Equivalence of the velocity and length gauge perturbation series

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A long-standing unresolved problem of the quantum mechanical perturbation theory of light-matter interaction is the existence of two distinct infinite perturbation series for a given transition amplitude in the so-called “velocity” and “length” gauges, that have hitherto resisted a demonstration of their mathematical equivalence. In addition, numerical calculations of the transition probability based on the two series (albeit, for practical reasons, only in their truncated forms) have frequently shown a significant discrepancy between them and/or with various experimental data. These and related difficulties have led some authors to argue in favor of the length gauge (e.g. [1, 2]) as opposed to the velocity gauge, since the former is based manifestly on a physically “true” energy operator [3]. Nevertheless, the principle of gauge invariance in quantum theory (e.g. [3, 4, 5]) requires that they ought to be equivalent.

The purpose of this Letter is to derive a “master” perturbation expansion for the quantum transition amplitude in a light field between the field-free initial and final atomic states in the minimal-coupling (MC) “velocity” gauge. The result is used to prove that the traditional “velocity” and “length” gauge perturbation series are equivalent infinite series representations or branches of the same amplitude function, that are equal but in a common domain of convergence (if it exists). More generally, we show that they constitute only two members of a one-parameter family of infinitely many branches of the given transition amplitude.

The Schrödinger equation of an atomic system interacting with an electromagnetic field, in the minimal-coupling (MC) transverse gauge is given by:

\[(\i \hbar \frac{\partial}{\partial t} - H_{MC}(t))\Psi_{MC}(t) = 0\]  \hspace{1cm} (1)

where, the total Hamiltonian of the interacting system is

\[H_{MC}(t) = \left(\frac{p_{op}^2}{2m} - \frac{1}{\i \hbar} A(t) \cdot A(t)\right) + e A_0(r)\]  \hspace{1cm} (2)

with the four-potential \(A_\mu \equiv (A_0(r), A(t))\) where, the scalar potential can be used to define the “atomic” potential, \(e A_0(r) = V_a(r)\), and \(A(t)\) is the transverse vector potential of the light field. In the usual electric dipole approximation (e.g. Bohr-radius/wavelength \(<< 1\)), the vector potential \(A(t)\) depends only on \(t\). As usual, the “atomic” Hamiltonian

\[H_a \equiv \frac{p_{op}^2}{2m} + V_a(r)\]  \hspace{1cm} (3)

provides a complete set of eigen-states

\[\sum_{\alpha \gamma} |\phi_{\alpha}^\gamma| < |\phi_{\gamma}^\gamma| = 1\]  \hspace{1cm} (4)

and eigen-energies, \(E_{\alpha}^\gamma\), which satisfy the eigenvalue equation:

\[H_a |\phi_{\gamma}^\gamma\rangle = E_{\gamma}^\gamma|\phi_{\gamma}^\gamma\rangle, \text{ all }\gamma.\]  \hspace{1cm} (5)

We define the “atomic” Green’s function \(G_a(t, t')\) by the equation

\[(\i \hbar \frac{\partial}{\partial t} - H_a(t))G_a(t, t') = \delta(t - t').\]  \hspace{1cm} (6)

Its solution is given by,

\[G_a(t, t') = -\frac{i}{\hbar} \theta(t-t')e^{-\i \hbar H_a(t-t')}\]

\[= -\frac{i}{\hbar} \theta(t-t') \sum_{\gamma \alpha} |\phi_{\gamma}^\alpha\rangle e^{-\i \hbar E_{\gamma}^\alpha(t-t')} < \phi_{\gamma}^\alpha|\]  \hspace{1cm} (7)

This can be easily verified by its substitution in Eq. (6) and noting that the derivative of the theta-function is the delta function. Finally, we define, for later use, the total Green’s function (or propagator) \(G_{MC}(t, t')\) associated with the minimal-coupling Hamiltonian \(H_{MC}(t)\), by the inhomogeneous differential equation:

\[(\i \hbar \frac{\partial}{\partial t} - H_{MC}(t))G_{MC}(t, t') = \delta(t - t').\]  \hspace{1cm} (8)

