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LINEAR RESPONSE THEORY FOR THE SPIN TRANSPORT

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We derive the "continuity-like" equation for the spin density in the system with SU(2) gauge potentials. Then we generalize the conventional Kubo formula for the spin transport, *i.e.*, the linear response of the spin current to both the external U(1) and SU(2) fields. The nonconservation of the spin density is shown to play an essential role in keeping the consistency of the generalized Kubo formula between different gauges.

Keywords: "Continuity-like" equation; generalized Kubo formula; consistency between different gauges.

1. Introduction

At The study on the transport properties of a certain material or some modelling systems has always been of great importance and the linear response theory is believed to be a useful tool in such investigations. Kubo formula,[1] as a pillar in the linear response theory, was firstly derived in the study of the electric conductivity in solids. Nowadays, spintronics,[2] which mainly deals with the active control and the manipulation of the spin degree in the material, has attracted more and more attentions for its promising applications in the future information technology. It becomes urgent to develop the corresponding Kubo formula for the spin transport which differs from the conventional one due to its non-Abelian feature.

Before we start the derivation of the generalized Kubo formula, it is worthwhile to investigate the continuity equation for the spin current. A general Hamiltonian including SU(2) gauge potentials for a single charged particle with spin is given by[3]

$$H = \frac{1}{2m}(\mathbf{p} - \frac{e}{c}\mathbf{A}(\mathbf{r},t) - \eta\boldsymbol{\mathcal{A}}^a(\mathbf{r},t)\tau^a)^2 + eA_0(\mathbf{r},t) + \eta\mathcal{A}_0^a(\mathbf{r},t)\tau^a, \tag{1}$$

where $(A_0, \mathbf{A})$ and $(\mathcal{A}_0^a, \boldsymbol{\mathcal{A}}^a)$ are the U(1) and SU(2) gauge potentials, respectively. The former refers to the traditional electromagnetic fields, while the later has been show to characterize spin-orbit couplings in certain semiconductors.[3] Usually, these gauge potentials consist of two parts, internal and external fields if any. τ^a stand for the generators of SU(2) algebra and η denotes the coupling strength of the SU(2) potentials. Hereafter, the indices a, b, c and d refer to the spin space while i and j

the spatial space, and repeated indices are summed over. In such a system, the state is described by a two-component wave function $\Psi(\mathbf{r},t)$. Multiplying the Schrödinger equation by $\Psi^\dagger(\mathbf{r},t)\hat{S}^a$ from the left, we obtain

$$i\hbar\Psi^\dagger(\mathbf{r},t)\hat{S}^a\partial_t\Psi(\mathbf{r},t) = \Psi^\dagger(\mathbf{r},t)\hat{S}^a H\Psi(\mathbf{r},t), \tag{2}$$

and its hermitian

$$-i\hbar[\partial_t\Psi^\dagger(\mathbf{r},t)]\hat{S}^a\Psi(\mathbf{r},t) = [H\Psi(\mathbf{r},t)]^\dagger\hat{S}^a\Psi(\mathbf{r},t), \tag{3}$$

with $\hat{S}^a$ the spin operator. Subtracting Eq. (3) from Eq. (2), we have

$$\begin{aligned}\frac{\partial}{\partial t}(\Psi^\dagger\hat{S}^a\Psi) = &-\frac{\partial}{\partial x_i}\frac{1}{2}\mathrm{Re}\Psi^\dagger\{\hat{S}^a,\frac{1}{m}(\mathbf{p}-\frac{e}{c}\mathbf{A}-\eta\boldsymbol{\mathcal{A}}^b\tau^b)_i\}\Psi + \eta\Psi^\dagger\epsilon^{abc}\mathcal{A}_0^b\hat{S}^c\Psi \\ &-\eta\epsilon^{abc}\mathcal{A}_i^b\frac{1}{2}\mathrm{Re}\Psi^\dagger\{\hat{S}^c,\frac{1}{m}(\mathbf{p}-\frac{e}{c}\mathbf{A}-\eta\boldsymbol{\mathcal{A}}^d\tau^d)_i\}\Psi,\end{aligned} \tag{4}$$

