Finite-time deviations from exponential decay in the case of spontaneous emission from a two-level hydrogenic atom

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For the first time to the authors' knowledge a mathematically rigorous method is used for treating finite-time deviations from the exponential decay in the case of spontaneous Lyman-α transitions in a two-level hydrogenic atom. First, in the so-called Weisskopf-Wigner model (where the rotating-wave approximation is implied) finite-time deviations with a rigorous validity range, based on accurate error estimations, are derived. Second, in order to obtain the frequency shift (Lamb shift), counter-rotating terms are taken into account by using a projection-operator method developed a decade ago by one of the present authors [J. Seke, Phys. Rev. A **21**, 2156 (1980)]. By means of this method, equations of motion for dipole-moment expectation values are derived without employing the usual Born approximation. These equations are solved by using the method of the Laplace transform and its inverse. Again finite-time deviations from the exponential decay of the dipole-moment expectation values with a definite validity range are obtained. Finally, it should be emphasized that all the results presented in this paper contain accurate error estimates which are absolutely necessary in a rigorous mathematical method.

I. INTRODUCTION

Long-time (asymptotic) deviations from exponential decay in the case of spontaneous emission from a single two-level atom have been shown by many authors (see, e.g., Refs. 1–3). All these authors have used the so-called dipole approximation, which was subject to criticism in our previous work[4] (hereafter to be referred to as I). Namely, in I we have shown that neglecting retardation effects in the atom-field interaction (dipole approximation) leads to an asymptotic result that differs significantly from that obtained without this approximation. For this reason, in the present paper no kind of dipole approximation will be made. This can be achieved by limiting ourselves to the case of the Lyman-α transition in a two-level hydrogenic atom.

In the present paper a twofold generalization of the results in I will be achieved. First, for the first time a rigorous mathematical method will be used for the estimation of the finite-time deviations from exponential decay in the Weisskopf-Wigner model of spontaneous emission[5] in which the rotating-wave approximation (RWA) is implied. In this connection the work of Robiscoe[6] should be acknowledged. By using a method which differs from ours, he derived finite-time deviations from exponential decay for the above model in the RWA. Unfortunately, he has given no error estimations for his approximations. This is, however, absolutely necessary for the determination of the validity range of the calculated deviations. On the contrary, the validity of all our present results is based on a very accurate estimation of the errors arising from the used approximations.

Second, since the RWA (applied in the Weisskopf-Wigner method) leads to an incorrect frequency shift (Lamb shift) in the oscillation frequency of the expectation values (EV's) of the dipole-moment operators, the inclusion of the counter-rotating (antiresonant) terms in the calculations is absolutely necessary. It should be mentioned that by including counter-rotating terms a correct frequency shift can be obtained only in the scope of the two-level model. In addition to this, the calculation of the correct frequency shift, of course, requires the inclusion of all the levels of the atom,[7–9] as well as taking into account the relativistic effects. In the present paper only the two-level model will be treated and thus the inclusion of the counter-rotating terms can be achieved by a special projection-operator technique,[10] which was developed a decade ago by one of the present authors (J.S.) by modifying the Robertson projection-operator method.[11] By using this special projection technique we are able to derive closed equations of motion (EM's) for the dipole-moment EV's *without making use of any kind of perturbation approximation as to the strength of the interaction* between the atom and the radiation field. This is an important fact, which makes possible a consistent comparison of the present results with those of the Weisskopf-Wigner method (where no kind of perturbative approximation was used). Unfortunately, this important fact was until now overlooked by all authors (see, e.g., Refs. 3 and 12–14), who, going beyond the RWA, have used new methods like projection-operator techniques[13,14] or Heisenberg equations of motion.[3,12] Namely, the authors applying these methods were forced to make a second-order perturbation approximation, the so-called Born approximation (BA), in order to obtain closed EM's for EV's. However, the application of the BA means that the approximation regarding the resonant terms in the interaction Hamiltonian is poorer than that of the Weisskopf-Wigner method.

In other words, only the elimination of the BA from the projection-operator technique makes it possible to obtain results that are superior to those of the Weisskopf-Wigner method. By using our special projection-operator method, where no kind of usual BA appears, we obtain closed integro-differential equations for the dipole-moment EV's as the only unknowns. In obtaining these equations we make a kind of RWA in the exact closed EM's. However, this RWA is very different from the RWA on the Hamiltonian itself, since it takes into account counter-rotating terms as far as to give the Lamb shift, which is correct only in the scope of the two-level model as mentioned above.

The equations for the dipole-moment EV's will be solved by using the Laplace transform and its inverse. Since logarithmic functions of complex variables appear, analytic continuation in the infinitely sheeted Riemann surface is necessary. Further, a mathematically rigorous, but very involved, localization and evaluation of the poles and their residue contributions provided with the respective error estimates will be given. Finally, for the first time, *finite-time deviations from the exponential decay* will be calculated *with a definite validity range* based on careful error estimations.

