Conserved geometric phase and group velocity

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In this paper we make use of the concept of conserved geometric phase and of group velocity, in conjunction with the representation theory, in order to derive some relevant physical quantities for the description of the dielectric and magnetic response of crystalline materials. As an application of the model, we derive the expression of the macroscopic dipole moment per unit volume, and the expression of the current induced by a uniform static external electromagnetic field.

INTRODUCTION

In 1983, in a milestone paper, M.V. Berry showed that a quantal system in an eigenstate, slowly transported around a circuit C, by varying parameters \( \beta \) in its Hamiltonian \( H_\beta \), will acquire a geometrical phase factor \( \Phi \) in addition to the dynamical phase factor. Moreover, in 1986 Y. Aharonov and J. Anandan showed that it is possible to define a new geometrical phase factor for any cyclic evolution of a quantum system, independently of the adiabatic approximation, and expressible as a gauge invariant quantity, including Berry’s case as a particular case.

In 1988, J.Zak showed also that it is possible to define a Berry’s phase for the dynamics of electrons in infinite periodic systems, suggesting how to label bands of a crystal by making use of the conserved geometric phase. In early nineties R.Resta and D.Vanderbilt showed, how to relate the conserved geometric phase to the macroscopic dipole moment per unit volume of a crystalline insulator. The model have been called by the authors the modern theory of polarization. In the following section, we shall review the concept of polarization in crystals, within the modern point of view.

POLARIZATION AND GEOMETRIC PHASE

The problem of the dielectric and magnetic response of matter, in condensed matter physics, have been intensively studied in the last decades (and references therein). A particularly interesting example is the treatment of the electronic structure of a crystalline material in an external uniform electrostatic field. The modern theory of polarization in crystals is one of the most important recent developments, in fact, the macroscopic polarization is a basic quantity used to describe, classically, dielectric media.

However a crystal is only a particular example of a quantal body and the classical concept of polarization extends also to non crystalline (disordered) systems, and it should not depend on the particular model system employed to perform explicit calculations.

As shown by Resta it is possible to define variations \( \Delta P \), of the dipole per unit volume of a crystal, due to a source, and given by

\[
\Delta P = P^{(1)} - P^{(0)} = \int_0^1 (\frac{\partial P}{\partial \lambda}) d\lambda
\]

Here \( \lambda \) is a dimensionless parameter depending on time; \( \lambda = 0 \) and \( \lambda = 1 \) represent the initial and the final states of the system, along a transformation that changes the periodic potential.

An explicit representation of \( P^{(\lambda)} \) in terms of the amplitudes \( u_{nk} \) of Bloch-states, has been derived by King-Smith and Vanderbilt:

\[
P^{(\lambda)} = \frac{e}{(2\pi)^3} \sum_n \int_{BZ} dk \langle u_{nk}^{(\lambda)} | \nabla_k | u_{nk}^{(\lambda)} \rangle
\]

where \( e > 0 \) is the absolute value of the charge of the electron, \( BZ \) is the Brillouin zone of the crystal and \( n \) is a discrete index, running over occupied bands.

Variations of this dipole per unit volume have been interpreted as the integrated electronic polarization current. According to the modern point of view, only variations of polarization are physical observables, completely independent of the periodic charge distribution. The charge density is represented by the squared modulus of the wave functions. Variations of polarization, instead, have been related to a Berry’s phase of the system. We shall try to clarify this statement in what follows.

GEOMETRIC PHASE AND V MATRIX

Here it is shown how to develop a calculation scheme in order to model the response of a body, in its steady states, to a static uniform electromagnetic field. The model is based on the concepts of group velocity and of conserved geometric phase. At this point we point out that we may assume definition of being valid even when a uniform static external field, is present in the system, as it is independent, i.e.
external, to the charge distribution of the quantal body (QB). In the following we shall always consider the states of the body of being implicitly dependent on external fields.