where we do not write out the arguments for simplicity and the curl bracket represents the anticommutator. By introducing the natural definitions of the spin density $s^a(\mathbf{r},t) = \Psi^\dagger\hat{S}^a\Psi$ and the spin current density $\hat{\mathbf{J}}^a(\mathbf{r},t) = \frac{1}{2}\mathrm{Re}\Psi^\dagger\{\hat{S}^a,\hat{\mathbf{v}}\}\Psi$ with the velocity of the particle $\hat{\mathbf{v}} = \frac{1}{m}(\mathbf{p}-\frac{e}{c}\mathbf{A}-\eta\boldsymbol{\mathcal{A}}^a\tau^a)$, we can rewrite Eq. (4) in a much compact form

$$(\frac{\partial}{\partial t} - \eta\vec{\mathcal{A}}_0\times)\vec{s}(\mathbf{r},\ t) + (\frac{\partial}{\partial x_i} + \eta\vec{\mathcal{A}}_i\times)\vec{J}_i(\mathbf{r},\ t) = 0, \tag{5}$$

where notations $\vec{s} = (s^1,\ s^2,\ s^3)$, $\vec{\mathcal{A}} = (\mathcal{A}^1,\ \mathcal{A}^2,\ \mathcal{A}^3)$ etc. are adopted. Eq. (5) is called "continuity-like" equation for the spin density[3] in the sense of the covariant formulation[a]. The extra parts $\eta\vec{\mathcal{A}}_i\times\vec{J}_i(\mathbf{r},\ t) - \eta\vec{\mathcal{A}}_0\times\vec{s}(\mathbf{r},\ t)$ which represents the precession of the spin will be shown to play a necessary role in keeping the consistency of the Kubo formula with different gauge fixings.

2. Linear Response to U(1) Fields with SU(2) Interaction

In this section, we derive the Kubo formula describing the linear response of the spin current to the U(1) electric field, which has been widely employed directly in the study of the spin Hall effect.[4] For this purpose, we separate the total many-body Hamiltonian which is constituted by the one in Eq. (1) into two parts: $H = H_0 + H'$, up to the first order of $\mathbf{A}_{\mathrm{ext}}$, with

$$\begin{aligned}H_0 &= \frac{1}{2m}\sum_l\Big(\hat{\boldsymbol{\pi}}_l^2 + eA_0(\mathbf{r}_l,t) + \eta\mathcal{A}_0^a(\mathbf{r}_l,t)\tau^a\Big),\\ H' &= \frac{-e}{2mc}\sum_l\Big(\hat{\boldsymbol{\pi}}_l\cdot\mathbf{A}_{\mathrm{ext}}(\mathbf{r}_l,t) + \mathbf{A}_{\mathrm{ext}}(\mathbf{r}_l,t)\cdot\hat{\boldsymbol{\pi}}_l\Big),\end{aligned} \tag{6}$$

where $\hat{\boldsymbol{\pi}}_l = \mathbf{p}_l - \frac{e}{c}\mathbf{A}_{\mathrm{int}}(\mathbf{r}_l,t) - \eta\boldsymbol{\mathcal{A}}_{\mathrm{int}}^a(\mathbf{r}_l,t)\tau^a$ stands for the dynamical momentum involving internal U(1) and SU(2) potentials if any. Throughout this paper, the

[a] In Eq. (5), we denote the spin density as $s^a(\mathbf{r},t)$ instead of $\sigma^a(\mathbf{r},t)$ in Ref. 3 to avoid ambiguity since the spin conductivity σ_{ij}^a will be discussed in the following sections.

