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TIME DEPENDENCE
in
QUANTUM MECHANICS

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Abstract

Time-dependent perturbation theory is formulated in a systematic way. The focus is shifted from the wavefunction to the unitary transformation that evolves the wavefunction from one slice of time to another. Perturbation theory is formulated in terms of a systematic iterative expansion of the unitary transformation in terms of the perturbing hamiltonian, expressed in the interaction representation. Two standard results are obtained in first order time-dependent perturbation theory. These are the Fermi Golden Rule for transition rates and the Lorentz line shape for radiative transitions, as formulated by Wigner and Weisskopf. Time-dependent perturbation theory is approached systematically in higher orders for a very specific perturbation of a very specific physical system, the simple harmonic oscillator subjected to a decaying exponential dipole driving term. Expansions are carried out to third order. These calculations suggest that a useful bookkeeping system be introduced for keeping track of the terms appearing in the perturbation series. This "diagrammatic technique" evolves, in a direct line, to the Feynman diagrams which keep the books for the perturbation theory called Quantum Electrodynamics. Some Lie Group theory is introduced and used to find an analytic expression for all transition amplitudes for any dipole-like perturbing potential. The analytic expression is compared with the systematic approximations at low orders for the exponentially decaying dipole forcing term where perturbation theory can be carried out explicitly to any order.

1 Introduction

The time-dependent Schrödinger equation is

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = H_0(x,p)\ \psi(x,t) \tag{1}$$

Eigenstates $\phi_j(x,t)$ with energy E_j of a time-independent hamiltonian $H_0(x,p)$ evolve in time by phase change:

$$\phi_j(x,t_2) = e^{-\frac{i}{\hbar}E_j(t_2-t_1)}\ \phi_j(x,t_1) \tag{2}$$

At this point it is useful to observe (for later suggestive purposes) that this time evolution can be expressed in the following form

$$\psi(x,t_2) = e^{-\frac{i}{\hbar}\int_{t_1}^{t_2} H_0(x,p)dt}\ \psi(x,t_1) \tag{3}$$

This expression is valid for any linear superposition of eigenstates of H_0: $\psi(x,t) = \sum_j c_j\phi_j(x,t)$. In this expansion the amplitudes $c_j(t)$ have the simple time dependence $c_j(t) = e^{-\frac{i}{\hbar}E_j t}\ c_j(0)$.

When the Hamiltonian is explicitly time-dependent, things become much more exciting. In such cases it is often the case that it is possible to express the Hamiltonian explicitly in the form

$$H(x,p;t) = H_0(x,p) + H_1(x,p;t) \tag{4}$$

In this decomposition we usually take the time-independent part of $H(x,p;t)$, H_0, as a hamiltonian that we can treat rather easily - even solve analytically if that is useful. All the time dependence is contained in the second term, $H_1(x,p;t)$, which is the source of transitions among the eigenstates of H_0. It is convenient to suppress the coordinate- and momentum-dependence of the interaction hamiltonian: $H_1(x,p;t) \to H_1(t)$.

2 Unitary Transformation U

In this section we shift the usual focus of time-dependent perturbation theory away from the amplitudes in the expansion of a state vector $\psi(x,t) = \sum a_j(t)\phi_j(x)$ to the time-dependent piece of the hamiltonian, $H_1(t)$, that causes transitions among the eigenstates of H_0.

2.1 Schrödinger Equation for U

The time dependence of the wavefunction $\psi(x,t)$ can be shifted to the unitary transformation that relates the wavefunction at some initial time $\psi(t_1)$ with the wavefunction at any later time via $\psi(x,t_2) = U(t_2,t_1)\psi(x,t_1)$:

$$i\hbar\frac{\partial}{\partial t}\ U(t,t_1)\psi(x,t_1) = H(x,p;t)\ U(t,t_1)\psi(x,t_1) \tag{5}$$

This equation must hold for any initial wavefunction $\psi(x,t_1)$. Therefore it is independent of this wavefunction, and must hold for the unitary transformation. The unitary transformation therefore also obeys the time-dependent Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\ U(t,t_1) = H(x,p;t)\ U(t,t_1) \tag{6}$$

2.2 Formal Solution for U

When the interval between the two times in U is small, U is approximated to lowest (first) order by

$$U(t+dt,t) = I - \frac{i}{\hbar}H(t)\ dt \quad (+\text{h.o.t.}) \tag{7}$$

To first order this operator is unitary: $U^{-1}(t+dt,t) = U^\dagger(t+dt,t)$. A finite-time unitary solution can be built up by multiplying together lots of small-time approximations computed along a discretization of the time interval:

$$U(t_n,t_0) =$$

$$(I - \tfrac{i}{\hbar}H(\tau_n)\Delta t_n)(I - \tfrac{i}{\hbar}H(\tau_{n-1})\Delta t_{n-1})\cdots(I - \tfrac{i}{\hbar}H(\tau_2)\Delta t_2)(I - \tfrac{i}{\hbar}H(\tau_1)\Delta t_1) \tag{8}$$

Here the $\Delta t_j = t_n - t_{j-1}$ are differences between successive closely spaced times and the $\tau_j = \frac{1}{2}(t_n + t_{j-1})$ are averages of the same closely spaced times.

The product above can be written as

$$U(t_n,t_0) = \prod_{j=1}^{n}(I - \frac{i}{\hbar}H(\tau_j)\Delta t_j) = \mathcal{T}\ EXP\left(-\frac{i}{\hbar}\int_{t_0}^{t_n} H(t)\ dt\right) \tag{9}$$

The symbol $\mathcal{T}$ ("time-ordered product") is introduced as an explicit reminder that the order of the factors in the product is important. If the hamiltonian does not explicitly depend on time ($H(t) \to H(*)$) we can further refine this expression:

$$U(t,t_0) = \lim_{n\to\infty}\left(I - \frac{i}{\hbar}H(*)\left(\frac{(t-t_0)}{n}\right)\right)^n = EXP\left(-\frac{i}{\hbar}\int_{t_0}^{t} H(*)\ dt\right) \tag{10}$$

Once the unitary transformation $U(t,t_0)$ has been determined it can be used to compute how the amplitudes of the eigenstates $\phi_j(x)$ in the expansion of a wavefunction $\psi(x,t) = \sum_j c_j(t)\phi_j(x)$ evolve in time:

$$c_j(t) = \int dx\ \phi_j^*(x)\ U(t,t_0)\ \psi(t_0) = \sum_k\ \langle j|U(t,t_0)|k\rangle\ c_k(t_0) \tag{11}$$

When $H_1(t) \neq 0$ the amplitudes $c_k(t)$ are no longer simply phase factors, so that $|c_k(t)|^2 \neq$ cst. We will use this equation extensively to compute transition amplitudes and probabilites, as well as other important quantities, in the following sections.

