Causality in the Fermi Problem and the Magnus expansion

J. S. Ben-Benjamin

Institute for Quantum Science and Engineering, Texas A&M University, Texas, USA.

Abstract

In 1932, Fermi presented a two-atom model for determining whether quantum mechanics is consistent with causality, and concluded that indeed it is. In the late 1960’s, Shirokov and others found that Fermi’s approximations may not have been sound, and when corrected, Fermi’s model shows non-causal behavior. We show that if instead of time-dependent perturbation theory, the Magnus expansion is used to approximate the time-evolution operator, causality does follow.

1 Introduction

In his 1932 review article on the quantum theory of radiation, Fermi sought to show that quantum theory gives causal results [1]. Fermi devised the following model: At time \( t = 0 \), a pair of stationary two-level atoms, \( A_R \) and \( A_L \), a distance \( R \) apart, where atom \( A_R \) is initially in the excited state and atom \( A_L \) is initially in the ground state, and no photons are present (See Fig. 1). Immediately after time \( t = 0 \), the probability that atom \( A_R \) is in the ground state becomes non-zero. The question Fermi asked is: When does the probability amplitude, \( A \), that \( A_L \) is excited become non-zero?

The model involves two spacetime events: Atom \( A_R \) starts decaying at \((t_R, z_R)\) and atom \( A_L \) starts becoming excited at \((t_L, z_L)\); quantum mechanics is consistent with causality if the probability amplitude \( A \) is zero for \( |t_L - t_R| < |z_L - z_R|/c \). Using his model, Fermi found that indeed, quantum theory is consistent with causality.

![Diagram of the Fermi model](image)

Figure 1: Initial conditions of the Fermi model. Two atoms are separated by a distance \( R \): The one on the left, \( A_L \) at position \( z_L \), is initially in the ground state, and the one on the right, \( A_R \) at position \( z_R \), is initially in the excited state; no photons are present. The initial state is \( |\psi(t = 0)\rangle = |b, a, 0\rangle \), where \( |0\rangle \) is the field vacuum state, and \( |b\rangle \) and \( |a\rangle \) are the ground and excited atomic states, respectively.
Sometime later, Shirokov showed that Fermi made some simplifying assumptions in his calculation, without which, his model yields non-causal predictions [2]. Specifically, Shirokov found that the ground state atom could become excited instantaneously. These results have been widely discussed, and views generally belong to one of the following: (a) Quantum theory should give causal answers, including in the Fermi model [1, 3, 4, 5, 6], (b) the Fermi model leads to absurd results because it is non-physical [2, 7, 8], (c) the Fermi model is not physically-realizable, but if one modifies it, causal predictions could be obtained [9, 10], and (d) quantum theory’s prediction of an instantaneous effect is physically correct.

The present paper is in the first camp. In Sec. 2 we show that causality is restored in the Fermi model if the state is evolved using the Magnus expansion of the time-evolution operator. In Sec. 3 we discuss the rotating wave approximation as it relates to causality. To illustrate the Magnus expansion method for a simple case, in the appendix we present an exactly solvable problem.

2 The Fermi problem and the Magnus expansion

To find the probability amplitude,

\[ A = \langle a, b, 0 | \hat{U}(t, 0) | b, a, 0 \rangle, \] (1)

that the state \( |b, a, 0\rangle \) at time \( t = 0 \) evolves into the state \( |a, b, 0\rangle \) at some later time \( t \), we use the Magnus expansion method. As we explain in the appendix, to second order, the Magnus expansion gives that the time-evolution operator is approximately the sum of three terms,

\[ \hat{U} = \mathbb{I} + \hat{M}_1 + \hat{M}_2. \] (2)