index l refers to the lth particle. Without losing generality, we take the electric fields to be of single-frequency $\mathbf{E}(\mathbf{r},t) = \mathbf{E}(\mathbf{q},\omega)\ e^{i\mathbf{q}\cdot\mathbf{r}-i\omega t}$ and choose the gauge $A_0 = 0$, which leads to $\mathbf{A}(\mathbf{r},t) = \frac{c}{i\omega}\mathbf{E}(\mathbf{r},t) = \frac{c}{i\omega}\mathbf{E}(\mathbf{q},\omega)e^{i\mathbf{q}\cdot\mathbf{r}-i\omega t}$. Hereafter we omit the subscript specifying the external field for simplicity. In the literature of many-body theory, the charge current is given by $\hat{\mathbf{J}}(\mathbf{r}) = \frac{e}{2m}\sum_l(\hat{\boldsymbol{\pi}}_l\delta(\mathbf{r}-\mathbf{r}_l) + \delta(\mathbf{r}-\mathbf{r}_l)\hat{\boldsymbol{\pi}}_l)$ which is matrix-valued due to the SU(2) gauge potentials in the dynamic momentum. As a result, the interaction can be rewritten as

$$H' = -\frac{1}{c}\int d\mathbf{r}\ \hat{J}_i(\mathbf{r})A_i(\mathbf{r},t) = -\frac{1}{i\omega}\hat{J}_i(\mathbf{q})E_i(\mathbf{q},\omega)e^{-i\omega t}, \tag{7}$$

with $\hat{J}_i(\mathbf{q})$ the Fourier image of the spin current. Based on the definition for a single particle, the spin current is defined as

$$\hat{\mathbf{J}}^a(\mathbf{r}) = \frac{\eta}{4m}\sum_l\Big[\{\tau^a,\hat{\boldsymbol{\pi}}_l\}\delta(\mathbf{r}-\mathbf{r}_l) + \delta(\mathbf{r}-\mathbf{r}_l)\{\tau^a,\hat{\boldsymbol{\pi}}_l\}\Big]. \tag{8}$$

At zero temperature, the spin current is evaluated for the ground state of the system. In the interaction representation, the state $|\psi(t)\rangle$ of the system at time t is related to the eigenvector $|\phi\rangle$ of H_0 by the S-matrix, i.e. , $|\psi(t)\rangle = S(t,-\infty)|\phi\rangle$. Up to the linear order of $H'_I(t')$, $S(t,-\infty) = 1 - \frac{i}{\hbar}\int_{-\infty}^{t} dt' H'_I(t')$, where $H'_I(t') = e^{iH_0t'/\hbar}H'e^{-iH_0t'/\hbar}$. Thus the total spin current including the external U(1) gauge potential $\mathbf{A}(\mathbf{r},t)$ reads

$$\begin{aligned}\langle\mathcal{J}_i^a(\mathbf{r},t)\rangle &= \langle\hat{J}_i^a(\mathbf{r},t)\rangle - \frac{e}{mc}A_i(\mathbf{r},t)s^a(\mathbf{r},t)\\ &= \frac{E_j(\mathbf{r},t)}{\hbar\omega}\int_{-\infty}^{t} dt' e^{i\omega(t-t')}e^{-i\mathbf{q}\cdot\mathbf{r}}\langle[\hat{J}_i^a(\mathbf{r},t),\hat{J}_j(\mathbf{q},t')]\rangle_0 + \frac{ie\delta_{ij}}{m\omega}s^a(\mathbf{r},t)E_j(\mathbf{r},t)\\ &\equiv \sigma_{ij}^a(\mathbf{q},\omega;\mathbf{r})E_j(\mathbf{r},t).\end{aligned} \tag{9}$$