It is already known, in condensed matter physics, that the macroscopic electronic dipole moment per unit volume, of an insulator is related to a conserved geometric phase\[^3\,^4\]. Here, we show how to obtain a conserved geometric phase in absence of external electromagnetic fields. We start our discussion presenting in this section part of the work of Zak\[^1\,^4\], in order to introduce the reasoning which led us to derive results reported in the following section. Firstly, we derive the conserved geometric phase making use of a matrix that we shall call V matrix. V is obtainable from the expectation values of the group velocity operator\[^3\,^1\].

In analogy to \[^1\,^1\,^4\], if we now derive eq.(3) with respect to \(k\) we obtain

\[
\frac{\hbar}{m} (-i\hbar \nabla_q + \hbar k) u_{n,k}(q) + H_{0,k} \nabla_q u_{n,k}(q) = \nabla_k \epsilon_n u_{n,k}(q) + \epsilon_n \nabla_k u_{n,k}(q) \tag{4}
\]

Multiplying eq.(4) on the left by \(u_n^*\), dividing by \(\hbar\) and integrating with respect to \(q\) in the super-cell we obtain

\[
v_{mn} = \langle u_{m,k} | v | u_{n,k} \rangle = -i \omega_{mn} d_{mn} + \frac{1}{\hbar} \nabla_k \epsilon_n \delta_{mn} \tag{5}
\]

where we write the transition frequencies as \(\omega_{mn} = \frac{\epsilon_m - \epsilon_n}{\hbar}\) and

\[
v = \frac{(-i\hbar \nabla_q + \hbar k)}{m} \tag{6}
\]

is the group velocity operator as shown in ref.\[^3\]. Coefficients \(v_{mn}\) are the matrix elements of the V matrix.

In the following, we shall express \(\langle u_{m,k} | v | u_{n,k} \rangle\) as also \(\langle m | v | n \rangle\) in order to simplify the notation.

Matrix elements \(d_{mn}\) are defined as

\[
d_{mn} = \langle u_{m,k} | \nabla_k | u_{n,k} \rangle \tag{7}
\]

and because of the normalization condition of the complex wave functions \(u_{nk}\) follows that

\[
d_{mn}^* = -d_{mn} \tag{8}
\]

also implying that the diagonal fields are real. From eq.(5) follows

\[
d_{mn} = i \frac{v_{mn}}{\omega_{mn}} m \neq n \tag{9}
\]

\[
v_{nn} = \frac{1}{\hbar} \nabla_k \epsilon_n m = n \tag{10}
\]

Let us first note that the trace of the velocity operator, evaluated with respect to the occupied bands, is

\[
\text{Tr}(v_{mn}) = \sum_n v_{nn} = \sum_n \frac{1}{\hbar} \nabla_k \epsilon_n = v(k) \tag{11}
\]

that is an invariant quantity because of its geometric nature. It represents the electronic current density of the system, in \(k\) space, once multiplied by the electronic charge \(e\),

\[
j(k) = e \text{Tr}(v_{mn}) = ev(k) \tag{12}
\]

By relation (10) in the appendix, and taking the curl of vectors \(d_{nn}\) it is possible to define

\[
\nabla \times d_{nn} = i \int \nabla_k u_{n,k}^*(q) \times \nabla_k u_{n,k}(q) dq \tag{13}
\]

as already shown by Zak\[^1\,^4\]. Also, by equation (11) follows that

\[
i \nabla_k u_{n,k}(q) = \sum_m d_{mn} u_{m,k}(q) \tag{14}
\]

and combined with eq.(12) gives

\[
\nabla \times d_{nn} = i \sum_{m \neq n} d_{mn} \times d_{nn} \tag{15}
\]

Making use of eq.(9) we obtain

\[
\nabla \times d_{nn} = i \sum_{m \neq n} d_{mn} \times d_{nn} = i \sum_{m \neq n} \frac{v_{mn} \times v_{mn}}{\omega_{mn}^2} \tag{16}
\]