2.3 Iterative Solution of U

It is useful to find a multiplicative decomposition for the unitary transformation $U(t)$ to mirror the form of the additive decomposition of the Hamiltonian in Eq.(4). We define $U(t) = U_0(t)U_1(t)$ following this analogy:

$$\begin{array}{ccccc} H(t) & = & H_0 & + & H_1(t) \\ U(t) & = & U_0(t) & \times & U_1(t) \end{array} \tag{12}$$

The equation of motion for the unitary transformations are:

$$i\hbar\frac{\partial U_0(t)}{\partial t}\ U_1(t) + U_0(t)\ \left\{i\hbar\frac{\partial U_1(t)}{\partial t}\right\} = H_0\ U_0(t)U_1(t) + H_1(t)\ U_0(t)U_1(t) \tag{13}$$

with $U_0(t) = e^{-\frac{i}{\hbar}H_0 t}$. The first term on the left is equal to the first term on the right. The equation of motion for $U_1(t)$ is obtained by multiplying by the inverse of $U_0(t)$:

$$i\hbar\frac{\partial U_1(t)}{\partial t} = \left\{U_0^{-1}\ H_1(x,p;t)\ U_0(t)\right\}\ U_1(t) = H_{\rm int}(t)\ U_1(t) \tag{14}$$

where

$$H_{\rm int}(t) = U_0^{-1}\ H_1(x,p;t)\ U_0(t) \qquad\qquad U_0(t) = e^{-\frac{i}{\hbar}H_0 t} \tag{15}$$

The result is that the part of the unitary transformation, $U_1(t)$, that contains information about the interaction induced by the time-dependent Hamiltonian $H_{\rm int}(x,p;t)$ obeys a simple time-dependent Schrödinger equation whose hamiltonian is $H_{\rm int}(t) = U_0^{-1}\ H_1(x,p;t)\ U_0(t)$.

Time dependence in Quantum Mechanics has been treated in three different ways, called Representations. These are the Schrödinger Representation, the Heisenberg Representation, and intermediate between these two, the Interaction Representation. If $\mathcal{O}$ is an operator that is not explicitly time dependent, then the time dependence of the operator $\mathcal{O}$ and the wave function ψ in these three representations is summarized as follows:

Representation	$\mathcal{O}$	ψ
Schrödinger	No	Yes
Interaction	Yes	Yes
Heisenberg	Yes	No

Somewhat surprisingly, the Interaction Representation, in which both the operator *and* the wavefunction are explicitly time dependent, is the most useful to work in. These three Representatations are described in more detail in Appendix **A**.

Equation (14) can be solved iteratively. The formal solution is

$$U(t,-\infty) - I = -\frac{i}{\hbar}\ \int_{-\infty}^{t} dt_1\ H_{\rm int}(t_1)\ U(t_1,-\infty) \tag{16}$$

The unitary transformation is the identity at equal times $t_2 = t_1$, in particular at $t \to -\infty$: $U(-\infty, -\infty) = I$. Equation (16) is an integral equation: the transformation to be determined is expressed in terms of itself. This can be rearranged and iterated, to give

$$U(t,-\infty) = I - \frac{i}{\hbar}\int_{-\infty}^{t} dt_1\, H_{\rm int}(t_1)\left\{I - \frac{i}{\hbar}\int_{-\infty}^{t_1} dt_2\, H_{\rm int}(t_2)\left\{I - \frac{i}{\hbar}\int_{-\infty}^{t_2} dt_3\, H_{\rm int}(t_3)\ \{...\}\right\}\right\} \tag{17}$$

In principle, this expansion should be carried out to all orders; in practice, it is usually truncated at first or second order. This means the truncation involves one or two integrals; one or two occurrances of the hamiltonian. To second order, this expansion is

$$U(t,-\infty) = I + \left(-\frac{i}{\hbar}\right)\int_{-\infty}^{t} dt_1\, H_{\rm int}(t_1) + \left(-\frac{i}{\hbar}\right)^2 \int_{-\infty}^{t} dt_1\, H_{\rm int}(t_1)\int_{-\infty}^{t_1} dt_2\, H_{\rm int}(t_2) \tag{18}$$

Often the interaction hamiltonian is proportional to a coupling constant, which we will call g below. Then the iterative expansion for the unitary transformation can be regarded as a "Taylor series" in the coupling constant g, and the coefficient of g^n consists of all terms that arise in nth order of the perturbation theory.

3 First Order Theory

In principle, perturbation theory should be carried out to all orders. In practice significant results can be obtained using only first order time-dependent perturbation theory. In this Section we introduce two of the classical results of first order theory. These are Fermi's Golden Rule for computing the transition rates from an excited state, and the Lorentz line shape of a radiative transition from an excited state to a lower lying state. This line shape, derived by Wigner and Weisskopf, holds for absorption as well as emission (detailed balance).

In both applications we compute the matrix element for transition from an initial state ϕ_K to final state(s) ϕ_j. In first order the matrix element of interest is

$$-\frac{i}{\hbar}\int_{-\infty}^{t} dt_1 \langle j|H_{\rm int}(t_1)|K\rangle c_K(t) = -\frac{i}{\hbar}\int_{-\infty}^{t} dt_1 \langle j|e^{+\frac{i}{\hbar}H_0 t_1} H_1(t_1) e^{-\frac{i}{\hbar}H_0 t_1}|K\rangle c_K(t_1)$$

$$\to -\frac{i}{\hbar}\int_{-\infty}^{t} dt_1\ e^{+\frac{i}{\hbar}E_j t_1}\ \langle j|H_1(t_1)|K\rangle\ e^{-\frac{i}{\hbar}E_K t_1}\ c_K(t_1) \tag{19}$$

In the two examples to follow, we will assume that the state ϕ_K is excited at $t = 0$ with $c_K(t) = 0,\ t < 0$ and $c_K(t = 0) = 1$. Under this approximation the integrals in the following two sections extend from 0 to t.

3.1 Fermi Golden Rule

We consider first the case where the initial state at $t = 0$ is some excited state ϕ_K of the time-independent hamiltonian H_0. As a time-dependent interaction $H_1(t)$ is turned on, this excited state typically decays to lower lying levels. As an example, think of the deexcitation of the hydrogen atom in "vacuum" from the $2P$ state to the $1S$ state by emission of a photon. The lifetime of the $2P$ state against radiative deexcitation is about 10^{-8} sec. The lifetime can be estimated using Fermi's Golden Rule, which we derive starting from the amplitude equations (11).