The total Hamiltonian \(H_{MC}(t)\) can always be written as a sum of two terms, in infinitely many ways:

\[H_{MC}(t) = H_s(t) + V_s(t); s = 1, 2, 3, \cdots \infty\]  \hspace{1cm} (9)
where, \( V_s(t) \equiv H_{MC}(t) - H_s(t) \), and the basis Hamiltonian \( H_s(t) \) can be used to define the associated basis Green’s functions, \( G_s(t, t') \), by the equations:

\[
(i\hbar \frac{\partial}{\partial t} - H_s(t))G_s(t, t') = \delta(t - t'); \ s = 1, 2, 3, \ldots \infty. \tag{10}
\]

Eq. (10) can be solved in terms of the linearly independent complete set of fundamental solutions, \( \phi_j^{(s)}(t) > 0; s = 1, 2, 3, \ldots, \infty; all j. \)

Explicitly, we have:

\[
G_s(t, t') = -\frac{i}{\hbar} \theta(t - t') \sum_{allj} |\phi_j^{(s)}(t) > < \phi_j^{(s)}(t')|. \tag{11}
\]

We may now expand the total Green’s function, \( G_{MC}(t, t') \), using any basis Green’s function, \( G_s(t, t') \), in an infinite series,

\[
G_{MC}(t, t') = G_s(t, t') + \int dt_1 G_s(t, t_1) D_{MC}(t_1, t')
\]

\[
\times G_s(t_1, t_1') + \int \int dt_1 dt_2 G_s(t_1, t_1) D_{MC}(t_2, t') \times G_s(t_2, t_2')
\]

\[+ \cdots; s = 1, 2, 3, \ldots, \infty. \tag{13}
\]

where we have introduced the (inhomogeneous Schrödinger operator):

\[
D_{MC}(t, t') \equiv [(H_{MC}(t) - i\hbar \frac{\partial}{\partial t}) + i\hbar \delta(t - t')]
\tag{14}
\]

which, in this way, depending on the total Hamiltonian \( H_{MC}(t) \), and not on its various partitions. The symbol \( \int \) above stands for the integration over the entire time axis: \( \int \equiv \int_{-\infty}^{\infty} \). We may note, parenthetically, that the presence of the theta-function in the explicit representation of a Green’s function, Eq. (12), automatically accounts for the appropriate domains of the intermediate time integrations in Eq. (13). Eq. (13) is a solution of the Green’s equation (8). This can be verified as follows: First, we apply (13) on (12) and use (10) to get,

\[
D_{MC}(t, t')G_s(t, t') = [(H_{MC}(t) - i\hbar \frac{\partial}{\partial t}) + i\hbar \delta(t - t')]G_s(t, t')
\]

\[
= [(H_s(t) - i\hbar \frac{\partial}{\partial t})G_s(t, t') + V_s(t)G_s(t, t')
\]

\[+ i\hbar \delta(t - t')G_s(t, t')] = -\delta(t - t') + V_s(t)G_s(t, t') + \delta(t - t')\theta(t - t')\]

\[\times \sum_{allj} |\phi_j^{(s)}(t) > < \phi_j^{(s)}(t')| = -\delta(t - t') + V_s(t)G_s(t, t') + \delta(t - t')\theta(t - t')\]

\[= V_s(t)G_s(t, t'); s = 1, 2, 3 \cdots, \infty. \tag{15}
\]

where, \( V_s(t) \equiv H_{MC}(t) - H_s(t) \), and in the last step we have used the fact that an integration variable, say \( t_{n+1} \), in any of the integrations in the series (13), always approaches its upper limit, say \( t_n \), as: \( \lim(t_n - t_{n+1}) = 0^+ \), \( \theta(t_n - t_{n+1}) = 1 \). Second, substituting Eq. (15) in Eq. (13) we may sum the series on the right hand side as,