in agreement with Berry and Zak’s derivations\[^1\,^4\]. We can evaluate then the flux of the field given by eq.(16), through the closed surface \(S\) of the Brillouin zone in \(k\) space, containing a closed curve \(C\).
We may either write
\[
\int_S dS \cdot \text{Im} \sum_{m \neq n} \frac{v_{mn} \times v_{nm}}{\omega_{mn}^2} = \int_S dS \cdot \nabla_k \times d_{mn}
\]
\[
= \oint_C d_{nn} \cdot dl = \phi_n(C)
\]
(16)
or in a different way,
\[
\int_S dS \cdot \text{Im} \sum_{m \neq n} d_{mn} \times d_{nm} = \int_S dS \cdot \nabla_k \times d_{nn}
\]
\[
= \oint_C d_{nn} \cdot dl = \phi_n(C)
\]
(17)
where \( \text{Im} \) stands for imaginary. After a summation over \( n \), we find
\[
\sum_n \phi_n(C) = \Phi(C)
\]
(18)
being \( \Phi(C) \) is the conserved geometric phase. In view of eq.(15) we note that \( \nabla_k \times d_{nn} \) is the trace of the Berry’s curvature [4], while instead \( d_{nn} \) is Berry’s connection [4].

Let us calculate the averaged trace of fields \( d_{nn} \), integrated over the Brillouin zone in reciprocal space, or in other words
\[
\bar{P} = e \bar{d}
\]
\[
= \frac{e}{(2\pi)^3} \sum_n \int_{BZ} dk < m_k | \nabla_k | n >
\]
\[
= \frac{e}{(2\pi)^3} \int_{BZ} dk \text{Tr}(d_{nn})
\]
\[
= e \int_{BZ} \frac{dk}{(2\pi)^3} \bar{d}
\]
where \( e \) is the electronic charge. The circuit integral of the field \( \bar{P} \) defined as
\[
\int_C \bar{P} \cdot dl = e \Phi(C)
\]
(20)
is
\[
\int_C P \cdot dl = e \Phi(C)
\]
Eq.(10) is coincident with results found in ref.[21, 22] (see also [21, 22, 23, 24] for its use in numerical calculations). Because of that we can associate to \( P \) the meaning of macroscopic dipole moment per unit volume of the system, in its steady states.

Berry’s phase instead is given by eq.(21), so that we may think of a classification of materials, as a function of values of \( \Phi(C) \), directly related to definition (20).

Moreover, we may calculate the conserved phase \( \Phi(C) \), not only by the knowledge of matrix elements of \( V \), as in eq.(16), but also by the knowledge of matrix elements \( d_{mn} \) by eq.(17). A discussion about degeneracies of the energy spectrum can be found in references [1, 2, 3, 14, 21, 22, 23, 24].

For what stated in [21], and by results given in [31] the reasoning may be directly extended to a many-body theory.

In that context the expression (15) will be generalized by eq.(18) of [31],
\[
v_{mn} = < m | \frac{1}{\hbar} \nabla_k H | n >
\]
(22)
being \( H \) the \( k \) dependent Hamiltonian of the problem. In the following, we extend the problem, to the case of an external uniform magnetostatic field present in the system.

\[\text{V MATRIX IN MAGNETIC FIELDS}\]

In this section we generalize the problem to the case of an external uniform magnetostatic field \( B^0 \) present in the system. The Hamiltonian operator is given by
\[
H_k \equiv \frac{1}{2m}(-\hbar \nabla_q + \hbar k + \frac{e}{c} B^0 \times i \nabla_k)^2 + V(q)
\]
(23)
The corresponding expression of the group velocity operator is then,
\[
v(B^0) = \frac{1}{\hbar} \nabla_k H_k
\]
(24)
so that matrix elements of the velocity operator are expressible as follows
\[
v_{mn}(B^0) = < m | v(B^0) | n > = -i \omega_{mn} d_{mn}
\]
\[
+ \frac{1}{\hbar} \nabla_k \epsilon d_{nn} + \frac{e}{mc} B^0 \times d_{mn}
\]
(25)
In analogy with (11), the current density is
\[
\mathbf{j}(k) = e \text{Tr}(v_{mn}) = e v(k) + \frac{1}{c} \omega_{cycl} \mathbf{b} \times \mathbf{P}
\]
(26)
being \( b \) a unit vector parallel to the direction of the magnetic field and \( \omega_{cycl} = \frac{eB_0}{mc} \) the cyclotron frequency of an electron. Moreover, by equation (26) and (48) we can calculate the divergence of the current as follows
\[
\nabla \cdot j(k) = e \nabla \cdot v - \frac{1}{c^2} \omega_{cycl} b \cdot \text{rot} P
\]  
(27)

