbol{Q},\omega)=\sum_{K=0}^{2s}C_K(\boldsymbol{Q},\omega)T^{(K)}_{\alpha\beta,\gamma\delta} \tag{94}$$

where $\boldsymbol{Q}=\boldsymbol{k}+\boldsymbol{k}'$ is the sum of external momenta. The cooperon eigenfunctions for each irreducible mode are

$$C_K(\boldsymbol{Q},\omega)=\frac{1}{\tau}\frac{\chi_K}{-\mathrm{i}\omega+DQ^2+1/\tau_c(K)} \tag{95}$$

with characteristic cooperon dephasing times

$$\tau_c(K) = \tau \frac{\chi_K}{1-\chi_K} \tag{96}$$

that depend directly on the crossed eigenvalues χ_K.

In applications to weak localization, one needs the integrated cooperon, both over momenta and spin indices, that counts arbitrary loops of counter-propagating amplitudes. Up to a normalization

$$P_c(\omega) = \sum_{\boldsymbol{Q}} \sum_{\gamma} C_{\alpha\gamma,\gamma\alpha}(\boldsymbol{Q},\omega) = \sum_{K=0}^{2s} w_K \sum_{\boldsymbol{Q}} C_K(\boldsymbol{Q},\omega) \tag{97}$$

where the cooperon spin-channel weights w_K are determined by the crossed contraction $w_K = \sum_\gamma T^{(K)}_{\alpha\gamma,\gamma\alpha}$ that corresponds to the sum over all final spin states $\beta = \gamma$ in the maximally crossed diagrams of figure 1(*b*). Using the recoupling formula (16), one finds

$$w_K = \sum_{K'} R_s(K,K') \sum_{\gamma} \mathcal{T}^{(K')}_{\alpha\alpha,\gamma\gamma} = R_s(K,0) = (-)^{2s+K} \frac{2K+1}{2s+1}. \tag{98}$$

Remarkably, although the integrated cooperon describes a renormalization of intensity diffusion (the scalar diffuson mode $K = 0$), in general all the cooperon modes $K = 0, \ldots, 2s$ contribute with non-zero weights [23].

Taking again the case of electronic elastic and spin-flip scattering as an example, the singlet and triplet channel weights are $w_0 = -\frac{1}{2}$ and $w_1 = \frac{3}{2}$, and the effective eigenvalues are

$$\chi_K^{\text{eff}} = \frac{\gamma_e + \gamma_m \chi_K}{\gamma} = 1 - \frac{\gamma_m}{\gamma}(1-\chi_K). \tag{99}$$

For a small spin-flip scattering rate $\gamma_m/\gamma \ll 1$, the corresponding dephasing rates are

$$\frac{1}{\tau_c(K)} = \frac{1-\chi_K}{\tau_m}. \tag{100}$$

Inserting the spin-flip eigenvalues $\chi_0 = -1$ and $\chi_1 = \frac{1}{3}$, the singlet and triplet dephasing times are $\tau_c(0) = \tau_m/2$ and $\tau_c(1) = 3\tau_m/2$. If the eigenvalues (99) in the numerator of (97) are approximated by unity, the integrated spin-flip cooperon finally reads

$$P_c(\omega) = \sum_{\boldsymbol{Q}} \left[\frac{3}{2} \frac{1}{-\mathrm{i}\omega + D\boldsymbol{Q}^2 + 2/3\tau_m} - \frac{1}{2} \frac{1}{-\mathrm{i}\omega + D\boldsymbol{Q}^2 + 2/\tau_m} \right]. \tag{101}$$

The coupling to the uncontrolled degrees of freedom of magnetic impurities dephases both the singlet and triplet channels irreversibly and leads to a drastic decrease of weak localization effects in disordered electronic samples. A similar effect is found for the weak localization of photons scattered by cold atoms with degenerate dipole transitions [9].

Note that in the case of electronic spin–orbit scattering, the triplet channel with positive weight $w_1 = \frac{3}{2}$ is also rapidly damped, whereas the singlet channel with negative weight $w_0 = (-)^{2s}/(2s+1) = -\frac{1}{2}$ survives and leads to antilocalization and a positive magnetoresistance [10] which appears here as characteristic for any half-integer spin.