\[
G_{MC}(t, t') = G_s(t, t') + \int dt_1 G_s(t_1, t_1) V_s(t_1) \times [G_s(t_1, t')
\]

\[+ \int dt_2 G_s(t_1, t_2) V_s(t_2)G_s(t_2, t_1') + \cdots]

\[= G_s(t, t') + \int dt_1 G_s(t_1, t_1) \times [G_{MC}(t_1, t')]
\tag{16}
\]

where, we have used the fact that the quantity in the square brackets above is equal to the series itself. Next, operating on the last equation from the left with \( (i\hbar \frac{\partial}{\partial t} - H_{MC}(t)) \), noting Eq. (10), and carrying out the resulting delta-function integration at once, we get,

\[
(i\hbar \frac{\partial}{\partial t} - H_{MC}(t))G_{MC}(t, t') = \delta(t - t') + V_s(t)G_{MC}(t, t')
\tag{17}
\]

Finally, on transposing the last term to the left hand side and using Eq. (9) we arrive at,

\[
(i\hbar \frac{\partial}{\partial t} - H_{MC}(t))G_{MC}(t, t) = \delta(t - t')
\tag{18}
\]

which agrees with Eq. (5); q.e.d. Thus, Eq. (13) provides a general series solution for the total Green’s function \( G_{MC}(t, t') \) for an arbitrary choice of the basis Hamiltonian \( H_s(t) \), and the associated basis Green’s function \( G_s(t, t') \). We may choose,

\[
H_s(t) = H_{\lambda}(t) = \frac{(p_{op} - \frac{e}{c} A(t))^2}{2m} + V_a(r) - \frac{e}{c} \dot{A}(t) \cdot r
\tag{19}
\]

where \( \lambda \) is a real number. The associated Green’s function \( G_{\lambda}(t, t') \) is defined by

\[
(i\hbar \frac{\partial}{\partial t} - H_{\lambda}(t))G_{\lambda}(t, t') = \delta(t - t')
\tag{20}
\]

We find its exact solution to be,

\[
G_{\lambda}(t, t') = \frac{i}{\hbar} \theta(t - t') e^{i\lambda \frac{e}{c} \dot{A}(t) \cdot r}
\]

\[\times \sum_{allj} |\phi_j^{(s)}(t) > e^{-\frac{i}{\hbar} H_a(t-t')} < \phi_j^{(s)}(t')|
\]

\[\times e^{-i\lambda \frac{e}{c} \dot{A}(t') \cdot r'}
\]

\[= e^{\lambda \frac{e}{c} \dot{A}(t) \cdot r} G_s(t, t') e^{-i\lambda \frac{e}{c} \dot{A}(t') \cdot r'}
\tag{21}
\]

The validity of the above solution can be established without difficulty by substituting Eq. (21) in Eq. (20), and simplifying by noting the definition (14) and using,

\[
(p_{op} - \frac{e}{c} A(t))^2 e^{i\lambda \frac{e}{c} \dot{A}(t) \cdot r} = e^{\lambda \frac{e}{c} \dot{A}(t) \cdot r} p_{op}^2.
\tag{22}
\]
We now substitute \( G_\lambda(t, t') \equiv G_\lambda(t, t') \) in Eq. (13) for the total Green’s function, to get:

\[
G_{MC}(t, t') = (G_\lambda(t, t') + \int dt_1 G_\lambda(t_1, t_1) D_{MC}(t_1, t') G_\lambda(t_1, t_2) \times \lambda e^{iA(t) \cdot r} G_\lambda(t_2, t') + \cdots )
\]

\[
eq e^{iA(t) \cdot r} G_\lambda(t, t') + \int dt_1 G_\lambda(t_1, t_1) D_{MC}(t_1, t_2) G_\lambda(t_1, t_2) \times \lambda e^{iA(t) \cdot r} G_\lambda(t_2, t') + \cdots
\]

\[
G_{MC}(t_1, t_2) D_{MC}(t_1, t_2) G_\lambda(t_2, t') + \cdots ) e^{-iA(t') \cdot r' r'}
\]

\[
= e^{iA(t) \cdot r} G_\lambda(t, t') + \int dt_1 G_\lambda(t_1, t_1) D_{MC}(t_1, t_2) G_\lambda(t_1, t_2) \times \lambda e^{iA(t) \cdot r} G_\lambda(t_2, t') + \cdots
\]

\[
G_\lambda(t_1, t_2) D_{MC}(t_1, t_2) G_\lambda(t_2, t_2) G_\lambda(t_2, t') + \cdots ) e^{-iA(t') \cdot r' r'}
\]