In the following section we shall derive another vectorial field, that is directly related to the curl of the dipolar magnetic field and the following relation obtained by the definition of another vectorial field. By eq.(19) is valid the following relation
\[
\omega_{cycl} \cdot b \times \text{rot} P = J^S
\]  
(30)

where \( S \) stands for symmetric combination. After a summation over \( m \neq n \) we obtain
\[
J^S_n = \sum_{m \neq n} \left[ \frac{V_{mn}^{(B^0)} \times V_{nm}^{(B^0)} + V_{mn}^{(B^0)} \times V_{nm}^{(B^0)}}{2\omega_{mn}} \right]
\]  
(29)

being \( \text{rot} d_{mn} = \nabla_k \times d_{mn} \).

By eq.(20) is valid the following relation
\[
\frac{\omega_{cycl}}{c} b \times \text{rot} P = J^S
\]  
(30)

where
\[
J^S = e \sum_n J^S_n = e v^S
\]  
(31)

Definition (20) also implies that
\[
\int_V dV \nabla \cdot J^S = -b \cdot \int_S dS \times \text{rot} P
\]  
(32)

We associate the meaning of a current to the field \( J^S \), whose source is related to the rotational properties of \( P \). An alternative derivation of the above results can be obtained by the definition of another vectorial field. By the following relation
\[
[V_{mn}^{(B^0)} \times d_{nn}] = -i\omega_{mn}(d_{mn} \times d_{nm}) + \frac{e}{mc} (B^0 \times d_{mn}) \times d_{nm}
\]  
(33)

we find
\[
I^A_n = i \sum_{m \neq n} [d_{mn} \times v_{mn}^{(B^0)}] - [d_{nn} \times v_{nm}^{(B^0)}]
\]  
(34)

directly derivable by \( d_{mn} \) and \( v_{mn} \) matrix elements, it is clear that \( I^A_n \equiv V^S_n \) and we can define
\[
J^S = e \sum_n I^A_n
\]  
(35)

APPEARANCE OF THE GEOMETRIC PHASE

Taking the vectorial product of \( B^0 \) and the field \( v^S_n \) we obtain
\[
B^0 \times v^S_n = \frac{e|B_0|^2}{mc} b \times (b \times \text{rot} d_{mn})
\]  
(36)

Let us exclude the cases \( \text{rot} P = 0 \), and \( \text{rot} P \) parallel to \( b \).

Dividing eq.(36) by \( |B_0|^2 \), summing over \( n \) and calculating the flux of \( v^S_n \) over the surface \( S \) of the Brillouin zone, containing a closed curve \( C \) we obtain
\[
-\int_S dS \cdot (b \times v^S) = \frac{\omega_{cycl}}{c} \int_S dS \cdot \text{rot} d
\]  
(37)

Multiplying eq.(37) by the electronic charge and bearing in mind eq.(21) we obtain
\[
b \cdot \int_V dV \text{rot} J^S = -\frac{e}{c} \int_S dS \cdot (b \times J^S) = \frac{\omega_{cycl} e}{c} \Phi(C)
\]  
(38)
LOW POWERS OF $\frac{1}{c}$

Bearing in mind definition (26), we can write at first order of powers of $\frac{1}{c}$

$$[V_{mn}^{(B^0)} \times V_{mn}^{(B^0)}] \sim \omega^2_{mn} d_{mn} \times d_{mn} + i\omega_{mn} \frac{B^0}{mc} \times (d_{mn} \times d_{nm})$$

(39)

Defining

$$V_A^{mn} = \frac{[V_{mn}^{(B^0)} \times V_{mn}^{(B^0)} - V_{mn}^{(B^0)} \times V_{mn}^{(B^0)}]}{2}$$

(40)

dividing by $\omega^2_{mn}$, and summing over $m \neq n$ we obtain

$$V_A^n = i \sum_{m \neq n} \omega^2_{mn} \left( \frac{V_{mn}^{(B^0)} \times V_{mn}^{(B^0)} - V_{mn}^{(B^0)} \times V_{mn}^{(B^0)}}{2\omega^2_{mn}} \right)$$