Initially $c_K(0) = 1$, $c_j(0) = 0$ unless $j = K$. Over a short time, during which $c_K(t) \simeq 1$ and the other $c_j(t)$ $(j \neq K)$ remain sufficiently small, the amplitudes are well approximated by

$$c_j(t) = -\frac{i}{\hbar}\int_0^t dt' \langle j|H_1(t')|K\rangle e^{\frac{i}{\hbar}(E_j - E_K)t'} \tag{20}$$

It is useful at this point to assume that the matrix element of $H_1(t)$ has a single Fourier contribution:

$$\langle j|H_1(t')|K\rangle = A_{jK}(\omega)e^{+i\omega t'} \tag{21}$$

Using this representation in the integral above (Eq.(20)) we find

$$c_j(t) = -\frac{i}{\hbar}\ A_{jK}(\omega)\ \frac{e^{\frac{i}{\hbar}(E_j - E_K)t + i\omega t} - 1}{i(\omega_{jK} + \omega)} \tag{22}$$

where $E_j - E_K = \hbar\omega_{jK}$. It is useful to set $\omega_{jK} + \omega = \kappa$. Then

$$\begin{aligned} c_j(t) &= -\frac{A_{jK}(\omega)}{\hbar}\ \frac{e^{i\kappa t} - 1}{\kappa} \\ &= -\frac{A_{jK}(\omega)}{\hbar}\ e^{i\kappa t/2}(it)\ \frac{(e^{i\kappa t/2} - e^{-i\kappa t/2})/2i}{\kappa t/2} \end{aligned} \tag{23}$$

$$|c_j(t)|^2 = \frac{|tA_{jK}(\omega)|^2}{\hbar^2}\frac{\sin^2(\kappa t/2)}{(\kappa t/2)^2}$$

In many cases the initial state can make a transition to many final states. This occurs, for example, in the decay of a hydrogen atom from a state $|nlm\rangle$ to a state $|n'l'm'\rangle$. Although the initial and final *atomic* states are nondegenerate (except for spin), the photon of energy $\hbar\omega = \hbar c|\mathbf{k}| = E_{|nlm\rangle} - E_{|n'l'm'\rangle}$ can be emitted in any direction on the sphere surface. To compute the transition rate, we must add up the transition probability over all possible final photon states. This is

$$\begin{aligned} \sum_j |c_j(t)|^2 &= \sum_j \frac{t^2|A_{jK}(\omega)|^2}{\hbar^2} \frac{\sin^2(\frac{\kappa t}{2})}{(\frac{\kappa t}{2})^2} \\ &\rightarrow \int \frac{t^2|A_{jK}(\omega)|^2}{\hbar^2} \frac{\sin^2(\frac{\kappa t}{2})}{(\frac{\kappa t}{2})^2} \rho(E)\, dE \end{aligned} \tag{24}$$

In this last expression we have assumed: (**i**) that the sum can be replaced by an integral, that is, the final states are closely spaced; (**ii**) that the matrix element $\langle j|H_{\rm int}|K\rangle$ is the same over all the transitions that conserve energy (see the delta function below); and (**iii**) that the number of available final states of energy E_j is represented by the density of states function $\rho(E)$. We note that $dE = dE_j = \frac{2\hbar}{t} d(\frac{\kappa t}{2})$. Replacing $\frac{\kappa t}{2} \rightarrow x$ the expression above reduces to

$$\rightarrow \frac{2\hbar}{t} \frac{t^2|A_{jK}(\omega)|^2}{\hbar^2} \int_{-\infty}^{+\infty} \frac{\sin^2(x)}{x^2}\, dx \tag{25}$$

The function under the integral ($\left(\frac{\sin(x)}{x}\right)^2$) is extremely sharply peaked around $x = 0$ and the area under this nonnegative curve is π. We can therefore replace this integral by $\pi\delta(x) = \pi\delta(E_j + \hbar\omega - E_K)$. The result is the Fermi Golden Rule for the transition rate out of an excited state ϕ_K:

$$\frac{d}{dt}\sum_j |c_j(t)|^2 = \frac{2\pi}{\hbar}|A_{jK}(\omega)|^2\, \rho(E_j)\, \delta(E_j + \hbar\omega - E_K) \tag{26}$$

This expression determines the transition rate out of a state ϕ_K that is occupied with probability one at time $t = 0$. The delta function imposes conservation of energy: The initial energy E_K is equal to the final energy $E_j + \hbar\omega$, where $\hbar\omega$ is the energy of the single photon (recall that we are doing first order perturbation theory) that is emitted in this transition.

If we assume the excited state population ϕ_K undergoes an exponential decay of the form $e^{-\gamma t}$, then the decay rate out of this state at short times ($t \rightarrow 0$) is $-\frac{d}{dt}e^{-\gamma t}|_{t\rightarrow 0} = \gamma$. Therefore the lifetime of this excited state is $\tau = 1/\gamma$, the reciprocal of the decay rate.

3.2 Wigner-Weisskopf (Lorentz) Line Shape

The second classical application of first order time-dependent perturbation theory leads to a description of the line shape of many radiative transitions. We assume as before that initially a state ϕ_K is excited, and that it decays due to the interaction hamiltonian $H_{\rm int}(t)$. We assume that the amplitude of this state is no longer +1 throughout the time of interest, but that the amplitude decays in such a way that $|c_K(t)|^2 = e^{-\gamma t}$. In short, we take $c_K(t) = e^{-\gamma t/2}$. The transition amplitude to state ϕ_j is

$$c_j(t) = -\frac{i}{\hbar}\, A_{jK}(\omega)\, \frac{e^{\frac{i}{\hbar}(E_j - E_K)t + i\omega t - \gamma t/2} - 1}{i(\omega - \omega_{Kj}) - \gamma/2} \tag{27}$$

This simplifies considerably in the long time limit $t \to \infty$. The square of the transition probability amplitude in this limit is a function of the frequency ω: this function has a Lorentzian line shape:

$$|\tilde{c}_j(\omega)|^2 = \frac{|A_{jK}(\omega)|^2/\hbar^2}{(\omega - \omega_{Kj})^2 + (\gamma/2)^2} \tag{28}$$

We note that the half width at half height is $\gamma/2$, so the full width at half height is the decay rate, as computed using Fermi's Golden Rule. The intensity of the line $|A_{jK}(\omega)|^2/\hbar^2$ is proportional (up to the density of states) to the decay rate.

4 Simple Harmonic Oscillator

In this section we treat the simple harmonic oscillator subjected to a dipole forcing term:

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2 - e\mathcal{E}(t)x \to \hbar\omega(a^\dagger a + \frac{1}{2}) - e\mathcal{E}(t)\sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a) = H_0 + H_1(t) \tag{29}$$

The eigenstates of $H_0 = \hbar\omega(a^\dagger a + \frac{1}{2})$ are $\phi_n(x)$ and are represented by $|n\rangle$. They satisfy $H_0|n\rangle = (n + \frac{1}{2})\hbar\omega|n\rangle = E_n|n\rangle$. Further, we express the electric field dependence in the form $\mathcal{E}(t) = \mathcal{E}_0 f(t)$, where $\mathcal{E}_0$ scales the field strength and $f(t)$ expresses its time-dependence.