Explicitly, Eq. (2) is [12],

\[ \hat{U}(t, 0) = \mathbb{I} + \int_0^t \frac{dt'}{i\hbar} \hat{V}(t') + \int_0^t \frac{dt'}{i\hbar} \int_0^{t'} \frac{dt''}{i\hbar} \left[ \hat{V}(t'), \hat{V}(t'') \right], \] (3)

where the interaction Hamiltonian is \( \hat{V} = \hat{V}_L + \hat{V}_R \), with

\[ \hat{V}_j(t) = g_j \left( \hat{\sigma} e^{-i\omega t} + \text{H.a.} \right) \sum_\nu \sqrt{\nu} \left( \hat{a}_\nu e^{-i\nu(ctz_j)/c} + \text{H.a.} \right), \] (4)

and where \( j \) is ‘L’ or ‘R’ (standing for the left and right atoms respectively), and the \((\pm)\) sign corresponds to left-moving and right-moving waves. In Eq. (4), \( g_j = \omega_j \sqrt{\hbar/\epsilon_0 L} \), and the operators \( \hat{\sigma}^\dagger = |a\rangle \langle b| \) and \( \hat{\sigma} = |b\rangle \langle a| \) are the atomic raising and lowering operators. The field creation and annihilation operators of frequency \( \nu \), \( \hat{a}_\nu^\dagger \) and \( \hat{a}_\nu \), interact locally and therefore are evaluated at the atomic position \( z_j \).

Since the Fermi model involves two atomic state changes, two contributions of the interaction Hamiltonian are required. Therefore only the third term in Eq. (3), \( \hat{M}_2 \), contributes to the amplitude \( A \),

\[ A = \int_0^t dt' \int_0^{t'} dt'' C(z', t'; z'', t''), \] (5)
where \( C(z', t'; z'', t'') \) is the matrix element of the commutator \( \langle a, b, 0 | \hat{V}(t') \hat{V}(t'') | b, a, 0 \rangle \), which involves two-spacetime events. The matrix element \( C \) is

\[
C(z', t'; z'', t'') = \pm \frac{\hbar}{i \pi \epsilon_0} \frac{\partial}{\partial R} \left\{ e^{i \omega_L t' - i \omega_R t''} \delta \left( t'' - t' \pm \frac{R}{c} \right) - e^{i \omega_L t'' - i \omega_R t'} \delta \left( t' - t'' \pm \frac{R}{c} \right) \right\},
\]

where \( R = z_R - z_L \). We therefore have that the probability amplitude \( A \) for the Fermi model is

\[
A = \pm \frac{\hbar}{i \pi \epsilon_0} \frac{\partial}{\partial R} \int_0^t dt' \int_0^{t''} dt'' \left\{ e^{i \omega_L t' - i \omega_R t''} \delta \left( t'' - t' \pm \frac{R}{c} \right) - e^{i \omega_L t'' - i \omega_R t'} \delta \left( t' - t'' \pm \frac{R}{c} \right) \right\}.
\]

The spacetime \( \delta \)-functions enforce that \( A \) remain exactly zero until at least a time \( R/c \) has passed, thus giving a causal prediction. Thus, the spacetime \( \delta \)-functions are crucial. These appear because the electric field operator is special and obeys Maxwell equations, which are causal.

Since \( R \) is positive and since the integration limits restrict \( t' \geq t'' \), we find that the first \( \delta \)-function in Eq. (7) could have a zero argument only for left-moving waves (+ sign), and that the second \( \delta \)-function could have zero argument only for right-moving waves (− sign). We note that even though the first \( \delta \)-function gives the left-moving wave contribution and the second \( \delta \)-function gives the right-moving wave contribution, it is not the case that the first consists of only co-rotating terms and that the second consists of only counter-rotating terms. Actually, each \( \delta \)-function requires both co-rotating and counter-rotating terms, as we discuss in Sec. 3.

These two processes are not distinguishable, and therefore add in amplitude. The left-propagating term is

\[
A_+ = \frac{\hbar}{i \pi \epsilon_0} \frac{\partial}{\partial R} \Theta(t - R/c) e^{i \omega_R R/c} \frac{e^{i(\omega_L - \omega_R)t} - e^{i(\omega_L - \omega_R)R/c}}{\omega_L - \omega_R},
\]

and the right-propagating term is

\[
A_- = \frac{\hbar}{i \pi \epsilon_0} \frac{\partial}{\partial R} \Theta(t - R/c) e^{-i \omega_R R/c} \frac{e^{i(\omega_L - \omega_R)t} - e^{i(\omega_L - \omega_R)R/c}}{\omega_L - \omega_R}.
\]