6. Summary and conclusion

In this paper, we have developed a systematic method to diagonalize the elementary spin scattering vertices which are the building block of diffuson and cooperon multiple scattering sequences for particles of arbitrary spin s. Our results therefore provide the conceptual

background for a truly unified description of the mesoscopic spin physics of electrons and photons. We have identified the relevant projectors onto invariant subspaces that are irreducible with respect to the rotation group. Once these operators have been obtained, the diagonalization allows us to transform the vertical coupling scheme for the scattering amplitudes into a horizontal scheme necessary for subsequent iteration of the multiple scattering sequence. We have obtained the diffuson and cooperon scattering eigenvalues as a function of the microscopic scattering mechanism, together with simple recoupling relations as well as useful sum rules. We have shown how these eigenvalues directly enter the expressions of the phase coherence times of weak localization.

The method presented here may be extended to non-scalar vertices such as the transverse photon propagator $\mathsf{G}(\boldsymbol{q})$ that was diagonalized exactly in [8]. This transverse propagator is no longer purely scalar at non-zero momentum transfer $\boldsymbol{q} \neq 0$, but contains quadrupolar parts coupling the modes $K = 0, 2$. A treatment of these non-scalar vertices would start from the expressions (36) and (51) of the present work and derive the appropriate projectors and eigenvalues. On a similar line of thought, light scattering by nematic crystals [24] as well as photon scattering vertices of atoms under the influence of an external magnetic field [22] require anisotropic diagonalization. Finally, these techniques may become useful for quantum computation schemes involving spin degrees of freedom (such as the one studied by Loss and di Vincenzo [25], to cite a paper employing a superoperator formalism quite similar to ours) or for entanglement characterization in irreducible representations of observable-induced tensor product spaces [26].

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Appendix. Photon scattering

A.1. Atomic vertex eigenvalues

For photons, polarization-dependent scattering proves more complicated than for electrons because of field transversality. The spin degrees of freedom are *not* decoupled from average propagation such that the complete diagonalization of the diffuson and cooperon series is much more involved. Nonetheless, the projection onto irreducible subspaces permits to derive all eigenvalues and projectors for isotropic photon vertices as well, as has been done in [8] for the case of photon scattering from degenerate atomic dipole transitions. For resonant photon scattering, the elementary interaction is of the form $V_{\mathrm{dip}} = -\boldsymbol{D} \cdot \boldsymbol{E}$ where the electric field operator $\boldsymbol{E}$, proportional to the polarization vector ε, creates or annihilates photons whereas the dipole operator $\boldsymbol{D}$ induces internal transitions between electronic states with angular momentum J_{g} and J_{e}. Obviously, the elementary interaction V_{dip} is of the same vectorial type as the electronic spin-flip vertex (1). The full photon scattering process, however, comprises the annihilation of the incident photon followed by the creation of the scattered one. Therefore, the full scattering amplitude is a second-order process in V_{dip}, and its elementary coupling coefficients s_K (see equation (30) of [8]) contain already all orders $K = 0, 1, 2$ obtained by the recoupling of two vector interactions of rank 1. The ladder and crossed eigenvalues are

then expressed in terms of $6j$- and $9j$-symbols. All relations between eigenvalues derived in section 4 apply to the photon case as well. The sum rule (83) has not been evaluated so far. For resonant photon scattering from a closed dipole transition $J_g \to J_e$, it reads

$$\sum_K (2K+1)\chi_K = \sum_K (2K+1)\lambda_K = \frac{3(2J_e+1)}{2J_g+1}. \tag{A.1}$$

The more general case of photon scattering from entire multiplets of hyperfine or fine structure dipole transitions can be treated as well [27]. In that case, the eigenvalues become frequency dependent, but all algebraic relations of the present work continue to hold.

A.2. Photon projectors

Concerning the projectors onto irreducible subspaces, it was shown in [8] that one and the same set of projectors

$$\mathcal{T}^{(0)}_{il,jk} = \tfrac{1}{3}\delta_{il}\delta_{jk}, \tag{A.2}$$

$$\mathcal{T}^{(1)}_{il,jk} = \tfrac{1}{2}(\delta_{ij}\delta_{kl} - \delta_{ik}\delta_{jl}), \tag{A.3}$$

$$\mathcal{T}^{(2)}_{il,jk} = \tfrac{1}{2}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl}) - \tfrac{1}{3}\delta_{il}\delta_{jk}, \tag{A.4}$$

diagonalizes both ladder and crossed vertex alike. Here, the indices i, j, k, l are Cartesian indices in configuration space $\mathbb{R}^3$.