The spin conductivity can be directly obtained after averaging over the whole system

$$\sigma_{ij}^a(\mathbf{q},\omega) = \frac{1}{\hbar\omega V}\int_{-\infty}^{t} dt'\ e^{i\omega(t-t')}\langle[\hat{J}_i^{\dagger a}(\mathbf{q},t),\hat{J}_j(\mathbf{q},t')]\rangle_0 + \frac{ie\delta_{ij}}{m\omega V}\int d\mathbf{r}s^a(\mathbf{r},t), \tag{10}$$

with V the volume of the system. A retarded current-current correlation function Q_{ij}^{ab} is introduced to calculate the spin conductivity:

$$Q_{ij}^a(\mathbf{q},t-t') = -\frac{i}{V}\ \theta(t-t')\langle[\ \hat{J}_i^{\dagger a}(\mathbf{q},t),\ \hat{J}_j(\mathbf{q},t')\ ]\rangle_0, \tag{11}$$

with its Fourier image in the frequency representation given by

$$Q_{ij}^a(\mathbf{q},\omega) = -\frac{i}{V}\int_{-\infty}^{+\infty} dt\ \theta(t-t')e^{i\omega(t-t')}\langle[\hat{J}_i^{\dagger a}(\mathbf{q},t),\ \hat{J}_j(\mathbf{q},t')\ ]\rangle_0. \tag{12}$$

As a result, we can rewrite the spin conductivity σ_{ij}^a in terms of the correlation function

$$\sigma_{ij}^a(\mathbf{q},\omega) = \frac{i}{\hbar\omega}\Big[Q_{ij}^a(\mathbf{q},\omega) + \frac{\hbar e\delta_{ij}}{mV}\int d\mathbf{r}s^a(\mathbf{r},t)\Big]. \tag{13}$$

The dc spin conductivity is finally obtained as the imaginary part of $\sigma^a_{ij}(\mathbf{q},\omega)$ by taking the limit $\omega \to 0$.[5]

One would wonder whether the Kubo formula still holds if choosing a zero-frequency electric field from the very beginning. The answer is positive as long as the continuity equation for the charge density holds. In the zero-frequency case, the interaction Hamiltonian is given by $H' = \int d\mathbf{r}\ \rho(\mathbf{r})A_0(\mathbf{r})$. By means of the method suggested by Luttinger, one needs to introduce the density matrix $f(t) = f_0 + \delta f(t)$ where f_0 refers to the density matrix with respect to the unperturbed Hamiltonian and $\delta f(t)$ is brought about by the perturbation H'. From the equation of motion for the perturbed part of the density matrix, $i\hbar\frac{\partial \delta f(t)}{\partial t} = [H_0, \delta f(t)] + [H', f_0]$, we can obtain a solution for $\delta f(t)$: $\delta f(t) = -\frac{1}{\hbar}\int_0^\infty dt \int_0^\beta d\beta'\ f_0 \frac{\partial}{\partial t} H'_I(-t - i\beta')$. With the help of the density matrix, the spin current can be then evaluated by taking the average

$$\langle \hat{J}^a_i(\mathbf{r},t)\rangle = \mathrm{tr}\big(f(t)\hat{J}^a_i(\mathbf{r})\big) = -\frac{1}{\hbar}\int_0^\infty dt \int_0^\beta d\beta' \mathrm{tr}\Big[f_0\ \frac{\partial}{\partial t}H'_I(-t - i\beta')\ \hat{J}^a_i(\mathbf{r})\Big], \quad (14)$$

where the equilibrium part of the current $\mathrm{tr}(f_0\hat{J}^a_i(\mathbf{r}))$ is assumed to be zero. The derivative of H'_I with respect to time t is calculated as $\partial_t H'_I(-t) = \int d\mathbf{r}\ \partial_t\rho(\mathbf{r},-t)A_0(\mathbf{r})$. The continuity equation for the charge density $\partial_t\rho + \nabla\cdot\mathbf{J} = 0$ leads to

$$\partial_t H'_I(-t) = -\int d\mathbf{r}\ E_i J_i(\mathbf{r},-t), \quad (15)$$

where the integration by parts has been used. Substituting it into Eq. (14), we obtain

$$\langle \hat{J}^a_i(\mathbf{r},t)\rangle = \frac{1}{\hbar}\int_0^\infty dt \int_0^\beta d\beta' \int d\mathbf{r}'\ \mathrm{tr}\Big[f_0 E_j J_j(\mathbf{r}', -t - i\beta')\hat{J}^a_i(\mathbf{r})\Big]. \quad (16)$$

