General form of the full electromagnetic Green function in materials physics

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\section*{Abstract}
In this article, we present the general form of the full electromagnetic Green function which is suitable for the application in bulk materials physics. In particular, we show how the seven adjustable parameter functions of the free Green function translate into seven corresponding parameter functions of the full Green function. Furthermore, for both the fundamental response tensor and the electromagnetic Green function, we discuss the reduction of the Dyson equation on the four-dimensional Minkowski space to an equivalent, three-dimensional Cartesian Dyson equation.

\textit{Keywords:} electrodynamics in media, Green function

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# Contents

1 Introduction .......................................................... 3

2 Basic techniques ................................................... 3
   2.1 Projector formalism ............................................. 3
   2.2 (3+1)-formalism .................................................. 5

3 Free electromagnetic Green function .............................. 6
   3.1 Definition ......................................................... 6
   3.2 General form ...................................................... 7
       3.2.1 Projector formalism ....................................... 7
       3.2.2 (3+1)-formalism .......................................... 8
   3.3 Temporal gauge .................................................. 9

4 Fundamental response tensor ...................................... 10
   4.1 Definition ......................................................... 10
   4.2 General form ...................................................... 11
   4.3 Proper response tensor ......................................... 12

5 Full electromagnetic Green function .............................. 14
   5.1 Definition ......................................................... 14
   5.2 General form ...................................................... 15
       5.2.1 Projector formalism ....................................... 15
       5.2.2 (3+1)-formalism .......................................... 18
   5.3 Temporal gauge .................................................. 21

6 Conclusion ............................................................ 22

A Cartesian, Minkowskian, and scalar equations ................. 24
1. Introduction

The full electromagnetic Green function with the ensuing relation to its free counterpart via the famous Dyson equation is a well-established object of study in quantum electrodynamics (see the standard textbooks [1, §7.1.1], [2, §7.5], [3, p. 189, Problem 9.2], or [4, Eqs. (9.87)–(9.88)]). By contrast, in ab initio materials physics one typically restricts attention to the so-called screened potential [5, 6], such that the relativistic Schwinger-Dyson equations [1, §10.1] can be reduced to their non-relativistic counterpart, the so-called Hedin equations [7, 8]. However, it first became obvious in plasma physics that the full electromagnetic Green function is a natural object to study in electrodynamics of materials as well (plasmas in this case), especially when it comes to the formulation of wave equations in media [9, §2.1].

This line of research has been resumed by the authors of the present article in their quest for a microscopic formulation of electrodynamics in media, which is both Lorentz covariant [10, 11] and in accordance with the common practice in ab initio materials physics [12]. In particular, it turned out that in condensed matter physics, the wave equation can be reformulated concisely in terms of the full electromagnetic Green function [13, §4.1.4]. Not surprisingly in this context, a succinct connection between the Cartesian dielectric tensor and the spatial part of the full electromagnetic Green function in the temporal gauge has been unearthed [14, Eq. (3.44)]. As this relation crucially hinges on the gauge condition for the Green function, these findings make it desirable to study the most general form of the full electromagnetic Green function in bulk materials, a problem which had already been solved for the free electromagnetic Green function in Ref. [15, §3.3].

Here, we address this issue as follows: After introducing some technicalities in Sct. 2 and a short review of the free Green function in Sct. 3, the basics of microscopic electrodynamics in materials—including, in particular, the fundamental response tensor—are introduced in Sct. 4. The central Sct. 5 then introduces the full Green function, derives its most general form, and discusses the reduction of the corresponding four-dimensional Dyson equation to its three-dimensional Cartesian version.

2. Basic techniques

2.1. Projector formalism

In this first subsection, we shortly assemble some technicalities which will be useful in the following. The Minkowskian longitudinal and transverse
projectors are operators acting on the four-dimensional Minkowski space as follows (see [15, §3.3]):

\[(P_L)_{\mu \nu}(k) = \frac{k^\mu k_\nu}{k^2}, \quad (2.1)\]

\[(P_T)_{\mu \nu}(k) = \eta_{\mu \nu} - \frac{k^\mu k_\nu}{k^2}, \quad (2.2)\]

where \(k^\mu = (\omega/c, \mathbf{k})^T\) denotes a four-wavevector, \(\eta_{\mu \nu} = \text{diag}(-1, 1, 1, 1)\) the Minkowski metric, and \(k^2 = k_\mu k^\mu = -\omega^2/c^2 + |\mathbf{k}|^2\). These operators being given, any Minkowski four-vector \(f(k) = f^\mu(k)\) can be uniquely decomposed into its longitudinal and transverse contributions,

\[f(k) = f_L(k) + f_T(k), \quad (2.3)\]

where \(f_L(k) = P_L(k)f(k)\) and \(f_T(k) = P_T(k)f(k)\). Similarly, any \((4 \times 4)\) Minkowski tensor \(M(k) = M^\mu_{\nu}(k)\) can be uniquely decomposed into four contributions,

\[M(k) = M_{LL}(k) + M_{LT}(k) + M_{TL}(k) + M_{TT}(k), \quad (2.4)\]

which are respectively defined as

\[M_{LL}(k) = P_L(k)M(k)P_L(k), \quad (2.5)\]
\[M_{LT}(k) = P_L(k)M(k)P_T(k), \quad (2.6)\]
\[M_{TL}(k) = P_T(k)M(k)P_L(k), \quad (2.7)\]
\[M_{TT}(k) = P_T(k)M(k)P_T(k). \quad (2.8)\]

In particular, a four-vector \(f\) is called Minkowski-transverse if

\[f_L = 0 \quad \text{and} \quad f_T = f, \quad (2.9)\]

and a Minkowski tensor \(M\) is called Minkowski-transverse if

\[M_{LL} = M_{LT} = M_{TL} = 0 \quad \text{and} \quad M_{TT} = M. \quad (2.10)\]

By contrast, the Cartesian longitudinal and transverse projectors are defined
as operators acting on the three-dimensional space \cite{15, §2.1}, i.e.,

\[
(P_L)_{ij}(k) = \frac{k_i k_j}{|k|^2},
\]

\[
(P_T)_{ij}(k) = \delta_{ij} - \frac{k_i k_j}{|k|^2}.
\]

For details on these operators, see Refs. \cite{14, §2.1} or \cite{15, §2.1}.