(23)

where,

\[
D_{MC}(t, t') \equiv e^{-iA(t) \cdot r} D_{MC}(t, t') e^{iA(t) \cdot r}
\]

\[
= \left\{ \left[ \frac{p_{op} + (\lambda - 1) \frac{e}{mc} A(t)^2}{2m} + V_\lambda(r) + \lambda e \frac{c}{c} A(t) \cdot r \right]
\]

\[
- i\hbar \frac{\partial}{\partial t} \right\} + \left( \frac{p_{op}^2}{2m} - V_\lambda(t) + i\hbar \delta(t - t') \right)
\]

\[
= \left\{ \left[ \frac{p_{op}^2}{2m} + V_\lambda(r) - i\hbar \frac{\partial}{\partial t} \right] + V_\lambda(t) + i\hbar \delta(t - t') \right\}
\]

(24)

and,

\[
V_\lambda(t) = [\frac{p_{op}^2}{2m} - V_\lambda(r) + (\lambda - 1)^2 \frac{e^2}{2mc} A^2(t)
\]

\[
+ \lambda \frac{e}{mc} A(t) \cdot r
\]

(25)

Operating with \( D_{MC}(t, t') \) from the left on to \( G_\lambda(t, t') \), noting Eq. (6), and calculating similarly as in the case of Eq. (10) above, we get:

\[
D_{MC}(t, t') G_\lambda(t, t') = \left\{ \left[ \frac{p_{op}^2}{2m} + V_\lambda(r) - i\hbar \frac{\partial}{\partial t} \right] G_\lambda(t, t')
\]

\[
+ V_\lambda(t) G_\lambda(t, t') + i\hbar \delta(t - t') G_\lambda(t, t') \right\}
\]

\[
= V_\lambda(t) G_\lambda(t, t').
\]

(26)

Finally, using Eq. (20) in Eq. (24), we obtain

\[
G_{MC}(t, t') = e^{iA(t) \cdot r} G_\lambda(t, t') + \int dt_1 G_\lambda(t_1, t_1) V_\lambda(t_1)
\]

\[
G_\lambda(t_1, t_2) V_\lambda(t_2) G_\lambda(t_2, t_2) G_\lambda(t_2, t') + \cdots ) e^{-iA(t') \cdot r' r'}
\]

\[
= e^{iA(t) \cdot r} G_\lambda(t, t') + \int dt_1 G_\lambda(t_1, t_1) D_{MC}(t_1, t_2) G_\lambda(t_1, t_2)
\]

\[
G_\lambda(t_2, t_2) V_\lambda(t_2) G_\lambda(t_2, t_2) G_\lambda(t_2, t') + \cdots ) e^{-iA(t') \cdot r' r'}
\]

(27)

This is a one-parameter family of infinite series representations of the total Green’s function \( G_{MC}(t, t') \), for any value of the real parameter \( \lambda \):

The transition amplitude, \( S^{f \rightarrow i}_{MC}(t_f, t_i) \), between the field-free reference states \( |f\rangle \):

\[
|\phi_f(t_i) \rangle = e^{iA(t) \cdot r} |f\rangle
\]

and

\[
< \phi_f(t_f) | = < \phi_f(t_f) | e^{iA(t_f) \cdot r'}
\]