Consequently, the dc SU(2) conductivity is obtained from the above equation after integrating $\mathbf{r}$ over the volume V,

$$\sigma^a_{ij} = \frac{1}{\hbar V}\int_0^\infty dt \int_0^\beta d\beta'\ \mathrm{tr}\Big[f_0 J_j(-t - i\beta')\ \hat{J}^a_i\Big]. \quad (17)$$

This result is consistent with the dc conductivity obtained from Eq.(10) as long as one chooses the representation of the eigenstates $|n\rangle$ of H_0.

3. Generalized Kubo Formula in Response to SU(2) Fields

Taking the SU(2) field as the perturbation, we have the interacting Hamiltonian as follow:

$$H' = \frac{-\eta}{2m}\sum_l \Big(\hat{\boldsymbol{\pi}}_l \cdot \boldsymbol{\mathcal{A}}^a_{\mathrm{ext}}(\mathbf{r}_l,t)\tau^a + \tau^a \boldsymbol{\mathcal{A}}^a_{\mathrm{ext}}(\mathbf{r}_l,t)\cdot\hat{\boldsymbol{\pi}}_l\Big). \quad (18)$$

Due to its non-Abelian feature, the SU(2) "electric" field[6] involves one more term of the gauge potentials than the U(1) field

$$E^a_i = -\partial_0\mathcal{A}^a_i - \partial_i\mathcal{A}^a_0 + \eta\epsilon^{abc}\mathcal{A}^b_0\mathcal{A}^c_i. \quad (19)$$

We also choose the single-frequency form for the SU(2) field and the gauge $\mathcal{A}_0^a = 0$. Thus $\mathcal{A}_i^a(\mathbf{r},t) = \frac{1}{i\omega}E_i^a(\mathbf{q},\omega)e^{i\mathbf{q}\cdot\mathbf{r}-i\omega t}$. Though the strategy in deriving the spin conductivity is much similar to the U(1) case, one should keep in mind that the algebra is totally different, which results in the appearance of more indices referring to the spin space. After careful formulation, the spin current evaluated for the ground states reads

$$\begin{aligned}\langle \mathcal{J}_i^a(\mathbf{r},t)\rangle &= \langle \hat{J}_i^a(\mathbf{r},t)\rangle - \frac{n_0\eta^2}{4m}\mathcal{A}_i^a(\mathbf{r},t)\\ &= \frac{E_j^b(\mathbf{r},t)}{\hbar\omega}\int_{-\infty}^{t} dt' e^{i\omega(t-t')}e^{-i\mathbf{q}\cdot\mathbf{r}}\langle[\hat{J}_i^a(\mathbf{r},t),\hat{J}_j^b(\mathbf{q},t')]\rangle_0 + \frac{i\eta^2 n_0}{4m\omega}\delta^{ab}\delta_{ij}E_j^b(\mathbf{r},t)\\ &\equiv \sigma_{ij}^{ab}(\mathbf{q},\omega;\mathbf{r})E_j^b(\mathbf{r},t),\end{aligned} \tag{20}$$

and the spin conductivity is obtained after averaging over the whole system

$$\sigma_{ij}^{ab}(\mathbf{q},\omega) = \frac{1}{\hbar\omega V}\int_{-\infty}^{t} dt'\ e^{i\omega(t-t')}\langle[\hat{J}_i^{\dagger a}(\mathbf{q},t),\hat{J}_j^b(\mathbf{q},t')]\rangle_0 + \frac{i\eta^2\ n_0}{4m\omega}\delta^{ab}\delta_{ij}, \tag{21}$$

where n_0 is the particle density. Some concrete examples for this generalized Kubo formula can be found in our previous paper.[7]