2.2. (3+1)-formalism

Although the theory of relativity is in principle completely symmetric with respect to space and time, it is useful for many purposes to formally break this manifest symmetry by decomposing any Minkowski four-vector into its temporal and spatial components. This is accomplished by the so-called (3+1)-formalism (see Refs. \cite{16, 17} for applications in general relativity, and \cite{10, 11} for applications in condensed matter physics). In this subsection, we shortly explain some aspects of this formalism as far as they are needed for the purposes of this article. First, we introduce the dimensionless Cartesian vector

\[
u := \frac{c k}{\omega},
\]

and the analogous Minkowski four-vector

\[
u^\mu := \frac{c k^\mu}{\omega}.
\]

Then, we can write the contravariant four-vector \(\nu^\mu\) as a \((4 \times 1)\)-matrix,

\[
u^\mu = \begin{pmatrix} 1 \\ \nu \end{pmatrix},
\]

and the corresponding covariant four-vector as a \((1 \times 4)\)-matrix,

\[
u_\nu = (-1, \nu^T).
\]

Furthermore, the projector \eqref{2.1} can be written in the \((3 + 1)\)-formalism as

\[
(P_L)^\mu_\nu = \frac{1}{|\nu|^2 - 1} \begin{pmatrix} -1 & \nu^T \\ -\nu & \nu \nu^T \end{pmatrix}.
\]
or equivalently as
\[
(P_L)_{\mu}^\nu = \frac{1}{|u|^2 - 1} \left( \begin{array}{c} 1 \\ u \end{array} \right) (-1, u^T). \tag{2.18}
\]

For later purposes, we also introduce the \((4 \times 3)\)-matrix
\[
\left( \begin{array}{ccc} u_1 & u_2 & u_3 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{array} \right), \tag{2.19}
\]
and the \((3 \times 4)\)-matrix
\[
\left( \begin{array}{ccc} -u_1 & 1 & 0 & 0 \\ -u_2 & 0 & 1 & 0 \\ -u_3 & 0 & 0 & 1 \end{array} \right). \tag{2.20}
\]

These auxiliary objects will become relevant in §5.2.2.

3. Free electromagnetic Green function

3.1. Definition

As a matter of principle, the fundamental equation of motion for the four-potential \(A^\nu(x)\) generated by the four-current \(j^\mu(x)\) reads
\[
(\eta^\mu_\nu \Box + \partial^\mu \partial_\nu) A^\nu(x) = \mu_0 j^\mu(x), \tag{3.1}
\]
where \(\Box = -\partial_\lambda \partial^\lambda\) is called the d’Alembert operator. A particular solution of this equation is given in terms of the (tensorial) free electromagnetic Green function \(D_0\) by
\[
A^\nu(x) = \int d^4x' (D_0)^\nu_\lambda(x - x') j^\lambda(x'), \tag{3.2}
\]
or in Fourier space by
\[
A^\nu(k) = (D_0)^\nu_\lambda(k) j^\lambda(k). \tag{3.3}
\]
Here, the free Green function fulfills per definitionem [15, § 3.3] the equation
\[
(\eta^\mu_\nu \Box + \partial^\mu \partial_\nu) (D_0)^\nu_\lambda j^\lambda = \mu_0 j^\mu. \tag{3.4}
\]
for any physical four-current, i.e., for any four-current which satisfies the continuity equation,
\[ \partial_\mu j^\mu = 0, \tag{3.5} \]
and which is hence Minkowski-transverse,
\[ P_T j = j. \tag{3.6} \]
On the other hand, the equation of motion (3.1) can be rewritten as
\[ \Box P_T A = \mu_0 j = \mu_0 P_T j, \tag{3.7} \]
and correspondingly, we obtain the defining equation for the (tensorial) electromagnetic Green function in the form
\[ \Box P_T D_0 P_T = \mu_0 P_T. \tag{3.8} \]
We note that this defining equation for the Green function is less restrictive than the one used by D. B. Melrose \[9, \text{Eq. (2.1.7)}\]; together with his Eq. (2.1.5), however, this approach does not allow one to identify the essential free parameters of the free Green function. In the following subsection, we will discuss the general solution of the above Eq. (3.8), which at the same time provides the general form of the free electromagnetic Green function.

3.2. General form
3.2.1. Projector formalism
As has been shown in Ref. \[15, \S 3.3\], the most general form of the free electromagnetic Green function reads
\[ (D_0)^\mu_\nu(k) = D_0(k) \left( \eta^\mu_\nu + \frac{ck^\mu}{\omega} f_\nu(k) + g^\mu(k) \frac{ck_\nu}{\omega} + \frac{ck^\mu}{\omega} h(k) \frac{ck_\nu}{\omega} \right), \tag{3.9} \]
where \( D_0(k) \) denotes the (scalar) Green function of the d’Alembert operator in Fourier space \[15, \S 3.1\],
\[ D_0(k, \omega) = \frac{\mu_0}{-\omega^2/c^2 + |k|^2}, \tag{3.10} \]
and where the complex parameter functions \( f_\nu, g^\mu \) and \( h \) can be chosen arbitrarily up to the constraints of Minkowski-transversality, i.e.,
\[ f_\nu(k) k^\nu = k_\nu g^\mu(k) = 0. \tag{3.11} \]
The above expression of the Minkowski tensor $D_0$ essentially coincides with the decomposition introduced in §2.1. More precisely, it is equivalent to