Both Amplitudes (8) and (9) exhibit causality because they are exactly zero for \( t < R/c \). The total probability amplitude for the Fermi problem is therefore \( A = A_+ + A_- \),

\[
A = -\frac{\hbar}{\pi \epsilon_0} \frac{\partial}{\partial R} \Theta(t - R/c) \left( e^{i \omega_R R/c} + e^{-i \omega_L R/c} \right) \times \frac{e^{i(\omega_L - \omega_R)t} - e^{i(\omega_L - \omega_R)R/c}}{\omega_L - \omega_R},
\]

which is causal.

### 3 The Rotating Wave Approximation

There are two contributions to the probability amplitude for the Fermi problem: (a) Atom \( A_R \) could transition to the ground state, emitting a photon which after a time \( R/c \) excites atom \( A_L \),
and (b) atom $A_L$ becomes excited and emits a photon, which a time $R/c$ later is absorbed by atom $A_R$, which transitions to the ground state. The second is the counter-rotating process, and not only does it contribute, it is in fact essential for causality.

We know that the quantized radiation Hamiltonian contains both co-rotating and counter-rotating terms, and that both have an essential role \[6\]; neglecting the counter-rotating terms (an approximation called “the rotating-wave approximation,” or RWA) is only appropriate in specific situations and only for calculating certain quantities \[14, 15, 16, 17, 18]. For example, even in the case in which the RWA is considered to be most appropriate (in the near-resonant two-level atom case), the counter-rotating terms have a significant contribution to the frequency shift of individual atoms \[17\]. This shows that ignoring the counter-rotating terms leads to non-causal results.

In the interaction Hamiltonian, Eq. (4), the terms that go as $\hat{\sigma} \hat{a}^\dagger$ and $\hat{\sigma}^\dagger \hat{a}$, are called co-rotating. It also contains counter-rotating terms; those go like $\hat{\sigma}^\dagger \hat{a}^\dagger$ and $\hat{\sigma} \hat{a}$, and do not (individually) conserve energy. The RWA amounts to neglecting the latter two terms, which would lead to the interaction Hamiltonian $\hat{V} = \hat{V}_L + \hat{V}_R$, where

$$
\hat{V}_j(t) \overset{\text{RWA}}{\longrightarrow} g_j \sum_\nu \sqrt{\nu} \left( \hat{\sigma}_j \hat{a}^\dagger_{\nu} e^{-i[\omega t - \nu(\epsilon t \pm z_j)/c]} + \text{H.a.} \right).
$$

One can show that using this purely co-rotating interaction Hamiltonian yields non-causal predictions. Specifically, the integrand in the Magnus expansion consists of functions other than $\delta$-functions. As discussed in Sec. 2, to be causal, the integrand must consist of only $\delta$-functions. The details will be published in a future paper.

4 Conclusion

The Fermi model has been widely used for discussing the issue of causality in quantum theory. While Fermi showed that the model implies causality, Shirokov and others have shown that it does not. We have shown that if one uses the Magnus expansion, one obtains causality in a straightforward way. Also, we have found that the the rotating wave approximation leads to non-causal results. That the Magnus expansion method gives causal results in the Fermi model may imply that causality is related to operator-ordering, as suggested in Ref. \[19\]; this is because the Magnus expansion uses a different operator-ordering than TDPT.

5 Acknowledgements

We would like to thank Professor M. O. Scully for insightful discussions, the Robert A. Welch Foundation (Grant No. A-1261), the Office of Naval Research (Award No. N00014-16-1-3054), the Air Force Office of Scientific Research (FA9550-18-1-0141), and the King Abdulaziz City for Science and Technology (KACST) grant for their the support.
References

[1] E. Fermi, “Quantum Theory of Radiation,” Rev. Mod. Phys. 4 87 (1932).

[2] M. I. Shirokov, “The Velocity of Electromagnetic Retardation in Quantum Electrodynamics,” Sov. J. Nulc. Phys. 4 774 (1967).