The matrix elements for this unitary transformation to zeroth, first, and second order can be computed directly from Eq.(18).

4.1 First Order

In this subsection we point out the deficiencies of first-order time-dependent perturbation theory. We assume that the oscillator is in its ground state $|0\rangle$ in the deep past and ask for the probability amplitude for transition to the jth excited state as a function of time. This is

$$\begin{aligned} c_j^{[1]}(t) &= -\tfrac{i}{\hbar}\int_{-\infty}^{t} dt' f(t') \left(-e\mathcal{E}_0\sqrt{\tfrac{\hbar}{2m\omega}}\right) e^{+ij\omega t'}\langle j|(a + a^\dagger)|0\rangle \\ &= -ig\int_{-\infty}^{t} e^{ij\omega t'} f(t')\ dt'\ \sqrt{1}\ \delta_{j,1} \end{aligned} \tag{30}$$

The superscript in square brackets ($^{[1]}$) identifies this contribution to the total amplitude as due to first-order time-dependent perturbation theory. In this expression we have collected all the physical parameters into a single coupling constant $g = -e\mathcal{E}_0/\sqrt{2m\hbar\omega}$ for clarity of presentation. The factor $e^{ij\omega t'}$ in the integral comes from the energy difference associated with the matrix element $e^{i(E_j - E_k)/\hbar}\langle j|H_1(t)|k\rangle$ (c.f., Eq.(19)). There is only one nonzero matrix element of the operator $(a + a^\dagger)$ between the initial state $|0\rangle$: that is to the excited

state $|1\rangle$, hence the matrix element $\sqrt{1} = \langle 1|a^\dagger|0\rangle$. There are no nonzero matrix elements to any other states in first order!

At an intuitive level, one might expect the dipole perturbation to excite the ground state into many possible higher levels, not just the first excited state. This intuition is correct. Nevertheless, this is impossible to achieve *in first order perturbation theory*. In short, while first order theory is adequate for many purposes (see previous section), it is not useful for others. To be explicit, the transition amplitude from $|0\rangle$ to $|j\rangle$, with $j > 0$, can be nonzero only in jth order perturbation theory (and higher). For this reason we turn to higher orders.

Even though only $c_1^{[1]}(t)$ is nonzero in first order perturbation theory, we might expect at an intuitive level that this amplitude carries much more information than is apparent. We find below in Sec. (4.5) that this intuition is correct. For the simple harmonic oscillator with dipole forcing, this piece of information can be used, together with one other piece of information obtained from second-order perturbation theory (c.f., Eq.(33)), to construct the complete analytic solution to the temporal evolution of the unitary transformation $U_1(t)$.

4.2 Second Order

In order to be able to make explicit and simple calculations, we make two useful assumptions:

a. The time dependence is simply a decaying exponential:

$$f(t) = 0, \quad t < 0 \qquad f(t) = e^{-at}, \quad 0 \le t \qquad (a > 0) \tag{31}$$

b. We search for the asymptotic value of the amplitude: $t \to \infty$.

In second order we have "dressed" matrix elements of $(a + a^\dagger)^2$ to compute, where "dressed" means that the operators in the expansion of this expression are multiplied by specific factors. When this bracket is opened up, we can see that the operator $a^\dagger a^\dagger$ connects $|0\rangle$ to the state $|2\rangle$, the operator $aa^\dagger$ connects $|0\rangle$ to the state $|0\rangle$, and the two operators $a^\dagger a$ and aa have no nonzero matrix elements. The two transition amplitudes, due to these two contributions, are

$$\begin{aligned} c_0^{[2]}(\infty) &= (-ig)^2 \int_0^\infty dt_1 e^{-a-i\omega t_1} \int_0^{t_1} dt_2 e^{-a+i\omega t_2} \langle 0|a|1\rangle\langle 1|a^\dagger|0\rangle \\ c_2^{[2]}(\infty) &= (-ig)^2 \int_0^\infty dt_1 e^{-a+i\omega t_1} \int_0^{t_1} dt_2 e^{-a+i\omega t_2} \langle 2|a^\dagger|1\rangle\langle 1|a^\dagger|0\rangle \end{aligned} \tag{32}$$

The matrix elements of the creation and annihilation operators are square roots of appropriate integers. Further, the double integrals are simple: $\int_0^\infty dx\ e^{-\alpha_1 x} \int_0^x dy e^{-\alpha_2 y} = \frac{1}{\alpha_1}\frac{1}{\alpha_1+\alpha_2}$. This result is shown in Appendix **B**. The result is

$$
\begin{aligned}
c_0^{[2]}(\infty) &= (-ig)^2 \quad \frac{\sqrt{1}}{a+i\omega} \quad \frac{\sqrt{1}}{2a} &&= \frac{(-ig)^2}{2a(a+i\omega)} = D \\
c_2^{[2]}(\infty) &= (-ig)^2 \quad \frac{\sqrt{2}}{a-i\omega} \quad \frac{\sqrt{1}}{2a-2i\omega} &&= \frac{c^{[1]}(\infty)^2}{\sqrt{2}}
\end{aligned}
\tag{33}
$$

From this result, one could almost get the (correct) impression that in nth order,

$$
c_n^{[n]}(\infty) = (-ig)^n \frac{\sqrt{n!}}{n!(a-i\omega)^n} = \frac{(-ig)^n}{\sqrt{n!}(a-i\omega)^n} = \frac{c^{[1]}(\infty)^n}{\sqrt{n!}} \tag{34}
$$

although one would be hard-pressed to guess other contributions to the transition amplitudes.

4.3 Third Order

In third order things get yet more complicated. There are three nonzero matrix elements of the operator $(a+a^\dagger)^3$ that must be computed. One ($a^\dagger a^\dagger a^\dagger$) connects the ground state $|0\rangle$ with state $|3\rangle$ and its contribution to the amplitude is given by Eq.(34). Two ($aa^\dagger a^\dagger$ and $a^\dagger aa^\dagger$) connect $|0\rangle$ with $|1\rangle$. In fact, they connect these two states with different amplitudes which interfere to some extent. The remaining five products of creation and annihilation operators have zero matrix elements starting from the ground state.