$$D_0(k) = D_{0,LL}(k) + D_{0,LT}(k) + D_{0,TL}(k) + D_{0,TT}(k), \quad (3.12)$$

where the four contributions are given by

$$D_{0,LL}(k) = \mathbb{D}_0(k) \left( 1 + \frac{c^2k^2}{\omega^2} h(k) \right) P_L(k), \quad (3.13)$$

$$D_{0,TT}(k) = \mathbb{D}_0(k) P_T(k), \quad (3.14)$$

as well as

$$(D_{0,LT})^\mu_\nu(k) = \mathbb{D}_0(k) \frac{ck^\mu}{\omega} f_\nu(k), \quad (3.15)$$

$$(D_{0,TL})^\mu_\nu(k) = \mathbb{D}_0(k) g^\mu(k) \frac{ck_\nu}{\omega}. \quad (3.16)$$

For later purposes, we now rewrite these results in the (3 + 1)-formalism.

### 3.2.2. (3+1)-formalism

In the (3 + 1)-formalism of §2.2, the constraints (3.11) imply that

$$f_\nu = (-u \cdot f, f^T) = f^T (-u, 1^T), \quad (3.17)$$

and

$$g^\mu = \begin{pmatrix} u \cdot g \\ g \end{pmatrix} = \begin{pmatrix} u^T \\ 1^T \end{pmatrix} g. \quad (3.18)$$

Combining Eqs. (2.15) and (3.17) we obtain

$$\frac{ck^\mu}{\omega} f_\nu = \begin{pmatrix} -u \cdot f & f^T \\ -(u \cdot f)u & uf^T \end{pmatrix}. \quad (3.19)$$

Similarly evaluating all other terms in Eq. (3.9) we arrive at

$$(D_0)^\mu_\nu = \mathbb{D}_0 \begin{pmatrix} 1 - u \cdot f - u \cdot g - h & f^T + (u \cdot g)u^T + hu^T \\ -(u \cdot f)u - g - hu & 1 + uf^T + gu^T + huu^T \end{pmatrix}. \quad (3.20)$$
with the scalar Green function given by Eq. (3.10) or equivalently by
\[ \mathbb{D}_0 \equiv \mathbb{D}_0(u, \omega) = \frac{1}{\varepsilon_0 \omega^2} \frac{1}{|u|^2 - 1}. \]  
(3.21)

We can also write this result as
\[ (D_0)_{\mu \nu} = \mathbb{D}_0 \left\{ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right\} + \left( \frac{1}{u} f^T(\leftarrow u, \uparrow 1) + \left( \frac{u^T}{1} \right) g (-1, u^T) + h \left( \frac{1}{u} \right) (-1, u^T) \right\}. \]  
(3.22)

The seven component functions given by \( f = (f_1, f_2, f_3)^T, g = (g_1, g_2, g_3)^T \) and \( h \) can be chosen arbitrarily, and each choice yields a tensorial Green function which satisfies the defining Eq. (3.8). In particular, we may consider special cases where
\[ f(u) = f(u) u, \]  
(3.23)
\[ g(u) = g(u) u, \]  
(3.24)
with scalar functions \( f \) and \( g \). Then, Eq. (3.20) simplifies to
\[ (D_0)_{\mu \nu} = \mathbb{D}_0 \left( \begin{array}{cc} 1 - (f + g)|u|^2 - h & (f + g|u|^2 + h)u^T \\ -(f|u|^2 + g + h)u & 1 + (f + g + h)uu^T \end{array} \right). \]  
(3.25)

This form of the electromagnetic Green function is particularly suitable for the recovery of the temporal gauge, as we will show in the next subsection.

3.3. Temporal gauge

It has been shown already in Ref. [15, Eqs. (3.57)–(3.59)] that the free Green function in the temporal gauge can be obtained by choosing the scalar functions \( f, g \) and \( h \) as follows:
\[ f(u) = \frac{1}{|u|^2 - 1}, \quad g(u) = 0, \quad h(u) = -f(u). \]  
(3.26)

In fact, by putting these functions into Eq. (3.25) we obtain
\[ (D_0)_{\mu \nu} = \mathbb{D}_0 \left( \begin{array}{cc} 0 & 0 \\ -u & 1 \end{array} \right), \]  
(3.27)
or in terms of the original variables \( k \) and \( \omega \),

\[
(D_0)^{\mu \nu}(k, \omega) = \mathcal{D}_0(k, \omega) \begin{pmatrix}
0 & 0 \\
-e\frac{k}{\omega} & 1
\end{pmatrix}.
\]  

(3.28)

As shown in Ref. [14, §2.2.1], this formula can also be derived directly from the equation of motion for the electromagnetic vector potential in the temporal gauge. We refer to Eq. (3.28) as the free electromagnetic Green function in the Minkowskian temporal gauge.

Furthermore, we have derived in Ref. [14, §2.2.2] an alternative form of the free electromagnetic Green function by replacing in the equation of motion the charge density with the current density via the continuity equation. Thus, the free electromagnetic Green function can be brought into the form

\[
(D_0)^{\mu \nu}(k, \omega) = \begin{pmatrix}
0 & 0 \\
\leftrightarrow & \mathcal{D}_0(k, \omega)
\end{pmatrix},
\]  

(3.29)

with the free Cartesian Green function

\[
\leftrightarrow \mathcal{D}_0(k, \omega) = \mathcal{D}_0(k, \omega) \left(1 - \frac{e^2|\mathbf{k}|^2}{\omega^2}P_L(k)\right),
\]  

(3.30)

which can also be written compactly as

\[
\leftrightarrow \mathcal{D}_0 = \mathcal{D}_0 (1 - uu^T).
\]  

(3.31)

The above form (3.29) of the free electromagnetic Green function can in turn be obtained from the general expression (3.25) by choosing

\[
f(u) = g(u) = \frac{1}{|u|^2 - 1}, \quad h(u) = \frac{1 + |u|^2}{1 - |u|^2}.
\]  

(3.32)

Correspondingly, we refer to Eq. (3.29) as the free electromagnetic Green function in the Cartesian temporal gauge.