[3] W. Heitler, S. T. Ma, “Quantum theory of radiation damping for discrete states,” Proc. R. Ir. Acad. 52 123 (1949).

[4] J. Hamilton, “Damping Theory and the Propagation of Radiation,” Proc. Phys. Soc. A 62 12 (1949).

[5] W. Heitler, The Quantum Theory of Radiation, Oxford (1964).

[6] M. O. Scully, M. S. Zubairy, Quantum Optics, Cambridge Univ. Press, New York (1997).

[7] G. C. Hegerfeldt, “Remark on causality and particle localization,” Phys. Rev. D 10 3320 (1974).

[8] G. C. Hegerfeldt, “Causality Problems for Fermi’s Two-Atom System,” Phys. Rev. Lett. 72 5 596 (1994).

[9] B. Ferretti, “Propagation of Signals and Particles,” in Old and New Problems in Elementary Particles, Acad. Press, New York (1968).

[10] M. I. Shirokov, “Signal velocity in quantum electrodynamics,” Sov. Phys. Usp. 21 345 (1978).

[11] W. Magnus, “On the exponential solution of differential equations for a linear operator,” Commun. Pure Appl. Math. VII 649 (1954).

[12] S. Blanes, F. Casas, J. A. Oteo, J. Ros, “The Magnus expansion and some of its applications,” Phys. Rep. 470 151 (2009).

[13] M. H. Stone, “On one-parameter unitary groups in Hilbert Space,” Ann. Math. 33 (3) 643 (1932).

[14] L. Mandel, D. Meltzer, “Theory of Time-Resolved Photoelectric Detection of Light,” Phys. Rev. 188, 198 (1969).

[15] G. S. Agarwal, “Rotating-wave approximation and spontaneous emission,” Phys. Rev. A 4 1778 (1971).

[16] G. S. Agarwal, Quantum Optics, Springer, Berlin (1974).

[17] P. L. Knight, L. Allen, “Rotating-wave approximation in coherent interactions,” Phys. Rev. A 7 368 (1973).

[18] H, Zheng, S.-Y. Zhu, M. S. Zubairy, “Quantum Zeno and anti-Zeno effects: without the rotating-wave approximation,” Phys. Rev. Lett. 101 200404 (2008).
Appendix: An exactly solvable model illustrating the Magnus method

We now present an exactly solvable model and use it to compare the Magnus expansion to time-dependent perturbation theory (TDPT). While causality is not an issue here, this model allows us to explicitly contrast the Magnus expansion method and TDPT.

Consider the Hamiltonian for a quantized single-mode radiation field due to a classical current, $\hat{H} = \hbar \omega \hat{a}^\dagger \hat{a} + g(\hat{a}^\dagger + \hat{a})$, which leads to the interaction potential

$$\hat{V}(t) = g(\hat{a}^\dagger e^{i\omega t} + \hat{a} e^{-i\omega t}).$$

The exact time-evolution operator is

$$\hat{U}_{\text{Exact}}(t, 0) = \exp\left[\frac{g}{\hbar \omega} \left\{ \hat{a} \left( e^{-i\omega t} - 1 \right) - \hat{a}^\dagger \left( e^{i\omega t} - 1 \right) \right\} \right].$$

We now contrast the exact time-evolution operator and the approximations obtained by TDPT and by the Magnus expansion method.

**Magnus expansion.** Since every unitary operator is the exponential of some anti-Hermitian operator \cite{13}, the time-evolution operator, which is unitary, may be written as $\hat{U} = \exp[\hat{M}]$. Following Magnus \cite{11, 12}, we write the exponent as $\hat{M} = \hat{M}_1 + \hat{M}_2 + \cdots$. In the Magnus expansion method, we truncate this sum and then expand the exponential in a power series, resulting in Eqs. (2) and (3).