We still need to connect these tensors to the diffuson (super-)projectors $\mathcal{T}^{(K)}$ derived in 3.3.1 and the seemingly different cooperon projectors $T^{(K)}$ derived in 3.5. Of course, all formulae of the present work are designed to apply to spin 1 as well. But spin 1 is special because its states transform under the fundamental representation SO(3) itself. This representation has the peculiar feature that its dimension is 3 and therefore equal to the dimension of the abstract group. For spin 1, one therefore can use either the standard spherical basis $\{|1q\rangle\}$ where $S^z|1q\rangle = q|1q\rangle$ is diagonal (and which was used throughout the present paper) or the Cartesian basis of $\mathbb{R}^3$ itself where the generators are $S^j_{kl} = -\mathrm{i}\epsilon_{ijk}$ (in this so-called adjoint representation, the generators are essentially given by the structure constants $f_{jkl} = -\epsilon_{jkl}$ of the Lie algebra SO(3)). Using the latter representation in the definitions (42) and (43), we indeed recover immediately (A.2) and (A.3).

In order to obtain the symmetric traceless projector $K = 2$, we have to push the calculation one step further. Extrapolating from the cases $K = 0, 1$, the construction rule for higher rank projectors (38) should be clear: they are complete contractions

$$\mathcal{T}^{(K)} = \sum_{i_1 i_2 \cdots i_K} O^{i_1 i_2 \cdots i_K} (O^{i_1 i_2 \cdots i_K}|\cdot) \tag{A.5}$$

of operators $O^{i_1 i_2 \cdots i_K}$ that are direct products of K copies of S^i with the appropriate symmetrization. Up to normalization, the operator of the $K = 2$ projector is

$$O^{ij} = S^i S^j - \sum_k (O^k|S^i S^j) O^k - (O^0|S^i S^j) O^0 \tag{A.6}$$

where $\sqrt{d_s} O^0 = \mathbb{1}$ pertains to the scalar projector (42). This construction is nothing but the Gram–Schmidt procedure used to orthogonalize the basis $\{e_n\}$ of a vector space according to $e_1 \mapsto e_1, e_2 \mapsto e_2 - (e_1 \cdot e_2)e_1$, etc. After short algebra, one finds

$$O^{ij} = \frac{1}{2}(S^i S^j + S^j S^i) - \frac{s(s+1)}{3}\delta_{ij}\mathbb{1} \tag{A.7}$$

without need for further normalization. This operator is manifestly symmetric and traceless by construction. Using $S^j_{kl} = -\mathrm{i}\epsilon_{ijk}$, we obtain the traceless symmetric projector (A.4) we sought to justify.

For particles of larger spin than $s = 1$ (or more general vertices with higher order irreducible components), the calculation of higher order projectors requires to compute traces of increasingly large products of spin operators, $\mathrm{tr}\{S^i S^j \cdots S^p\}$. Beyond the first terms $K = 0, 1, 2$, carrying out the traces becomes rapidly cumbersome, and the formulation (40) in terms of spherical components $T^{(K)}_q$ turns out to be more economic since the CG-coefficients automatically incorporate the correct symmetrization.

At this point, we have completely justified the diffuson tensors (A.2)–(A.4). However, at first sight the corresponding crossed projectors $T^{(K)}$ derived in 3.5 have nothing in common with them. But inserting the relevant transformation coefficients for $s = 1$

$$(R_1)_{K,K'} = \begin{pmatrix} 1/3 & -1/3 & 1/3 \\ -1 & 1/2 & 1/2 \\ 5/3 & 5/6 & 1/6 \end{pmatrix} \tag{A.8}$$

into the recoupling relation (60) yields indeed $T^{(K)}_{il,jk} = \mathcal{T}^{(K)}_{il,jk}$, $K = 0, 1, 2$. This proves that the diagonalization of spin 1 ladder and crossed vertices in Cartesian components involves the unique set of isotropic projectors (A.2)–(A.4). This is no longer the case for half-integer spins $s = \frac{1}{2}, \frac{3}{2}, \ldots$, because their $SU(2)$ representations are complex unitary which means that ladder and crossed vertices couple rotationally different objects. The same conclusion holds for integer spins $s = 2, 4, \ldots$, though they admit real orthogonal representations of SO(3). This is because the adjoint representation is not available and one has to work *a priori* with two distinct sets of projectors.

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