4. Fundamental response tensor

4.1. Definition

Within the limits of linear response theory, the basic quantity of electrodynamics in media is the fundamental response tensor defined as [15, §5.1]

\[
\chi^{\mu \nu}(x, x') = \frac{\delta f_\text{ind}(x)}{\delta A_\text{ext}^\nu(x')},
\]  

(4.1)
such that the induced four-current can be expanded in terms of the external four-potential as

$$j^\mu_{\text{ind}}(x) = \int d^4x' \chi^\mu_\nu(x, x') A^\nu_{\text{ext}}(x').$$  \hspace{1cm} (4.2)

The continuity equation for the induced four-current and its invariance under gauge transformations of the external four-potential imply the constraint relations

$$\partial_\mu \chi^\mu_\nu(x, x') = 0, \hspace{1cm} (4.3)$$

$$\partial'_\nu \chi^\mu_\nu(x, x') = 0. \hspace{1cm} (4.4)$$

In the homogeneous limit, response functions depend only on the coordinate difference, $\chi(x, x') = \chi(x - x')$, such that the expansion (4.2) can be written in Fourier space as a point-wise product,

$$j^\mu_{\text{ind}}(k) = \chi^\mu_\nu(k) A^\nu_{\text{ext}}(k).$$  \hspace{1cm} (4.5)

In this limit, the constraints (4.3)–(4.4) read

$$k\mu \chi^\mu_\nu(k) = \chi^\mu_\nu(k) k\nu = 0. \hspace{1cm} (4.6)$$

These equations will become particularly important for the description of the fundamental response tensor in the \((3 + 1)\)-formalism.

4.2. General form

In terms of the Minkowskian longitudinal and transverse projectors of §2.1 the constraints (4.6) can be written equivalently as

$$P_L(k) \chi(k) = \chi(k) P_L(k) = 0. \hspace{1cm} (4.7)$$

This implies that in the general decomposition

$$\chi = \chi_{LL} + \chi_{LT} + \chi_{TL} + \chi_{TT}, \hspace{1cm} (4.8)$$

only the last term is nonzero, i.e.,

$$\chi_{LL} = \chi_{LT} = \chi_{TL} = 0, \hspace{1cm} (4.9)$$

$$\chi_{TT} = \chi, \hspace{1cm} (4.10)$$
hence $\chi$ is a Minkowski-transverse tensor. Moreover, it follows that in the $(3+1)$-formalism the fundamental response tensor attains the form

$$\chi^\mu_\nu = \begin{pmatrix} -u^T \chi u & u^T \chi \\ -\chi u & \chi \end{pmatrix}.$$  

(4.11)

This can be written even more compactly as

$$\chi^\mu_\nu = \begin{pmatrix} u^T \chi \end{pmatrix} \begin{pmatrix} \chi^{-1} \chi u \end{pmatrix}.$$  

(4.12)

where we have used the matrices defined in Eqs. (2.19)–(2.20). In terms of the original variables $k$ and $\omega$, we thus obtain the well-known representation of the fundamental response tensor (see Ref. [15] and references therein)

$$\chi^\mu_\nu(k, \omega) = \begin{pmatrix} -\omega^2 k^T \chi(k, \omega) k & \frac{c}{\omega} k^T \chi(k, \omega) \\ -\frac{c}{\omega} \chi(k, \omega) k & \chi(k, \omega) \end{pmatrix}.$$  

(4.13)

In particular, this shows that the current response tensor, which is defined as the spatial part of the fundamental response tensor, already determines the whole fundamental response tensor—and thus, ultimately, all linear electromagnetic response properties (see Ref. [15, Sct. 6]).

4.3. Proper response tensor

Similarly as the (direct) fundamental response tensor introduced in §4.1, the proper fundamental response tensor is defined as the functional derivative of the induced four-current with respect to the total (i.e., external plus induced) four-potential, i.e.,

$$\tilde{\chi}^\mu_\nu(x, x') = \frac{\delta j^\mu_{\text{ind}}(x)}{\delta A^\nu_{\text{tot}}(x')}.$$  

(4.14)

This quantity satisfies the same constraints as the fundamental response tensor, Eqs. (4.3)–(4.4), and is therefore also Minkowski-transverse,

$$\tilde{\chi} = \tilde{\chi}^{\text{TT}}.$$  

(4.15)
Correspondingly, its general form in the homogeneous limit reads

\[
\tilde{\chi}^{\mu}_{\nu} = \begin{pmatrix}
-\mathbf{u}^T & \tilde{\mathbf{u}} \\
\tilde{\mathbf{u}} & \tilde{\chi}
\end{pmatrix}.
\] (4.16)

One can easily show by a functional chain rule that the fundamental response tensor is related to its proper counterpart by the Dyson-type equation

\[
\chi = \tilde{\chi} + \tilde{\chi}D_0\chi. \tag{4.17}
\]

We now draw a few direct conclusions from this equation. First, one shows easily that Eq. (4.17) implies the relations

\[
\chi = (1 - \tilde{\chi}D_0)^{-1}\tilde{\chi}, \tag{4.18}
\]

as well as

\[
1 + D_0\chi = (1 - D_0\tilde{\chi})^{-1}. \tag{4.19}
\]