In the U(1) case, we have shown that Kubo formula is consistent no matter whether the electric field is chosen to be of zero-frequency at the beginning. The key point is that the continuity equation for the charge density always hold. However, the SU(2) current density does not conserve as long as an SU(2) interaction is present. For example, the spin current density is not conservative if there exists the spin-orbit coupling or the Zeeman term. The nonconservation of the spin density leads to the "continuity-like" equation $\left(\frac{\partial}{\partial t} - \eta\vec{\mathcal{A}}_0\times\right)\vec{s}(\mathbf{r},\ t) + \left(\frac{\partial}{\partial x_i} + \eta\vec{\mathcal{A}}_i\times\right)\vec{J}_i(\mathbf{r},\ t) = 0$. On the other hand, the SU(2) "electric" field involves one more term of the gauge potentials than the U(1) field. In the following, we will show that these two features exactly make the generalized Kubo formula describing the response to the SU(2) field consistent. We choose the gauge $\partial_0\mathcal{A}_i^a = 0$ for the zero-frequency case and the SU(2) "electric" field reads $E_i^a = -\partial_i\mathcal{A}_0^a + \eta\epsilon^{abc}\mathcal{A}_0^b\mathcal{A}_i^c$. In such a case, the interaction is given by $H_I'(t) = \int d\mathbf{r}\ s^a(\mathbf{r},t)\mathcal{A}_0^a(\mathbf{r})$. The derivative of H_I' with respect to time t is calculated as

$$\partial_t H_I'(-t) = \int d\mathbf{r}\ \partial_t s^a(\mathbf{r},-t)\mathcal{A}_0^a(\mathbf{r}). \tag{22}$$

Using Eq. (5) and the integration by parts, we have

$$\partial_t H_I'(-t) = \int d\mathbf{r}\Big(\eta\epsilon^{abc}(\mathcal{A}_0^b\,s^c - \mathcal{A}_i^b J_i^c) - \partial_i J_i^a\Big)\mathcal{A}_0^a = -\int d\mathbf{r}\ E_i^a J_i^a(\mathbf{r},-t). \tag{23}$$

After some similar calculation as we shown for the U(1) external field, one can also draw a conclusion that the generalized Kubo formula indeed holds even if choosing the zero-frequency field at the beginning. Now it is clear that the spin procession terms, $\eta\vec{\mathcal{A}}_i\times\vec{J}_i(\mathbf{r},\ t) - \eta\vec{\mathcal{A}}_0\times\vec{s}(\mathbf{r},\ t)$, precisely compensate the extra term $\eta\epsilon^{abc}\mathcal{A}_0^b\mathcal{A}_i^c$ in the SU(2) field. This finally makes our theory self-consistent.

4. Summary

We have illustrated the derivation of the "continuity-like" equation for the spin density in the system with SU(2) gauge potentials, which is useful in proving the consistency of the generalized Kubo formula. For the demand in the spin transport, we generalized the conventional Kubo formula to describe the linear responses to both the external U(1) and SU(2) fields. We found that even though the spin density does not conserve in the present of the SU(2) gauge potentials, the processing terms $\eta\vec{\mathcal{A}}_i \times \vec{J}_i(\mathbf{r},\ t) - \eta\vec{\mathcal{A}}_0 \times \vec{s}(\mathbf{r},\ t)$ in the "continuity-like" equation exactly cancel the extra term $\eta\epsilon^{abc}\mathcal{A}_0^b\mathcal{A}_i^c$ in the SU(2) "electric" field, which keeps the consistency of our generalized Kubo formula between different gauge choices.

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