The two interfering contributions are

$$
\begin{aligned}
aa^\dagger a^\dagger \quad &\rightarrow \quad (-ig)^3\sqrt{2}\sqrt{2}\sqrt{1}\; I_3(a+i\omega, a-i\omega, a-i\omega) \quad = \quad \frac{(-ig)^3 \times 2}{(a+i\omega)(2a)(3a-i\omega)} \\
a^\dagger aa^\dagger \quad &\rightarrow \quad (-ig)^3\sqrt{1}\sqrt{1}\sqrt{1}\; I_3(a-i\omega, a+i\omega, a-i\omega) \quad = \quad \frac{(-ig)^3 \times 1}{(a-i\omega)(2a)(3a-i\omega)}
\end{aligned}
\tag{35}
$$

The third order iterated integrals $I_3(\alpha_1, \alpha_2, \alpha_3)$ are defined and evaluated in Appendix **B**. These two complex amplitudes must be added to the amplitude $c_1^{[1]}(\infty)$ computed from first-order time-dependent perturbation theory, to obtain a result correct to third order. This result is

$$
c_1^{[1]} + c_1^{[3]} = \frac{(-ig)}{a-i\omega} + \frac{(-ig)^3}{2a(a^2+\omega^2)} = c_1^{[1]} + c_1^{[1]} D \tag{36}
$$

where D has previously been defined in Eq.(33).

4.4 Harmonic Oscillator: Diagrammatic Methods

The amplitude for any transition from $|0\rangle$ to $|j\rangle$ is the sum of amplitudes from all orders in perturbation theory:

Figure 1: Application of diagrammatic rules to two third-order terms in the perturbation series expansion of the harmonic oscillator driven by a decaying exponential dipole interaction.

$$c_j(t) = \sum_{k=0}^{\infty} c_j^{[k]}(t) \xrightarrow{(1)} \sum_{k=j}^{\infty} c_j^{[k]}(t) \xrightarrow{(2)} \sum_{m=0}^{\infty} c_j^{[j+2m]}(t) \tag{37}$$

The first simplification (1) comes about because the interaction hamiltonian $H_1 \simeq (a + a^\dagger)$ can only connect adjacent eigenstates of H_0. The second simplification (2) comes about because each additional nonzero contribution must contain equal numbers of creation and annihilation operators.

The number of contributions to the amplitude $c_j^{[j+2m]}(t)$ increases rapidly; the rate of increase is a combinatorial problem. In order to compute these contributions explicitly a good bookkeeping system is called for. This system is a diagrammatic technique. (It evolves in a more or less direct line to Feynman diagrams.)

For the kth-order contributions:

1. Draw all diagrams leading in k steps from the initial eigenstate to the final eigenstate (e.g., $|0\rangle$ to $|j\rangle$).
2. Associate with each transition
   (a) A matrix element of the appropriate creation or annihilation operator.
   (b) A complex number $\alpha = a \pm i\omega$, with + for a step down and a − for a step up.
3. Associate the integral $I_k(\alpha_1, \alpha_2, \cdots, \alpha_k)$ to the diagram, with $\alpha_k = a - i\omega$ identified with the first transition (e.g., $|0\rangle$ to $|1\rangle$), proceeding from earlier (α_j, j larger) to later (j smaller) times.
4. Multiply together all the square root factors.

This series of rules is essentially the "Feynman Rules" for time-dependent perturbation theory for the simple harmonic oscillator with decaying dipole perturbation.

4.5 Harmonic Oscillator: Exact Solution

One small step in the "time-ordered product" can be written as

$$e^{\delta y^j X_j} e^{y^i X_i} = e^{(y+dy)^i X_i} \tag{38}$$

Here X_i are operators that span the Heisenberg Lie algebra, $e^{\delta y^j X_j}$ represents a small displacement (e.g., $e^{-\frac{i}{\hbar}H_1(t)dt}$), and $e^{y^i X_i}$ is a finite displacement. The infinitesimal displacements dy^i are linearly related to the displacements δy^j

$$dy^i = M(y)^i{}_j \delta y^j \tag{39}$$

The $p \times p$ matrices $M(y)^i{}_j$ (p is the dimension of the Lie algebra) can always be computed by matrix methods, as illustrated in Appendix **C**. For the Heisenberg algebra with $y^i X_i = ca^\dagger + ba + eI$ and $\delta y^i X_i = \delta c a^\dagger + \delta b a + \delta e I$, the relation is

$$\begin{bmatrix} dc \\ db \\ de \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -\frac{1}{2}l & +\frac{1}{2}r & 1 \end{bmatrix} \begin{bmatrix} \delta c \\ \delta b \\ \delta e \end{bmatrix} \tag{40}$$

For our purposes $dc = \delta c = -\frac{i}{\hbar} f^*(t) e^{+i\omega t} dt$ and $db = \delta b = -\frac{i}{\hbar} f(t) e^{-i\omega t} dt$ so that, recalling that $c(-\infty) = b(-\infty)$

$$\begin{array}{rcl} c(t) & = & (-i/\hbar) \int_{-\infty}^{t} f^*(t') e^{+i\omega t'} dt' \\ b(t) & = & (-i/\hbar) \int_{-\infty}^{t} f(t') e^{-i\omega t'} dt' = -c^*(t) \\ e(t) & = & \frac{1}{2}(D - D^*), \qquad D(t) = (-i/\hbar)^2 \int_{-\infty}^{t} dt_1 f^*(t_1) e^{+i\omega t_1} \int_{-\infty}^{t_1} dt_2 f(t_2) e^{-i\omega t_2} \end{array} \tag{41}$$

As a result, we have the closed form expression for the unitary transformation $U_1(t, -\infty)$:

$$U_1(t, -\infty) = e^{c(t)a^\dagger + b(t)a + e(t)I} = e^{c(t)a^\dagger} e^{D(t)I} e^{b(t)a} \tag{42}$$

The middle expression is obtained from Eq.(38). The rightmost expression is obtained from the middle expression using a disentangling theorem that can be constructed using the matrix methods described in Appendix **C**. It is this expression we will find most useful to use.

In this form it is not difficult to compute the transition amplitude from the ground state to the nth excited state:

$$A_{|n\rangle \leftarrow |0\rangle} = \langle n|U_0(t)U_1(t)|0\rangle = \langle n|U_0(t)|n'\rangle \ \langle n'|e^{ca^\dagger}|0\rangle \ \langle 0|e^{D(t)I}|0\rangle \ \langle 0|e^{ba}|0\rangle \tag{43}$$

The matrix $U_0(t)$ is diagonal, with $\langle n|U_0(t)|n'\rangle = e^{-i(n+\frac{1}{2})\omega t}\delta_{n,n'}$. Further, $\langle 0|e^{ba}|0\rangle = 1$ by simple Taylor expansion, $\langle 0|e^{D(t)I}|0\rangle$ is the c-number $e^{D(t)}$, and $\langle n|e^{ca^\dagger}|0\rangle = (c(t))^n / \sqrt{n!}$ by Taylor series expansion again. Putting this all together we find

$$A_{|n\rangle \leftarrow |0\rangle}(t) = e^{-i(n+\frac{1}{2})\omega t + D(t)} \ (c(t))^n / \sqrt{n!} \tag{44}$$

The transition probability from the ground state to $|n\rangle$ is therefore

$$P_{|n\rangle \leftarrow |0\rangle}(t) = e^{D(t)+D^*(t)} \ |c^*(t)c(t)|^n / n! \tag{45}$$

We point out here that our previous intuition that the amplitude $c_1^{[1]}(t)$ for the transition $|0\rangle \rightarrow |1\rangle$ that is computed in first order time-dependent perturbation theory is almost totally sufficient to compute *all* transition amplitudes, was in fact right on target. It is sufficient to compute the probabilities $P_{|n\rangle \leftarrow |0\rangle}(t)$ completely.