Furthermore, since both \(\chi\) and \(\tilde{\chi}\) are Minkowski-transverse tensors, we can replace \(D_0\) in Eq. (4.17) by its transverse projection, i.e.,

\[
\chi = \tilde{\chi} + \tilde{\chi}(D_0)_{TT}\chi, \tag{4.20}
\]

where \((D_0)_{TT} \equiv D_{0,TT}\) are two different notations for the same object. By means of the explicit expression (3.14), this can be further simplified to

\[
\chi = \tilde{\chi} + D_0\tilde{\chi}\chi, \tag{4.21}
\]

with the scalar Green function \(D_0\). From the ensuing formal expansion

\[
\chi = \tilde{\chi} + D_0\tilde{\chi}^2 + D_0^2\tilde{\chi}^3 + \ldots = \sum_{n=1}^{\infty} D_0^{n-1}\tilde{\chi}^n, \tag{4.22}
\]

we then deduce that the tensors \(\chi\) and \(\tilde{\chi}\) commute with each other, i.e.,

\[
\chi\tilde{\chi} = \tilde{\chi}\chi. \tag{4.23}
\]

Moreover, the Dyson-type equation (4.21) implies the following relations, which are analogous to Eqs. (4.18)–(4.19):

\[
\chi = X\tilde{\chi}, \tag{4.24}
\]

13
with the dimensionless Minkowski tensor \( X \) being given by
\[
X := 1 + D_0 \chi = (1 - D_0 \chi)^{-1}.
\] (4.25)

Finally, by choosing the free electromagnetic Green function \( D_0 \) in the Cartesian temporal gauge (see §3.3), the Dyson equation (4.17) translates into
\[
\begin{pmatrix}
-u^T \hat{\chi} u & u^T \hat{\chi} \\
-\hat{\chi} u & \hat{\chi}
\end{pmatrix}
= \begin{pmatrix}
-u^T \hat{\tilde{\chi}} u & u^T \hat{\tilde{\chi}} \\
-\hat{\tilde{\chi}} u & \hat{\tilde{\chi}}
\end{pmatrix}
\begin{pmatrix}
0 & 0 \\
0 & D_0
\end{pmatrix}
\begin{pmatrix}
-u^T \hat{\chi} u & u^T \hat{\chi} \\
-\hat{\chi} u & \hat{\chi}
\end{pmatrix}.
\] (4.26)

Performing the matrix multiplications explicitly, we thus obtain
\[
\begin{pmatrix}
-u^T \hat{\chi} u & u^T \hat{\chi} \\
-\hat{\chi} u & \hat{\chi}
\end{pmatrix}
= \begin{pmatrix}
-u^T \left( \hat{\chi} + \hat{\tilde{\chi}} D_0 \hat{\chi} \right) u & u^T \left( \hat{\chi} + \hat{\tilde{\chi}} D_0 \hat{\chi} \right) \\
-(\hat{\chi} + \hat{\tilde{\chi}} D_0 \hat{\chi}) u & \left( \hat{\chi} + \hat{\tilde{\chi}} D_0 \hat{\chi} \right)
\end{pmatrix},
\] (4.28)
from which we read off the Cartesian Dyson-type equation
\[
\hat{\chi} = \hat{\chi} + \hat{\tilde{\chi}} D_0 \hat{\chi},
\] (4.29)
which is hence equivalent to its well-known Minkowskian version (4.17).

5. Full electromagnetic Green function

5.1. Definition

The free electromagnetic Green function introduced in §3.1 can be characterized as the functional derivative of the four-potential with respect to its own generating four-current,
\[
(D_0)^\mu_\nu(x, x') = \frac{\delta A^\mu(x)}{\delta j^\nu(x')}. 
\] (5.1)

In the presence of materials, we introduce the analogous quantity [15, §5.2]
\[
D^\mu_\nu(x, x') = \frac{\delta A^\mu_{\text{tot}}(x)}{\delta j^\nu_{\text{ext}}(x')}, 
\] (5.2)
which is correspondingly called the full electromagnetic Green function. Using once more a functional chain rule, the full Green function can be related to its free counterpart and the fundamental response tensor as

\[ D = D_0 + D_0 \chi D_0. \]  

(5.3)

Alternatively, the full Green function can be related to its free pendant and the proper fundamental response tensor by the Dyson equation

\[ D = D_0 + D_0 \tilde{\chi} D, \]  

(5.4)

where we have used the identities

\[ (D_0)^\mu_\nu(x, x') = \frac{\delta A^\mu_{\text{ext}}(x)}{\delta j^\nu_{\text{ext}}(x')} = \frac{\delta A^\mu_{\text{ind}}(x)}{\delta j^\nu_{\text{ind}}(x')}. \]  

(5.5)

As a matter of principle, this Dyson equation—although derived within the context of condensed matter physics—is identical to the self-consistent equation for the full Green function used in quantum electrodynamics. Furthermore, with these equations we can finally specify the principal problem treated in this article. In fact, as has been reviewed in Sect. 3, the solution of the equation of motion (3.8) for the free Green function is not uniquely determined. Instead, its general form is given by Eq. (3.9), which involves seven freely adjustable parameter functions (namely, \( h(k) \), \( f(k) \), and \( g(k) \)). Consequently, the full Green function is not uniquely determined either. The question therefore arises what its general form looks like, and how the adjustable parameters of the free electromagnetic Green function translate into the corresponding adjustable parameters of the full Green function. These questions will be answered in the remaining part of this article.