(41)

Evaluating the flux over the surface $S$ of the Brillouin zone we find

$$\int_S dS \cdot [V_A^n] = \Phi_n(C)$$

(42)

If we instead consider also terms containing second powers of $\frac{1}{c}$, we instead obtain

$$\int_S dS \cdot [V_A^n] = \Phi_n(C) + \frac{1}{c^2} \sum_{m \neq n} \int_S dS \cdot \left[ \frac{\omega_{mn}^2}{\omega_{mn}^2} (b \cdot (d_{mn} \times d_{nm}))b \right]$$

(43)

Equations (46) and (33), in conjunction with eqs. (21) and eq. (30), clearly show that if the vectorial field $d$ is conservative (irrotational, rot $d = 0$), then the system would acquire a vanishing Berry’s phase, and the vectorial field $J^{S}$ would become vanishing by eq. (30). Moreover, if $d$ is conservative, the divergence of the current $j(k)$ will not be affected by the latter. In the case of $d$ not being conservative the flux of $j(k)$ over the surface of the Brillouin zone will be instead proportional to the projection, over the direction of the applied magnetostatic field, of the circulation of $d$ (or equivalently $P$) over the surface of the Brillouin zone.

POWER IN A UNIFORM STATIC ELECTROMAGNETIC FIELD

The group velocity is not explicitly dependent on a uniform electrostatic field $E_0$ eventually present in the system, so that all the results obtained above are equally right even if $E_0$ is present in the system. Bearing in mind eqs. (26) and eq. (19), we can express the work per unit time and per unit volume done by the electromagnetic field $(E_0, B^0)$ on the body as

$$W = E_0 \cdot J = E_0^0 \cdot \int_V dV \bar{j}(k)$$

$$= eE_0^0 \cdot \int_V dV \bar{v} + \frac{4\pi e^2}{mc^2} \bar{S} \cdot \bar{d}$$

(44)

being $\bar{S} = \frac{\bar{e}}{c^2} (E_0 \times B^0)$ the Poynting vector, associated to the electromagnetic field and $V$ the volume of the Brillouin zone in $k$-space.

CONCLUSIONS

The reported non-relativistic calculation scheme, may be useful for practical calculations of macroscopic electromagnetic properties of a quantal body interacting with a static external uniform electromagnetic field. It has been shown how to calculate the power density, the macroscopic polarization $\bar{P}$, and the electronic current induced by the presence of a uniform magnetostatic field $B^0$, making use of the concept of group velocity. It has been shown the reasoning in the case of the one-body approximation, and by construction it would apply to every first-principles calculation scheme based on periodic boundary conditions within a DFT scheme [30]. The above discussion can be extended to a ‘many-body’ theory because of what stated in [4]. Eq. (10) may help us for a theoretical classification of crystalline materials via the values of $\Phi(C)$, that are directly dependent on the dielectric properties of the material under consideration via eq. (21). We may also think that dielectric and magnetic properties of the crystalline material determine its geometrical properties too. In fact eq. (21) [48], eq. (40) show that if the vectorial field $d$ is conservative (irrotational, rot $d = 0$), then the system would acquire a vanishing Berry’s phase and the vectorial field $J^{S}$ would become vanishing by eq. (30). Nevertheless a proper theoretical solution of the problem requires a theoretical study of the ionic response as well as the electronic one, that we leave to a future work. The model presented above allows us to find several useful physical quantities in a clear and simple way, amenable of a straightforward physical interpretation.
APPENDIX

Vector Identities

\[ \nabla \times (fA) = f\nabla \times A + (\nabla f) \times A \]  
\[ A \times (B \times C) = (A \cdot C)B - (A \cdot B)C \]  
\[ (A \times B) \times (C \times D) = ((A \times B) \cdot D)C - ((A \times B) \cdot C)D \]  
\[ (\nabla \cdot A) \times B = B \cdot \nabla \times A - A \cdot \nabla \times B \]