4.6 A Comparison

In Sec. 4.4 we developed a diagrammatic method for computing transition amplitudes from the ground state to any excited state, to any order, for a very specific potential. This is the decaying exponential e^{-at}. This diagrammatic method was developed using the first-, second-, and third-order calculations as models. In the previous subsection we have constructed an analytic closed form representation for these amplitudes for any potential at any time.

Being physicists, a siren song calls us to compare these two results.

The comparison is simple. We choose $f(t) = e^{-at} = f^*(t)$ and carry out the integrals in Eq. (41) from 0 to ∞.

$$\begin{aligned} b(\infty) &= \frac{-ig}{a+i\omega} \\ c(\infty) &= \frac{-ig}{a-i\omega} = c_1^{[1]}(\infty) \\ D(\infty) &= \frac{(-ig)^2}{(a+i\omega)(2a)} = c_0^{[2]}(\infty) = D \end{aligned} \tag{46}$$

with the coupling strength $g = eE/\sqrt{2m\hbar\omega}$ as before. The expressions for $c_1^{[1]}(\infty)$ and $c_0^{[2]}(\infty) = D$ have previously been computed and are given in Eqs.(33). We find

Transition	Analytic Sec.4.5	0^{th}Order	1^{st}Order Sec.4.1	2^{nd}Order Sec.4.2	3^{rd}Order Sec.4.3
$\|0\rangle \rightarrow \|0\rangle$	e^D	1		D	
$\|0\rangle \rightarrow \|1\rangle$	$e^D c$		c		Dc
$\|0\rangle \rightarrow \|2\rangle$	$e^D c^2/\sqrt{2!}$			$c^2/\sqrt{2!}$	
$\|0\rangle \rightarrow \|3\rangle$	$e^D c^3/\sqrt{3!}$				$c^3/\sqrt{3!}$

(47)

Using these expressions in Eq.(45), we find for the transition probabilities the simple Poisson expression

$$P_{|n\rangle \leftarrow |0\rangle}(\infty) = \frac{K^n}{n!}\, e^{-K} \qquad K = \frac{(g/\hbar)^2}{a^2+\omega^2} \tag{48}$$

5 Summary and Conclusions

Time-dependent perturbation theory has been formulated in a systematic way. The hamiltonian is expressed in terms of a time-independent part H_0 and a time-dependent part $H_1(t)$. A unitary transformation $U(t)$ is computed in a basis of eigenstates ϕ_j of H_0. In this way it is possible to avoid consideration of the position-dependence of the unitary transformation, and map wavefunctions $\psi(x, t_1)$ on one time slice to wavefucntions $\psi(x, t_2)$ on another time slice without worrying about coordinate-dependence.

The unitary transformation $U(t) = U_0(t) \times U_1(t)$ is expressed in terms of a simple part, $U_0(t) = e^{-\frac{i}{\hbar}H_0 t}$, and a more complicated part that incorporates the time-dependent perturbation. The unitary transformation $U_1(t)$ satisfies the Schrödinger equation under the action of $H_1(t)$ in the interaction representation, $H_{\rm int}(t)$. This integral equation is solved iteratively.

Two profoundly important applications are described in first-order of this perturbative expansion. We construct Fermi's Golden Rule for transition rates from an excited state and derive the Lorentzian line shape for radiative transitions from an excited state, or absorptions from a lower-lying level.

Expansions to higher order are carried out systematically. We illustrate by example how this procedure works by using a perturbation for which closed form calculations are possible. This is the simple harmonic oscillator subject to a dipole driving term. This can be solved analytically for any time dependence using some Lie group theory. The calculations can also be carried out, order by order in closed form, for a particularly simple form of the driving term: a decaying exponential. The perturbation expansion is carried out to third order for this perturbation and the results are compared (by Taylor series) to the exact analytic calculation.

A diagrammatic method is introduced to take care of the bookkeeping involved in an all-orders perturbation series calculation involving this particular perturbation. From this diagrammatic representation it is only a short hop and skip to the Feynman rules for Feynman diagrams in the pertrubation theory called Quantum Electrodynamics.

Appendix A: Representations

The expectation value of an operator $\mathcal{O}$ is

$$\langle\psi(t)|\mathcal{O}|\psi(t)\rangle \tag{49}$$

The time evolution of the wave function can be expressed in several useful ways:

$$
\begin{array}{rcll}
|\psi(t)\rangle & = & U(t)|\psi(t)\rangle & U(t) = \mathcal{T} e^{-\frac{i}{\hbar}\int_0^t [H_0 + H_{\rm int}(t')]dt'} \\
|\psi(t)\rangle & = & U_0(t)U_1(t)|\psi(t)\rangle & U_0(t) = e^{-\frac{i}{\hbar}\int_0^t H_0 dt'} \\
 & & & U_1(t) = U(t)U_0^{-1}(t)
\end{array}
\tag{50}
$$

The time-integrated unitary transformation in the first line of Eq.(50) is time ordered ($\mathcal{T}$). The expectation value given in Eq.(49) can be expressed in three useful ways:

$$
\begin{array}{ll}
\langle\psi(0)|U_1^{-1(t)}U_0^{-1}(t) \underbrace{\mathcal{O}} \underline{U_0(t)U_1(t)|\psi(0)\rangle} & \text{Schrodinger Representation} \\
\langle\psi(0)|U_1^{-1(t)} \underbrace{U_0^{-1}(t)\mathcal{O}U_0(t)} \underline{U_1(t)|\psi(0)\rangle} & \text{Interaction Representation} \\
\langle\psi(0)| \underbrace{U_1^{-1(t)}U_0^{-1}(t)\mathcal{O}U_0(t)U_1(t)} \underline{|\psi(0)\rangle} & \text{Heisenberg Representation}
\end{array}
\tag{51}
$$

In the Schrödinger Representation the operator $\mathcal{O}$ remains time-independent if it is explicitly independent of time. All the time dependence is contained in the wave function, whose evolution is determined by the time-dependent Schrödinger equation. In the Heisenberg Representation it is the wave function that remains independent of time: all the time-dependence is thrown onto the operator $\mathcal{O}$. The Interaction Representation is intermediate between the two extremes: the operator $\mathcal{O}$ is time-dependent, and its time dependence is given by a simple unitary operator. It is the wavefunction that undergoes complicated time dependence. This time-dependence is governed by the unitary transformation $U_1(t)$. The time dependence (Yes) or independence (No) of operators $\mathcal{O}$ and wave functions ψ in these three representations is summarized here:

Representation	$\mathcal{O}$	ψ
Schrödinger	No	Yes
Interaction	Yes	Yes
Heisenberg	Yes	No

Appendix B: Iterated Integrals

B.1: Recursion Method

Time-dependent perturbation theory with a decaying exponential $f(t) = e^{-at}$ $(t \geq 0)$, $f(t) = 0, t < 0$, leads to a series of iterated integrals, the first three of which have the form

$$\begin{aligned}
\int_0^\infty dt_1 e^{-\alpha_1 t_1} &= \frac{1}{\alpha_1} \\
\int_0^\infty dt_1 e^{-\alpha_1 t_1} \int_0^{t_1} dt_2 e^{-\alpha_2 t_2} &= \frac{1}{\alpha_1}\,\frac{1}{\alpha_1+\alpha_2} \\
\int_0^\infty dt_1 e^{-\alpha_1 t_1} \int_0^{t_1} dt_2 e^{-\alpha_2 t_2} \int_0^{t_2} dt_3 e^{-\alpha_3 t_3} &= \frac{1}{\alpha_1}\,\frac{1}{\alpha_1+\alpha_2}\,\frac{1}{\alpha_1+\alpha_2+\alpha_3}
\end{aligned} \tag{52}$$

In these expressions $Re(\alpha_i) > 0$. Express the three integrals above as $I_1(\alpha_1)$, $I_2(\alpha_1, \alpha_2)$, and $I_3(\alpha_1, \alpha_2, \alpha_3)$. Observe that

$$\int_0^\infty dt_1 e^{-\alpha_1 t_1} \int_0^{t_1} dt_2 e^{-\alpha_2 t_2} \int_0^{t_2} dt_3 e^{-\alpha_3 t_3} = \int_0^\infty dt_1 e^{-\alpha_1 t_1} \int_0^{t_1} dt_2 e^{-\alpha_2 t_2} \left\{1 - e^{-\alpha_3 t_2}\right\}/\alpha_3 \tag{53}$$

With a little effort this equation can be re-expressed in the recursive form

$$\alpha_3\ I_3(\alpha_1, \alpha_2, \alpha_3) = I_2(\alpha_1, \alpha_2) - I_2(\alpha_1, \alpha_2 + \alpha_3) \tag{54}$$

This is easily seen to be satisfied using the results of Eq.(53). More generally we find the recursion relation

$$\alpha_{n+1}\ I_{n+1}(\alpha_1, \alpha_2, ..., \alpha_n, \alpha_{n+1}) = I_n(\alpha_1, \alpha_2, .., \alpha_n) - I_n(\alpha_1, \alpha_2, .., \alpha_n + \alpha_{n+1}) \tag{55}$$

It is now a straightforward matter to verify that the expression for $I_n(\alpha_1, \alpha_2, .., \alpha_n)$ expected from Eq.(52) leads to the expected form for $I_{n+1}(\alpha_1, \alpha_2, ..., \alpha_n, \alpha_{n+1})$. This recursion relation is initialized by $I_1(\alpha_1) = \frac{1}{\alpha_1}$.

B.2: Change of Variables

The integrals $I_n(\alpha_1, \alpha_2, \cdots, \alpha_n)$ can be done simply by change of variables. Define $\tau_i = t_i - t_{i+1},\ i = 1, 2 \cdots, n-1$ with $\tau_n = t_n$, so that $t_j = \sum_{i=j}^n \tau_i$ For $n = 3$ we find

$$\int_0^\infty \int_0^{t_1} \int_0^{t_2} e^{-\alpha\cdot\mathbf{t}} dt_1 \wedge dt_2 \wedge dt_3 = \int_0^\infty \int_0^\infty \int_0^\infty e^{-\mathbf{L}\cdot\tau} d\tau_1 \wedge d\tau_2 \wedge d\tau_3 \tag{56}$$

The change of variables is

$$\alpha\cdot\mathbf{t} = \begin{bmatrix} \alpha_1 & \alpha_2 & \alpha_3 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \tau_1 \\ \tau_2 \\ \tau_3 \end{bmatrix} = \mathbf{L}\cdot\tau \tag{57}$$

and $L_j = \sum_{i=1}^{j} \alpha_i$. The integrals over each τ extend from 0 to ∞ and the total integral factors to one independent integral for each τ, because of linearity in the exponent. The result is

$$I_3(\alpha_1, \alpha_2, \alpha_3) = \prod_{j=1}^{3} \int_0^\infty e^{-L_j \tau_j} d\tau_j = \prod_{j=1}^{3} \frac{1}{L_j} = \prod_{j=1}^{3} \frac{1}{\sum_{i=1}^{j} \alpha_i} \tag{58}$$

For the general case replace $3 \rightarrow n$.

Appendix C: Harmonic Oscillator - Another Exact Solution

Every once in a while a Quantum Mechanical time evolution problem comes along that can be solved analytically. The simple harmonic oscillator that we have been discussing is simple enough to fall into this category.

The secret weapon that allows an analytic solution to be constructed is Group Theory. In this theory there are some theorems of enormous power but of limited applicability for physics. Fortunately, their limited range of applicability encompases our current needs.

The requirements for this theory are that the hamiltonian of interest is a linear superposition of operators that close under commutation. Such operators are said to span a Lie Algebra. Under the EXPonential operation these operators map to elements in the associated Lie Group. While elements in the Lie Algebra can be multiplied by scalars, added, and their commutators can be constructed, elements in the Lie Group can only be multiplied together. The group operations are analogous to the unitary transformations that map quantum states at one time to states at a later time.

Here is the path we follow in this Appendix. We express the hamiltonian in terms of elements in the appropriate (Heisenberg) Lie algebra. Then the Schrödinger equation for $H_{\rm int}(t)$ is constructed. The unitary transformation is a very large matrix in the Fock representation, with basis states $|n\rangle$, $n = 0, 1, 2, \cdots$.

At this stage we begin to pull rabbits out of hats. The equation of motion is actually an equation for the evolution of an element in the Heisenberg Lie Group. It doesn't matter how the group operation is computed: specifically, it doesn't matter whether this group operation is computed abstractly or in some matrix representation, so long as the matrix representation is *faithful*, that is, 1:1. We introduce a simple faithful matrix representation for the group and its algebra. It is a 3×3 matrix representation. This matrix representation of the hamiltonian is **not hermitian** and the representation of the time-dependent evolution operator is **not unitary**. Nevertheless, and importantly, it **is faithful**. The group operation is computed in "closed" form for any driving function and any time. When the group operation is determined, it is mapped into the unitary infinite-dimensional representation very simply. Once the unitary representation has

been determined, all transition probability amplitudes can be determined. We reproduce the result obtained in Eq.(42) by this alternate method.