5.2. General form

5.2.1. Projector formalism

The most general form of the full Green function in the homogeneous limit follows from the Dyson equation (5.4), which uniquely determines \( D \) in terms of the free Green function \( D_0 \) and the proper fundamental response tensor \( \tilde{\chi} \) as a formal power series,

\[ D = D_0 + D_0 \tilde{\chi} D_0 + D_0 \tilde{\chi} D_0 \tilde{\chi} D_0 + \ldots \]  

(5.6)

Even more straightforwardly, however, the general form of \( D \) can be deduced from its representation (5.3) in terms of the free Green function \( D_0 \) and the
direct response tensor $\chi$. For this purpose, we use again the expansion of the full Green function,

$$D = D_{LL} + D_{LT} + D_{TL} + D_{TT}, \quad (5.7)$$

and the analogous expansions of the free Green function and the fundamental response tensor (which were investigated in §3.2.1 and §4.2). Multiplying Eq. (5.3) from left and right with $P_L$ or $P_T$, respectively, and using that $\chi$ is Minkowski-transverse, we obtain the four identities

$$D_{LL} = (D_0)_{LL} + (D_0)_{LT} \chi (D_0)_{TL}, \quad (5.8)$$

$$D_{LT} = (D_0)_{LT} + (D_0)_{LT} \chi (D_0)_{TT}, \quad (5.9)$$

$$D_{TL} = (D_0)_{TL} + (D_0)_{TT} \chi (D_0)_{TL}, \quad (5.10)$$

$$D_{TT} = (D_0)_{TT} + (D_0)_{TT} \chi (D_0)_{TT}. \quad (5.11)$$

With the concrete expressions (3.13)–(3.16) for the free Green function, we first obtain the longitudinal contribution of the full Green function,

$$(D_{LL})_{\mu \nu}(k) = (D_0)_{LL} + (D_0)_{LT} \chi (D_0)_{TL},$$

then the mixed contributions,

$$(D_{LT})_{\mu \nu}(k) = (D_0)_{LT} + (D_0)_{LT} \chi (D_0)_{TT},$$

and finally the transverse contribution,

$$(D_{TT})_{\mu \nu}(k) = (D_0)_{TT} + (D_0)_{TT} \chi (D_0)_{TT}. \quad (5.15)$$

By summing up all contributions, we arrive at the following general form of
the full electromagnetic Green function:

\[ D_{\mu \nu}(k) = \]  

\[ \mathcal{D}_0(k) \left( X_{\mu \nu}(k) + \frac{ck_{\mu}}{\omega} F_{\nu}(k) + G_{\mu}(k) \frac{ck_{\nu}}{\omega} + \frac{ck_{\mu}}{\omega} H(k) \frac{ck_{\nu}}{\omega} \right) , \]  

where the dimensionless tensor \( X \) was defined in Eq. \([4.25]\) and where the dimensionless functions \( F_{\nu}, G_{\mu}, H \) are related to their counterparts \( f_{\nu}, g_{\mu}, h \) in the analogous representation \([3.9]\) of the free electromagnetic Green function by the following equations:

\[ F_{\nu} = f_{\lambda} X^\lambda_{\nu} , \]  

\[ G_{\mu} = X^\mu_{\rho} g^\rho , \]  

\[ H = h + f_{\lambda} (X^\lambda_{\rho} - \eta^\lambda_{\rho}) g^\rho . \]  

One the one hand, the functions \( F_{\nu}, G_{\mu}, H \) can be regarded as parameter functions of the full Green function, which can be chosen arbitrarily up to the constraints of Minkowski-transversality (analogous to Eq. \([3.11]\)), i.e.,

\[ F_{\nu}(k) k_{\nu} = k_{\mu} G_{\mu}(k) = 0 . \]  

On the other hand, these functions are uniquely determined once their counterparts \( f_{\nu}, g_{\mu}, h \) in the free Green function are fixed. Thus, we can also derive an explicit expression of the full Green function in terms of the parameter functions of the free Green function: resubstituting the definition \([4.25]\) of \( X \) in Eqs. \([5.16]\)–\([5.19]\) and abbreviating \( u^\mu = ck^\mu/\omega \), we obtain

\[ D_{\mu \nu}(k) = \mathcal{D}_0 \left( \eta_{\mu \nu} + u^\mu f_{\nu} + g^\mu u_{\nu} + u^\mu h u_{\nu} \right) \]  

\[ + \mathcal{D}_0^2 \left( \chi^\mu_{\nu} + u^\mu f_{\lambda} X^\lambda_{\nu} + \chi^\mu_{\rho} g^\rho u_{\nu} + u^\mu (f_{\lambda} X^\lambda_{\rho} g^\rho) u_{\nu} \right) , \]  

or equivalently,

\[ D_{\mu \nu} = (D_0)^{\mu \nu} + \mathcal{D}_0^2 \left( \eta_{\mu \lambda} + u^\mu f_{\lambda} \right) \chi^{\lambda}_{\rho} \left( \eta^\rho_{\nu} + g^\rho u_{\nu} \right) , \]  

where the first term is just the free Green function given by Eq. \([3.9]\). In fact, this last equation can also be derived directly from Eq. \([5.3]\) by using the expression \([3.9]\) for the free Green function together with the constraints \([4.6]\) on the fundamental response tensor.
5.2.2. (3+1)-formalism

We now reformulate our results in the (3 + 1)-formalism, which will turn out to be useful for deriving the Cartesian Dyson equation in the following subsection. First, the tensor $X$ defined by Eq. (4.25) can be represented as

$$X^\mu_\nu = \left( \begin{array}{cc} 1 - D_0 \hat{u}^T \hat{X} \hat{u} & D_0 \hat{u}^T \hat{X} \\ - D_0 \hat{u} \hat{X} \hat{u} & 1 + D_0 \hat{X} \end{array} \right),$$

(5.23)

which follows from the corresponding expression (4.13) of the fundamental response tensor. In terms of the dimensionless matrix

$$\hat{X} := 1 + D_0 \hat{X},$$

(5.24)

which is the spatial part of the Minkowski tensor $X$, we obtain the equivalent representation

$$X^\mu_\nu = \left( \begin{array}{cc} 1 - u^T (\hat{X} - \hat{1}) u & u^T (\hat{X} - \hat{1}) \\ -(\hat{X} - \hat{1}) u & \hat{X} \end{array} \right).$$

(5.25)