J^8 FIELD

Let us evaluate the following quantity

\[ v_{mn}^{(B^0)} \times v_{nm}^{(B^0)} = \omega_{mn}^2 d_{mn} \times d_{nm} \]
\[ + \frac{e^2}{m^2 c^2} \left[ (B^0 \times d_{mn}) \times (B^0 \times d_{nm}) \right] \]
\[ - i\omega_{mn} \left[ d_{mn} \times \left( \frac{e}{mc} (B^0 \times d_{nm}) \right) \right] \]
\[ + i\omega_{nm} \left[ d_{nm} \times \left( \frac{e}{mc} (B^0 \times d_{mn}) \right) \right] \]  
\[ = \omega_{mn}^2 d_{mn} \times d_{nm} \]
\[ + \frac{e^2}{m^2 c^2} \left[ (B^0 \times d_{mn}) \times (B^0 \times d_{nm}) \right] \]
\[ + i\omega_{mn} \left[ d_{mn} \times \left( \frac{e}{mc} (B^0 \times d_{nm}) \right) \right] \]
\[ + \omega_{mn} \left[ d_{nm} \times \left( \frac{e}{mc} (B^0 \times d_{mn}) \right) \right] \]
\[ = \omega_{mn}^2 d_{mn} \times d_{nm} \]
\[ + \frac{e^2}{m^2 c^2} \left[ (B^0 \times d_{mn}) \times (B^0 \times d_{nm}) \right] \]

From eq. (49), making use of the vector identity (46), and the fact that \( \omega_{mn} = -\omega_{nm} \) we can recast the last two terms of eq. (49) as follows

\[ - i\omega_{mn} \left[ d_{mn} \times \left( \frac{e}{mc} (B^0 \times d_{nm}) \right) \right] \]
\[ + \omega_{mn} \left[ d_{nm} \times \left( \frac{e}{mc} (B^0 \times d_{mn}) \right) \right] \]
\[ = \frac{e}{mc} B^0 \times (d_{mn} \times d_{nm}) \]

so that

\[ v_{mn}^{(B^0)} \times v_{nm}^{(B^0)} = \omega_{mn}^2 d_{mn} \times d_{nm} \]
\[ + i\omega_{mn} \left[ d_{mn} \times \left( \frac{e}{mc} B^0 \times (d_{nm} \times d_{nm}) \right) \right] \]
\[ + \frac{e^2}{m^2 c^2} \left[ (B^0 \times d_{mn}) \times (B^0 \times d_{nm}) \right] \]
\[ = \omega_{mn}^2 d_{mn} \times d_{nm} \]
\[ + i\omega_{mn} \left[ d_{mn} \times \left( \frac{e}{mc} B^0 \times (d_{nm} \times d_{nm}) \right) \right] \]
\[ + \frac{e^2}{m^2 c^2} \left[ (B^0 \times d_{mn}) \times (B^0 \times d_{nm}) \right] \]
\[ = \omega_{mn}^2 d_{mn} \times d_{nm} \]
\[ + i\omega_{mn} \left[ d_{mn} \times \left( \frac{e}{mc} B^0 \times (d_{nm} \times d_{nm}) \right) \right] \]
\[ + \frac{e^2}{m^2 c^2} \left[ (B^0 \times d_{mn}) \times (B^0 \times d_{nm}) \right] \]

and define the following quantity,

\[ i \sum_{m \neq n} \frac{v_{mn}^{(B^0)} \times v_{nm}^{(B^0)}}{\omega_{mn}^2} = \text{rot } d_{mn} \]
\[ - \sum_{m \neq n} \frac{\omega_{cycl}}{\omega_{mn} c} \left[ \frac{d_{mn} \times d_{nm}}{\omega_{mn} c} \right] \]
\[ + i \sum_{m \neq n} \frac{\omega_{cycl}^2}{c^2 \omega_{mn}^2} \left[ \frac{d_{mn} \times d_{nm}}{\omega_{mn} c} \right] b \]
\[ = \frac{\omega_{cycl}^2}{c^2 \omega_{mn}^2} \left[ \frac{d_{mn} \times d_{nm}}{\omega_{mn} c} \right] b \]
\[ \]  
\[ \text{being } b \text{ a unit vector in the direction of the magnetic axis and } \omega_{cycl} \text{ is the electronic cyclotron frequency per unit magnetic field, defined as } \frac{\omega_{cycl}}{c} = \frac{e}{mc}. \]