(29)

that are prepared initially at \( t' = t_i \) and detected finally at a later time \( t = t_f \), where \( A(t, f) \) are arbitrary constant vector potentials, is:

\[
S^{f \rightarrow i}_{MC}(t_f, t_i) \equiv i\hbar < \phi_f(t_f) | G_{MC}(t_f, t_i) | \phi_i(t_i) >
\]

\[
= \delta f_i - \frac{i}{\hbar} \left( \int dt_1 < \phi_f(t_1) | V_{MC}(t_1) | \phi_i(t_1) >
\]

\[
+ \int \int dt_1 dt_2 < \phi_f(t_1) | V_{MC}(t_1, t_2) G_\lambda(t_1, t_2) | \phi_i(t_2) >
\]

\[
+ \cdots ; \lambda = 0
\]

(30)

where, we have used the total Green’s function \( G(t, f) \) given by Eq. (27), cancelled the phase factors depending on the arbitrary (constant) vector potentials, and simplified by putting,

\[
< \phi_f(t_f) | G_\lambda(t_f, t_i) = - \frac{i}{\hbar} < \phi_f(t_f) | \phi_i(t_i) >
\]

\[
and
\]

\[
G_\lambda(t, t_i) | \phi_i(t_i) > = - \frac{i}{\hbar} | \phi_i(t_i) > .
\]

(31)

Note that the above expression (30) holds for any value of the real parameter \( \lambda \), and thus constitutes a “master” expansion of the transition amplitude derived in the minimal-coupling (MC) “velocity” gauge. It provides a one-parameter family of infinitely many series representations or branches of the amplitude function \( S^{f \rightarrow i}_{MC}(t_f, t_i) \). We may choose, for instance, the parameter \( \lambda = 0, 1, \text{or } \frac{1}{2} \) on the right hand side of Eq. (30), and get, respectively, the three expansions of the transition amplitude:

\[
S^{f \rightarrow i}_{MC}(t_f, t_i) = \delta f_i - \frac{i}{\hbar} \left( \int dt_1 < \phi_f(t_1) | V_{MC}(t_1) | \phi_i(t_1) >
\]

\[
+ \int \int dt_1 dt_2 < \phi_f(t_1) | V_{MC}(t_1, t_2) G_\lambda(t_1, t_2) | \phi_i(t_2) >
\]

\[
+ \cdots ; \lambda = 0
\]

\[
= \delta f_i - \frac{i}{\hbar} \left( \int dt_1 < \phi_f(t_1) | V_{MC}(t_1) | \phi_i(t_1) >
\]

\[
+ \int \int dt_1 dt_2 < \phi_f(t_1) | V_{MC}(t_1, t_2) G_\lambda(t_1, t_2) | \phi_i(t_2) >
\]

\[
+ \cdots ; \lambda = 1
\]

\[
= \delta f_i - \frac{i}{\hbar} \left( \int dt_1 < \phi_f(t_1) | V_{MC}(t_1) | \phi_i(t_1) >
\]

\[
+ \int \int dt_1 dt_2 < \phi_f(t_1) | V_{MC}(t_1, t_2) G_\lambda(t_1, t_2) | \phi_i(t_2) >
\]

\[
+ \cdots ; \lambda = 1
\]

(34)

(33)

(35)
where, from Eq. (25),

\[ V_{\text{vel}}(t) = (-\frac{e}{mc} \mathbf{A}(t) \cdot \mathbf{p}_o + \frac{e^2}{2mc^2} A^2(t)); \lambda = 0 \]
\[ V_{\text{len}}(t) = (\frac{e}{c} \mathbf{A}(t) \cdot \mathbf{r}) = (-e \mathbf{E}(t) \cdot \mathbf{r}); \lambda = 1 \]
\[ V_{\text{hyb}}(t) = \left( \frac{1}{2} [V_{\text{vel}}(t) + V_{\text{len}}(t)] - \frac{e^2}{4mc^2} A^2(t)]; \lambda = \frac{1}{2} \] (36)