For calculations in the present paper, we use the Hamiltonian for a single two-level hydrogenic atom (system A) interacting with the radiation field (system R):

$$H=H_0+H_{AR}\ , \tag{1.1}$$

where

$$H_0=\omega_0 S^z\otimes I_R+\int_0^\infty d\omega\,\omega a^+(\omega)a^-(\omega)\otimes I_A \quad (\hbar=1) \tag{1.2}$$

is the unperturbed Hamiltonian (I_A and I_R are the unit operators in the Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_R$ of systems A and R) and

$$\begin{aligned} H_{AR}&=-\frac{e}{mc}\mathbf{A}\cdot\mathbf{P}\\ &=\int_0^\infty d\omega[g(\omega)a^-(\omega)-g^*(\omega)a^+(\omega)]\otimes(S^+-S^-) \end{aligned} \tag{1.3}$$

is the interaction Hamiltonian which neither implies the RWA nor ignores retardation effects (dipole approximation). Here S^z and $S^\pm$ are atomic population-inversion and dipole-moment operators, respectively, defined by

$$\begin{aligned} &S^z=\tfrac{1}{2}(|1\rangle\langle 1|-|2\rangle\langle 2|),\quad S^+=|1\rangle\langle 2|,\quad S^-=|2\rangle\langle 1|\ ,\\ &[S^+,S^-]=2S^z,\quad [S^z,S^\pm]=\pm S^\pm\ , \end{aligned} \tag{1.4}$$

with

$$\begin{aligned} |1\rangle&=|n_1=2,\ j_1=1,\ m_1=0\rangle\ ,\\ |2\rangle&=|n_2=1,\ j_2=0,\ m_2=0\rangle \end{aligned} \tag{1.5}$$

as the excited state and ground state of an hydrogenic atom in the case of the Lyman-α transition ($2P\rightarrow 1S$). Here we chose $m_1=0$, but our further calculation as well as the final results are independent of the choice of m_1 (i.e., the treatment of the other two cases with $m_1=\pm 1$ is quite identical). The symbols $a^\pm(\omega)$ denote the creation and annihilation operators for a photon with frequency ω, and quantum numbers $j=1$, $m=m_1-m_2=0$ (which follows from the selection rules), and $\tau=0$ (electric multipole field). The coupling constant $g(\omega)$ includes all the retardation effects and is given by[15]

$$g(\omega)=\left[\frac{\lambda}{2\pi}\right]^{1/2}\frac{(-i)\omega^{1/2}}{[1+(\omega/\Omega)^2]^2},\quad \lambda=\frac{\gamma}{\omega_0},\quad \Omega=\frac{3c}{2a_0} \tag{1.6}$$

where $\gamma\approx 10^8\ \mathrm{s}^{-1}$ is the Einstein coefficient for spontaneous Lyman-α radiation, $\omega_0\approx 10^{16}\ \mathrm{s}^{-1}$ is the energy separation of the two atomic levels, and $a_0\approx 10^{-9}$ cm is the Bohr radius.

For one-photon states the following normalization relations hold:

$$\begin{aligned} &\langle V|V\rangle=1,\quad \langle\omega,j,m,\tau=0|V\rangle=0\ ,\\ &\langle\omega,j,m,\tau=0|\omega',j',m',\tau'=0\rangle=\delta(\omega-\omega')\delta_{jj'}\delta_{mm'}\ ,\\ &a^+(\omega)|V\rangle=|\omega,j=1,\ m=0,\ \tau=0\rangle\ , \end{aligned} \tag{1.7}$$

($|V\rangle$ is the vacuum state).

The paper is organized as follows. In Sec. II we derive finite-time deviations from the exponential decay in the RWA. In Sec. III by using a special projection-operator method we derive closed EM's for the dipole-moment EV's by taking into account the influence of the counter-rotating terms. In Sec. IV these EM's will be treated analytically by using the Laplace transform and its inverse. In Sec. V the path of the integration on the Riemann surface will be adequately deformed in order to obtain the contribution of the Weisskopf-Wigner pole yielding the exponential decay and an integral describing the deviation from the exponential decay. In Sec. VI this deviation will be estimated for finite and asymptotic times. In Sec. VII we draw a conclusion. In Appendix A we evaluate some integrals used in preceding sections. In Appendix B we describe the fixed-point method and use it for approximate evaluation of the poles. In Appendix C the argument principle is used for the determination of the number of poles and zeros. Their localization is also performed. In Appendix D approximations for the integrands of Secs. II and VI are given.