We can write

\[ [v_{mn}^{(B^0)} \times v_{nm}^{(B^0)}] = \omega_{mn}^2 d_{mn} \times d_{nm} \]
\[ + i\omega_{mn} \left[ d_{mn} \times \left( \frac{e}{mc} B^0 \times (d_{nm} \times d_{nm}) \right) \right] \]
\[ + \frac{e^2}{m^2 c^2} \left[ (B^0 \times d_{mn}) \times (B^0 \times d_{nm}) \right] B^0 \]
and

\[
\langle \mathbf{v}^{(\mathbf{B}^0)} \times \mathbf{v}^{(\mathbf{B}^0)} \rangle = \omega_n^2 n m d_{mn} \times d_{nm} \\
+ i \omega_n \frac{e}{mc} B^0 \times (d_{mn} \times d_{nm}) \\
+ \frac{e^2}{mc^2} (B^0 \cdot (d_{mn} \times d_{nm})) B^0 \\
= -\omega_n^2 n m d_{mn} \times d_{nm} \\
+ i \omega_n \frac{e}{mc} B^0 \times (d_{mn} \times d_{nm}) \\
- \frac{e^2}{mc^2} (B^0 \cdot (d_{mn} \times d_{nm})) B^0 \\
= -[\mathbf{v}^{(\mathbf{B}^0)} \times \mathbf{v}^{(\mathbf{B}^0)}] \\
+ 2 \omega_n \frac{e}{mc} B^0 \times (d_{mn} \times d_{nm})
\]

eq. (55) and eq. (56) imply then

\[
\mathbf{v}_n^S = \frac{\mathbf{v}^{(\mathbf{B}^0)} \times \mathbf{v}^{(\mathbf{B}^0)} + \mathbf{v}^{(\mathbf{B}^0)} \times \mathbf{v}^{(\mathbf{B}^0)}}{2 \omega_n} \\
= i \frac{e}{mc} B^0 \times (d_{mn} \times d_{nm})
\]

Also, summing over \(m \neq n\) we find

\[
\mathbf{v}_n^S = \sum_{m \neq n} \left[ \frac{\mathbf{v}^{(\mathbf{B}^0)} \times \mathbf{v}^{(\mathbf{B}^0)} + \mathbf{v}^{(\mathbf{B}^0)} \times \mathbf{v}^{(\mathbf{B}^0)}}{2 \omega_n} \right] \\
= \frac{e}{mc} B^0 \times i \sum_{m \neq n} (d_{mn} \times d_{nm}) = \frac{e}{mc} B^0 \times \text{rot} d_{mn}
\]

eq. (57) and eq. (58) implies

\[
\frac{\omega \rho d}{e} \mathbf{b} \times \text{rot} \mathbf{P} = \mathbf{J}^S
\]

where

\[
\mathbf{P} = e \mathbf{d} = e \sum_n d_{nn}
\]

and

\[
\mathbf{J}^S = e \sum_n \mathbf{v}_n^S = e \mathbf{v}^S
\]

1A field

Let us write the following quantity

\[
\langle \mathbf{v}^{(\mathbf{B}^0)} \times \mathbf{d}_{mn} \rangle = -i \omega_m (d_{mn} \times d_{nm}) \\
+ \frac{e}{mc} (B^0 \times d_{mn}) \times d_{mn}
\]

We find

\[
i \sum_{m \neq n} \langle \mathbf{v}^{(\mathbf{B}^0)} \times \mathbf{d}_{mn} \rangle - \langle \mathbf{v}^{(\mathbf{B}^0)} \times \mathbf{d}_{mn} \rangle = \frac{e}{mc} B^0 \times \text{rot} \mathbf{d}_{mn}
\]

(63)