The first two series (33) and (34) are readily recognized, on comparing the expressions of the respective interaction series, traditionally obtained in the “velocity” and the “length” gauges, respectively. Thus, they are seen to be nothing but two equivalent infinite series representations (branches) of the same amplitude function \( S_{MC}^{t_f, t_i}(t_f, t_i) \) and, hence, are but equal in their common domain of convergence (assuming, it exists) [2]. We may add that at present, little, if any thing, is known regarding the convergence properties of these infinite series representations of the same amplitude function. The third expansion (35) provides another equivalent series representation (in terms of a “hybrid interaction”) of the same amplitude by choosing \( \lambda = \frac{1}{2} \), and so on for any other equivalent series. Before concluding, we point out that there is no difficulty in deriving a “master” expansion, analogous to Eq. (30), from the total Hamiltonian given in the “length” gauge (or for that matter in any other gauge) by proceeding exactly analogously as shown above – it leads to the same conclusion of the mathematical equivalence of the two traditional perturbation series, in the velocity and length gauges, in a common domain of convergence, as demonstrated above.

To conclude, starting explicitly in the minimal-coupling (MC) “velocity” gauge, we have derived a “master” perturbation expansion (30) for generating a one-parameter family of equivalent infinite series representations of a given transition amplitude. The result is used to demonstrate (Eqs. (33) and (34)) that the two well-known perturbation series, traditionally obtained in the “velocity” and “length” gauges, are only two equivalent infinite series representations or branches of the same amplitude function \( S_{MC}^{t_f, t_i}(t_f, t_i) \), and hence, are equal in their common domain of convergence (provided that the latter exists).

We note that the Taylor series representation in the first line of (37) above (which converges for \( |kr \cos \theta| < 1 \)) and the Bessel-Legendre series representation in the third line, have in general different domains of convergence. They constitute two series representations (branches) of the plane wave function appearing on the left hand side; they are only equal at any point within the common domain of convergence (as can be checked for example at a point satisfying e.g. \( |kr \cos \theta| < 1, (\theta \neq 0, \pi) \)). It goes without saying that their partial sums up to the same number of terms (e.g. the second and the fourth lines) may not necessarily agree numerically. Finally, It is worth noting that a given asymptotic series could be often usefully transformed into another infinite series having an extended domain and/or a faster rate of convergence, for example, by a Shank’s transformation [8].

[1] W. E. Lamb Jr., Phys. Rev. 85, 259 (1952).
[2] K.-H. Yang, Ann. Phys. (N.Y.) 101, 62 (1976).
[3] C. Cohen-Tannoudji, B. Diu and F. Laloë, Quantum Mechanics (Hermann/Wiley, Paris, 1977).
[4] V. Fock, Zeit. für Physik 39, 226 (1926).
[5] F.H.M. Faisal, J.Phys. B 40, F145 (2007); Phys. Rev. A 75,063412 (2007).
[6] In the present context, the general field-free condition is \( \mathbf{E}(t_i, f) = -\frac{1}{\lambda} \mathbf{A}(t_i, f) = 0, \) for \( \mathbf{A}(t_i, f) \) arbitrary constants or 0, for any given values of \( t_i, f \) (including the asymptotic values \( t_i, f = \mp \infty \)). The general field-free atomic reference states are given by the fundamental solutions of the Schrödinger equation associated with the reference Hamiltonian (19): \( H_s(t_i, f) = (p_o^2 - \frac{\lambda}{\lambda} \mathbf{A}(t_i, f))^2/2m + V_a(r); \) the corresponding initial and final reference states are thus the same as given in Eqs. (25) and (29) in the text.
[7] This may be illustrated by the following two well-known infinite series representations of the same plane wave function:

\[ e^{ikr \cos \theta} = \sum_{n=0}^{\infty} (ikr \cos \theta)^n/n! = 1 + (ikr \cos \theta)/1! - (kr \cos \theta)^2/2! + \cdots = \sum_{n=0}^{\infty} (2n + 1)^n j_n(kr) P_n(\cos \theta) \]

\[ = j_0(kr) + (3i)j_1(kr) P_1(\cos \theta) - 5j_2(kr) P_2(\cos \theta) + \cdots \]