The Heisenberg Algebra/Group has the following simple faithful 3×3 matrix representation.

$$\begin{array}{c} \text{Algebra} \\ \left[\begin{array}{ccc} 0 & b & d \\ 0 & a & c \\ 0 & 0 & 0 \end{array}\right] \end{array} \stackrel{EXP}{\longrightarrow} \begin{array}{c} \text{Group} \\ \left[\begin{array}{ccc} 1 & B & D \\ 0 & A & C \\ 0 & 0 & 1 \end{array}\right] \end{array} \tag{59}$$

The parameters (a, b, c, d) describing elements in the Lie algebra are related to those, (A, B, C, D), describing elements in the Lie group by carrying out the exponential expansion and sum. This can be done in closed form, but we do not need these general, somewhat complicated results. The elements in the Lie algebra are related to the creation and annihilation operators as follows:

$$\hbar\omega(\hat{n}+\frac{1}{2})+ra^\dagger+la+dI \rightarrow \left[\begin{array}{ccc} 0 & l & d \\ 0 & \hbar\omega & r \\ 0 & 0 & 0 \end{array}\right] \tag{60}$$

Caution: An objection is often raised that in this representation the matrix representing the operator $a\dagger$ is not the transpose of the matrix representing the operator a. An even louder objection is raised that the matrix representing the identity operator $I = [a, a^\dagger]$ is not the unit 3×3 matrix I_3. These objections are not to the point. The only property that matters is that the operators, and the matrices representing the operators, have identical (isomorphic) commutation relations. As long as they do, the theorems that allow us to simplify the equation of motion calculations are valid.

The time-dependent hamiltonian in this nonhermitian representation is

$$H = H_0 + H_1(t) = \hbar\omega(\hat{n}+\frac{1}{2})+f^*(t)a^\dagger+f(t)a \rightarrow \left[\begin{array}{ccc} 0 & f(t) & 0 \\ 0 & \hbar\omega & f^*(t) \\ 0 & 0 & 0 \end{array}\right] \tag{61}$$

The 3×3 group operation that represents $U_0(t)$ is

$$EXP(-\frac{i}{\hbar}H_0 t) \rightarrow \left[\begin{array}{ccc} 1 & 0 & 0 \\ 0 & e^{-i\omega t} & 0 \\ 0 & 0 & 1 \end{array}\right] \tag{62}$$

From this it is a simple matter to compute the nonhermitian representation of $H_{\rm int}(t)$

$$H_{\rm int}(t) = U_0^{-1}H_1(t)U_0(t) \rightarrow \left[\begin{array}{ccc} 0 & f(t)e^{-i\omega t} & 0 \\ 0 & 0 & f^*(t)e^{+i\omega t} \\ 0 & 0 & 0 \end{array}\right] \tag{63}$$

and the Schrödinger equation for the 3×3 nonunitary representation of $U_1(t)$:

$$i\hbar\frac{d}{dt}\begin{bmatrix}1 & B & D\\ 0 & A & C\\ 0 & 0 & 1\end{bmatrix} = \begin{bmatrix}0 & f(t)e^{-i\omega t} & 0\\ 0 & 0 & f^*(t)e^{+i\omega t}\\ 0 & 0 & 0\end{bmatrix}\begin{bmatrix}1 & B & D\\ 0 & A & C\\ 0 & 0 & 1\end{bmatrix} \quad (64)$$

Initially the unitary matrix is the identity operator, so our initial conditions are $A = 1$ and $B = C = D = 0$.

From this we derive immediately the equation describing the evolution of the time-dependent group parameter $A(t)$: $dA/dt = 0$, so that $A = 1$ for all times.

The equations of motion for B and C are (recall $B(-\infty) = C(-\infty) = 0$)

$$\begin{aligned} i\hbar\frac{dB}{dt} = f(t)e^{-i\omega t} \quad &\Rightarrow \quad B(t) = \frac{-i}{\hbar}\int_{-\infty}^{t} dt' f(t')e^{-i\omega t'} \\ i\hbar\frac{dC}{dt} = f^*(t)e^{+i\omega t} \quad &\Rightarrow \quad C(t) = \frac{-i}{\hbar}\int_{-\infty}^{t} dt' f^*(t')e^{+i\omega t'} = -B^*(t) \end{aligned} \quad (65)$$

and since $i\hbar\dot{D} = f(t)e^{-i\omega t}C(t)$

$$D(t) = \left(\frac{-i}{\hbar}\right)^2 \int_{-\infty}^{t} dt' f(t')e^{-i\omega t'} \int_{-\infty}^{t'} dt'' f^*(t'')e^{+i\omega t''} \quad (66)$$

Next, we express the functions $B(t), C(t), D(t)$ in terms of coefficients $b(t), c(t), d(t)$ in the Lie algebra through the exponential relation

$$\begin{bmatrix}1 & B & D\\ 0 & 1 & C\\ 0 & 0 & 1\end{bmatrix} = EXP\begin{bmatrix}0 & b & d\\ 0 & 0 & c\\ 0 & 0 & 0\end{bmatrix} = \begin{bmatrix}1 & b & d+\frac{1}{2}bc\\ 0 & 1 & c\\ 0 & 0 & 1\end{bmatrix} \quad (67)$$

From this matrix equation we relate the parameters B, C, D describing the group operation in its 3×3 matrix representation with the coefficients b, c, d of the appropriate operators in the Lie algebra of this group:

$$\begin{aligned} b(t) &= B(t) \\ c(t) &= C(t) \\ d(t) &= D(t) - \frac{1}{2}B(t)C(t) \end{aligned} \quad (68)$$

With these results it is possible to construct the unitary transformation mapping any initial state at $t \to -\infty$ to a state at any time t. In the hermitian representation the operators in the Lie algebra $\hat{n}, a^\dagger, a, [a, a^\dagger] = I$ have their standard Quantum Mechanics interpretation as "$\infty \times \infty$" matrices with matrix elements $\langle r|a^\dagger|s\rangle = \sqrt{r}\ \delta_{r,s+1}$, etc. The unitary representation of this transformation is

$$U(t) = U_0(t)U_1(t) = EXP\left(-i(\hat{n} + \frac{1}{2})\omega\right) EXP\left(b(t)a + c(t)a^\dagger + d(t)I\right) \quad (69)$$

In many cases only the lowest lying states are initially populated, so it is convenient rewrite the second exponential in normally ordered form. This disentangling result is easily constructed in the 3×3 matrix representation, and is

$$EXP\left(b(t)a + c(t)a^\dagger + d(t)I\right) = EXP\left(c(t)a^\dagger\right) EXP\left(D(t)I\right) EXP\left(b(t)a\right) \quad (70)$$

This is exactly the expression achieved in Eq.(43) by different means.