Next, the Minkowski-transverse functions $F_\nu$ and $G^\mu$ defined in the previous subsection can be written as

$$F_\nu = (-u \cdot F, F^T),$$

(5.26)

and

$$G^\mu = \left( \begin{array}{c} u \cdot G \\ G \end{array} \right),$$

(5.27)

which is analogous to Eqs. (3.17)–(3.18). By putting these expressions into Eq. (5.16) and performing the matrix multiplications, we arrive at the following expression of the full Green function in the (3 + 1)-formalism:

$$D^\mu_\nu = D_0 \left( \begin{array}{cc} 1 - u^T (\hat{X} - \hat{1}) u & u^T (\hat{X} - \hat{1}) \\ -(\hat{X} - \hat{1}) u & \hat{X} \end{array} \right)$$

$$+ D_0 \left( \begin{array}{cc} -u \cdot F - u \cdot G - H & F^T + (u \cdot G) u^T + H u^T \\ -(u \cdot F) u - G - H u & u F^T + G u^T + H uu^T \end{array} \right).$$

(5.28)
Using once more the relation (5.24) we can write this result equivalently as

\[ D_{\mu \nu} = D_0^2 \left( -u^T \chi \ u \ u^T \chi \right) \]

\[ + D_0 \left( 1 - u \cdot F - u \cdot G - H \ F^T + (u \cdot G) u^T + H u^T \right) \]

\[ - (u \cdot F) u - G - H u \ u^T \ \\
\]

where the second term is now precisely analogous to Eq. (3.20) for the free
Green function.

To proceed further, we express the parameter functions \( F, G \) and \( H \) in terms of their counterparts \( f, g \) and \( h \) appearing in the free Green function. Thus, we rewrite Eq. (5.17) as

\[ (-u \cdot F, F^T) = (-u \cdot f, f^T) \]

\[ + D_0 (-u \cdot f, f^T) \left( -u^T \chi \ u \ u^T \chi \right) \]

from which we obtain after a straightforward calculation,

\[ F^T = f^T + D_0 f^T (1 - uu^T) \chi \]

Similarly, Eq. (5.18) implies that

\[ G = g + D_0 \chi (1 - uu^T) g \]

and from Eq. (5.19) we obtain

\[ H = h + D_0 f^T (1 - uu^T) \chi (1 - uu^T) g \]

Putting these results into Eq. (5.29) yields after a lengthy but straightforward calculation the following general expression of the full electromagnetic Green function:

\[ D_{\mu \nu} = (D_0)^\mu \nu \]

\[ + D_0^2 \left( f^T u \ u^T \chi \right) \]

\[ + D_0 \left( 1 - uu^T + uf^T \right) \chi \]

\[ (-g^T u, 1 - uu^T + g^T uu^T) \]

\[ + 19 \]
where we have introduced the functions

\[
    f_u(u) := u + (\hat{\nu} - uu^T) f(u), \quad (5.35)
\]

\[
    g_u(u) := u + (\hat{\nu} - uu^T) g(u). \quad (5.36)
\]

Note that the first term on the right-hand side of Eq. (5.34) is just the free Green function, which as a \((4 \times 4)\)-matrix is given in terms of \(f\), \(g\) and \(h\) by Eq. (3.20). By contrast, the second term depends on the current response tensor and formally involves the multiplication of a \((4 \times 3)\)-matrix, a \((3 \times 3)\)-matrix and a \((3 \times 4)\)-matrix.

We conclude this subsection with a few remarks concerning our result (5.34). First, an even shorter derivation of this expression in the \((3 + 1)\)-formalism can be given by starting from Eq. (5.22) of the previous subsection, which also relates the full Green function to the parameter functions of the free Green function (but in the manifestly Lorentz-covariant formalism). Expressing \(f_\nu\), \(g_\mu\) and \(\chi_{\mu \nu}\) in terms of their respective spatial parts via Eqs. (3.17), (3.18) and (4.12) leads directly to the result (5.34).

Secondly, using the representation (3.31) of the free Cartesian Green function, we can rewrite Eqs. (5.31)–(5.33) compactly as

\[
    F^T = f^T (\hat{\nu} + \hat{\nu} D_0 \hat{\chi}), \quad (5.37)
\]

\[
    G = (\hat{\nu} + \hat{\nu} \hat{D}_0) g, \quad (5.38)
\]

\[
    H = h + \hat{D}_0^{-1} f^T \hat{D}_0 \hat{\chi} \hat{D}_0 g. \quad (5.39)
\]

Correspondingly, the result (5.34) is equivalent to

\[
    D^\mu_{\nu} = (D_0)^\mu_{\nu}
\]

\[
    + \left( \frac{\hat{D}_0 u^T + f^T \hat{D}_0}{\hat{D}_0 \hat{1} + u f^T \hat{D}_0} \right) \hat{\chi} \left( -\hat{D}_0 u - \hat{D}_0 g, \hat{D}_0 \hat{1} + \hat{D}_0 g u^T \right). \quad (5.40)
\]

Finally, in the special case where \(f\) and \(g\) are parallel to \(u\) and given by
Eqs. (3.23)–(3.24) the definitions (5.35)–(5.36) also simplify to
\[ f_u(u) = f_u(u) u, \quad (5.41) \]
\[ g_u(u) = g_u(u) u. \quad (5.42) \]
with the respective scalar functions being defined as
\[ f_u(u) = 1 + (1 - |u|^2) f(u), \quad (5.43) \]
\[ g_u(u) = 1 + (1 - |u|^2) g(u). \quad (5.44) \]
This case will be important in the following subsection.