In fact, by making use of definition (41), the vector identity (30), eq. (38), and the relation \(\omega_m = -\omega_m\), we find

\[
\langle \mathbf{v}^{(\mathbf{B}^0)} \times \mathbf{d}_{mn} \rangle - \langle \mathbf{v}^{(\mathbf{B}^0)} \times \mathbf{d}_{mn} \rangle = \\
= -i \omega_m (d_{mn} \times d_{nm}) + \frac{e}{mc} (B^0 \times d_{mn}) \times d_{mn} \\
- [-i \omega_m (d_{mn} \times d_{nm}) + \frac{e}{mc} (B^0 \times d_{mn}) \times d_{mn}] \\
= -i \omega_m (d_{mn} \times d_{nm}) + \frac{e}{mc} (B^0 \times d_{mn}) \times d_{mn} \\
- [-i \omega_m (d_{mn} \times d_{nm}) + \frac{e}{mc} (B^0 \times d_{mn}) \times d_{mn}] \\
= -i \omega_m (d_{mn} \times d_{nm}) + \frac{e}{mc} (B^0 \times d_{mn}) \times d_{mn} \\
+ i \omega_m (d_{mn} \times d_{nm}) - \frac{e}{mc} (B^0 \times d_{mn}) \times d_{mn} \\
= \frac{e}{mc} (B^0 \times d_{mn}) \times d_{nm} - \frac{e}{mc} (B^0 \times d_{mn}) \times d_{mn} \\
= \frac{e}{mc} [-d_{mn} \times (B^0 \times d_{mn}) + d_{mn} \times (B^0 \times d_{mn})] \\
= \frac{e}{mc} [-d_{mn} \times (B^0 \times d_{mn}) + d_{mn} \times (B^0 \times d_{mn})] \\
+ (d_{mn} \times d_{nm}) B^0 - (d_{mn} \times B^0) d_{mn} \\
= \frac{e}{mc} [(d_{mn} \times B^0) d_{mn} - (d_{mn} \times B^0) d_{nm}] \\
= \frac{e}{mc} B^0 \times (d_{mn} \times d_{nm})
\]

(64)

By definition (25) and eq. (8) follows that

\[
\sum_{m \neq n} [d_{mn} \times \mathbf{v}^{(\mathbf{B}^0)}] - [d_{mn} \times \mathbf{v}^{(\mathbf{B}^0)}] = \frac{e}{mc} B^0 \times \text{rot} \mathbf{d}_{mn}
\]

(65)

is a pure imaginary field.

Also we may re-write eq. (65) as

\[
\mathbf{1}^A = i \sum_{m \neq n} [d_{mn} \times \mathbf{v}^{(\mathbf{B}^0)}] - [d_{mn} \times \mathbf{v}^{(\mathbf{B}^0)}]
\]

(66)

We can evaluate the following flux over the surface of BZ (Brillouin zone) in k space, containing a closed curve
\[ C, \]
\[
= \sum_n \left[ \int_S dS \cdot 1^n \right] \]
\[
= \sum_n \omega_{\text{cycl}} \int_S dS \cdot (b \times \text{rot} \, d_{nn}) \]
\[
= \sum_n \omega_{\text{cycl}} \int_V dV \nabla \cdot (b \times \text{rot} \, d_{nn}) \]
\[
= - \sum_n \omega_{\text{cycl}} \int_V dV b \cdot (\nabla \times \text{rot} \, d_{nn}) \tag{67} \]
\[
= -\omega_{\text{cycl}} \int_V dV b \cdot (\nabla \times d) \]
\[
= -\omega_{\text{cycl}} b \cdot \int_V dV (\nabla \times b) \]
\[
= -\omega_{\text{cycl}} b \cdot \int_S dS \times \text{rot} \, d \]

where in the third line has been used Gauss’s theorem (divergence theorem), and \( \omega_{\text{cycl}} = \frac{e}{2m} \) is the cyclotron frequency per unit magnetic field and \( B^0 = |B^0| \mathbf{b} \), being \( \mathbf{b} \) the direction of the magnetic axis. Equations [67] and \( \int_S \) imply also

\[
\int_V dV \nabla \cdot J^S = -b \cdot \int_S dS \times \text{rot} \, P \tag{68} \]

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