For the potential in Eq. (12), the terms $\hat{M}_1$ and $\hat{M}_2$ are [see Eq. (3)]

$$\hat{M}_1 = \frac{g}{\hbar \omega} \left\{ \hat{a} \left( e^{-i\omega t} - 1 \right) - \hat{a}^\dagger \left( e^{i\omega t} - 1 \right) \right\},$$

and

$$\hat{M}_2 = \frac{ig^2}{(\hbar \omega)^2} \left( \omega t - \sin(\omega t) \right).$$

Since $\hat{M}_2$ is proportional to the identity operator, the exponential form of $\hat{U}$ is $\exp[\hat{M}_1 + \hat{M}_2] = \exp[\hat{M}_2] \exp[\hat{M}_1]$, where we have truncated the exponent to the first two terms $\hat{M} \simeq \hat{M}_1 + \hat{M}_2$, but the resulting operator is still unitary. Explicitly,

$$\hat{U} \simeq \exp \left[ \frac{ig^2}{(\hbar \omega)^2} \left( \omega t - \sin(\omega t) \right) \right] \exp \left[ \frac{g}{\hbar \omega} \left\{ \hat{a} \left( e^{-i\omega t} - 1 \right) - \hat{a}^\dagger \left( e^{i\omega t} - 1 \right) \right\} \right].$$

Eq. (16) is almost the same as the exact time-evolution operator $\hat{U}_{\text{Exact}}$ in Eq. (13): The two expressions become equal if we approximate $\sin(\omega t) \simeq \omega t$, that is, $\hat{M}_2 \simeq 0$. However, should we...
want to approximate Eq. (16) further, we would keep the overall scalar factor, \( \exp[\hat{M}_2] \), and expand the exponential of \( \hat{M}_1 \) in a power series. This approach gives

\[
\hat{U}_{\text{Mag}} = \exp \left[ \frac{ig^2}{\hbar^2 \omega^2} \left( \omega t - \sin(\omega t) \right) \right] \\
\times \left\{ \hat{1} + \frac{g}{\hbar \omega} \left[ \left( e^{-i\omega t} - 1 \right) \hat{a} - \left( e^{i\omega t} - 1 \right) \hat{a}^\dagger \right] \right\},
\]

which is close to unitary: When calculating \( \hat{U}_{\text{Mag}}^\dagger \hat{U}_{\text{Mag}} \), the leading term is the identity \( \hat{1} \), the term first-order in \( g \) is zero, and the second-order term oscillates like \( \sin^2(\omega t/2) \) with time and decreases with the square of the photon energy. Explicitly

\[
\hat{U}_{\text{Mag}}^\dagger \hat{U}_{\text{Mag}} = \hat{1} + \left( \frac{g}{\hbar \omega} \right)^2 \sin^2 \left( \frac{\omega t}{2} \right) \left[ e^{i\omega t/2} \hat{a}^\dagger + e^{-i\omega t/2} \hat{a} \right]^2,
\]

which is approximately unitary for large photon frequency \( \omega \).

**Time-dependent perturbation theory.** To second-order, TDPT gives

\[
\hat{U}_{\text{TDPT}} = \hat{1} + \frac{g}{\hbar \omega} \left[ \left( e^{i\omega t} - 1 \right) \hat{a}^\dagger - \left( e^{-i\omega t} - 1 \right) \hat{a} \right]
\]

\[
+ \frac{g^2}{\hbar^2 \omega^2} \left[ \left( i\omega t + e^{-i\omega t} - 1 \right) \hat{a} \hat{a}^\dagger - \left( i\omega t - e^{i\omega t} + 1 \right) \hat{a}^\dagger \hat{a} \right]
\]

\[
- \left( e^{-2i\omega t} - 1 \right) \hat{a} \hat{a} + \left( \frac{e^{2i\omega t} - 1}{2} - e^{i\omega t} + 1 \right) \hat{a}^\dagger \hat{a}^\dagger \right].
\]

From Eq. (19), we see that the TDPT time-evolution operator increases linearly in time, that is, \( \hat{U}_{\text{TDPT}}(t, 0) \propto t \). Therefore, TDPT yields predictions for the total probability that diverge as \( t^2 \). In contrast, the Magnus expansion approximation for the time-evolution operator, \( \hat{U}_{\text{Mag}} \), does not diverge in this way. This, of course, does not show that the Magnus expansion method is always better than TDPT.