5.3. Temporal gauge

It follows directly from Eq. (3.32) that in the Cartesian temporal gauge,
\[ f_u(u) = g_u(u) = 0. \quad (5.45) \]
Thus, the general expression (5.34) of the full Green function simplifies to
\[
D_{\mu\nu} = \begin{pmatrix} 0 & 0 \\ 0 & \hat{D}_0 \end{pmatrix} + \hat{D}_0^2 \begin{pmatrix} 0 \\ \hat{1} - uu^T \end{pmatrix} \hat{\chi} (0, \hat{1} - uu^T) \quad (5.46)
\]
\[
= \begin{pmatrix} 0 & 0 \\ 0 & \hat{D}_0 \end{pmatrix} + \begin{pmatrix} 0 \\ \hat{D}_0 \end{pmatrix} \hat{\chi} (0, \hat{D}_0), \quad (5.47)
\]
where we have used again Eq. (3.31). Multiplying out the matrices, we find that the full Green function is of the same form as the free Green function,
\[
D_{\mu\nu} = \begin{pmatrix} 0 & 0 \\ 0 & \hat{D} \end{pmatrix}, \quad (5.48)
\]
and the full Cartesian Green function is related to its free counterpart by
\[
\hat{D} = \hat{D}_0 + \hat{D}_0 \hat{\chi} \hat{D}_0. \quad (5.49)
\]
This is a Cartesian version of Eq. (5.3) which had been our starting point for deriving the general form of the full Green function. Together with the
relation \([4.29]\) between the direct and the proper current response tensor, Eq. \((5.49)\) implies the corresponding Cartesian Dyson equation
\[
\hat{\mathbb{D}} = D_0 + \hat{\mathbb{D}}_0 \hat{\chi} \hat{\mathbb{D}},
\]  
(5.50)

which constitutes a main result of this article. While we have derived Eqs. \((5.49)\) and \((5.50)\) from the general form of the full Green function, these equations can also be deduced directly from their more fundamental Minkowskian counterparts, Eqs. \((5.3)\) and \((5.4)\), by using the free Green function in the Cartesian temporal gauge, Eq. \((3.29)\), together with the general representation \((4.13)\) of the fundamental response tensor.

6. Conclusion

We have derived the most general form of the full electromagnetic Green function, both in the manifestly Lorentz-covariant formalism (see Eq. \((5.16)\)), and in the \((3 + 1)\)-formalism which is more suitable for application in condensed matter physics (see Eq. \((5.29)\)). These results generalize the corresponding expressions for the free electromagnetic Green function, Eqs. \((3.9)\) and \((3.20)\), which had been derived already in Ref. [15]. In particular, we have shown that the full Green function depends on seven complex parameter functions \((F, G, H)\), which can be chosen arbitrarily, but which are uniquely determined once the corresponding parameter functions \((f, g, h)\) of the free Green function are fixed. Thus, we could also express the full Green function in terms of the parameter functions of the free Green function, both in the manifestly Lorentz-covariant formalism (see Eq. \((5.22)\)), and in the \((3 + 1)\)-formalism (see Eqs. \((5.34)\)–\((5.36)\), or Eq. \((5.40)\)).

As a further outcome of this analysis being of a more practical value, we have derived Cartesian Dyson equations both for the full electromagnetic Green function (see Eqs. \((5.50)\)) and for the fundamental response tensor (see Eq. \((4.29)\)). These allow for a reduction of their original four-dimensional Lorentz formulation to a more economic three-dimensional formulation still being exact and hence encapsulating the complete information.

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### Minkowskian Cartesian

| Minkowskian | Cartesian |
|-------------|-----------|
| $\chi = \tilde{\chi} + \tilde{\chi} D_0 \chi$ | $\chi = \tilde{\chi} + \tilde{\chi} D_0 \chi$ |
| $D = D_0 + D_0 \chi D$ | $\hat{D} = \hat{D}_0 + \hat{D}_0 \hat{\chi} \hat{D}$ |
| $D = D_0 + D_0 \chi D_0$ | $\hat{D} = \hat{D}_0 + \hat{D}_0 \hat{\chi} \hat{D}_0$ |

Table 1: Exact Dyson-type equations.

### Cartesian Scalar

| Cartesian | Scalar |
|-----------|--------|
| $\hat{\chi} = \tilde{\chi} + \tilde{\chi} D_0 \chi$ | $\chi = \tilde{\chi} + \tilde{\chi} v \chi$ |
| $(\hat{\varepsilon}_r)^{-1} = 1 + \hat{D}_0 \hat{\chi}$ | $\varepsilon_r^{-1} = 1 + v \chi$ |
| $\hat{\varepsilon}_r = 1 - \hat{D}_0 \hat{\chi}$ | $\varepsilon_r = 1 - v \tilde{\chi}$ |

Table 2: Current response tensor and dielectric tensor (left column: exact relations, right column: relations between longitudinal response functions which are valid in the isotropic limit).
A. Cartesian, Minkowskian, and scalar equations

In this appendix, we compare some relations between Cartesian tensors, which were derived in this article, to their already well-known Minkowskian counterparts, as well as to their analogous scalar relations which are commonly used in electronic structure physics.

Concretely, Table 1 summarizes the Dyson-type relations between the free electromagnetic Green function $D_0$, the full electromagnetic Green function $D$, the (direct) fundamental response tensor $\chi$, and the proper fundamental response tensor $\tilde{\chi}$. Importantly, the more economic Cartesian equations are actually equivalent to their Minkowskian counterparts (provided that we choose the Cartesian temporal gauge, see §3.3). The Cartesian equations correspond to Eqs. (4.29), (5.49), and (5.50) in the main text, whereas the Minkowskian versions are derived, for example, in Ref. [15, §5.2].

Furthermore, Table 2 summarizes relations between the dielectric tensor and the (direct or proper) current response tensor. In the homogeneous limit, where longitudinal and transverse response functions decouple, the general tensor relations can be reduced to simpler scalar relations, which are commonly employed in first-principles materials physics. These scalar relations involve the (direct) density response function $\chi$, the proper density response function $\tilde{\chi}$, and the longitudinal dielectric function $\varepsilon_r$. In particular, in these formulae the scalar Coulomb kernel $v$ replaces the free Cartesian Green function. For a derivation of these relations, see [14, §3.4 and §5.1].

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