II. FINITE-TIME DEVIATIONS FROM EXPONENTIAL DECAY IN THE RWA

In I, by applying the RWA to the interaction Hamiltonian in Eq. (1.3), we have already derived an asymptotic result for the probability amplitude $b_1(t)$ for finding a two-level hydrogenic atom in the excited state and no photons in the radiation field [cf. Eqs. (4.11) and (4.12) in I].

In order to have an estimate for $b_1(t)$ for finite times, we must give a more detailed derivation of the results in I. The starting point is our initial-value problem [cf. Eq. (4.3) in I]

$$\dot{b}_1(t)=-\frac{\lambda}{2\pi}\int_0^\infty d\omega\, f(\omega)\int_0^t d\tau\, e^{i(\omega_0-\omega)\tau}b_1(t-\tau)\ . \tag{2.1}$$

Here $b_1(0)$ is given an initial value of $b_1(t)$ and $f(\omega)$ is the natural smooth cutoff function

$$f(\omega)=\frac{\omega\Omega^8}{(\Omega^2+\omega^2)^4}\ . \tag{2.2}$$

In order to solve Eq. (2.1) we apply the Laplace transformation[16]

$$\hat{b}_1(z)=\int_0^\infty b_1(t)e^{-tz}dt\ ,$$

so that we get a new (algebraic) equation for the function $\hat{b}_1(z)$,

$$\hat{b}_1(z)=b_1(0)\Big/\left[z+\frac{\lambda}{2\pi}\int_0^\infty\frac{d\omega\, f(\omega)}{z-i(\omega_0-\omega)}\right]\ . \tag{2.3}$$

Still following the lines in I, we substitute $u=iz+\omega_0$ and introduce a new function

$$\hat{B}_1(u)=-i\hat{b}_1(-iu+i\omega_0)=\frac{b_1(0)}{u-\omega_0+(\lambda/2\pi)I(u)}\ , \tag{2.4}$$

with

$$\begin{aligned}I(u)&=\int_0^\infty\frac{d\omega\, f(\omega)}{\omega-u}\\&=-\frac{C_1(u)}{\Omega^6}+\frac{C_2(u)\pi}{2\Omega}\\&\quad+f(u)[-\log(u)+\ln\Omega+i\pi]\ ,\end{aligned} \tag{2.5}$$

$$C_1(u)=\frac{f(u)}{12}(11\Omega^6+18\Omega^4u^2+9\Omega^2u^4+2u^6)\ , \tag{2.6}$$

$$C_2(u)=\frac{f(u)}{16\Omega^4u}(5\Omega^6-15\Omega^4u^2-5\Omega^2u^4-u^6)\ . \tag{2.7}$$

Here, we use the convention $\log(u)$ for the multivalued natural logarithm of a complex variable [for the evaluation of $I(u)$ see Appendix A].

Next we note that the Laplace inversion (and substitution $z=-iu+i\omega_0$) yields

$$b_1(t)=\frac{e^{i\omega_0 t}}{2\pi i}\int_C e^{-itu}\hat{B}_1(u)du\ , \tag{2.8}$$

where C is according to Fig. 1. Note that the integrand of Eq. (2.8) is analytic for $\mathrm{Im}(u)>0$ and "lives" on the Riemann surface of $\log(u)$. According to Fig. 1, we deform the path of integration C to the path K. This choice is rather special, and was also used by Davidovich and Nussenzveig.[9] It has the following advantage. In I (where the path C was used) singularities appear around $u=-i\Omega$, whose influence on the error terms is hard to estimate. However, by the special choice for K, we may completely avoid dealing with these singularities, since none of them is passed in the process of deforming C into K. That is to say, the integrand in Eq. (2.8) behaves much better along K, because we are "far away" from the singularities around $u=-i\Omega$, so that less technical work with estimates has to be done.

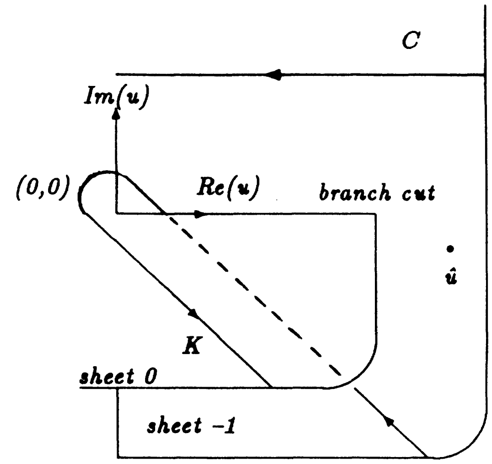

FIG. 1. Path of integration C in Eq. (2.8) and the deformed path K on the Riemann sheets 0 and -1 used in Eq. (2.15). The Weisskopf-Wigner pole $\hat{u}$ on sheet -1 is crossed in the process of deformation.

In Appendix B we apply the fixed-point method for finding approximate values of the poles and give a rigorous error estimation. Here we summarize the results. The approximate value u_1 of the Weisskopf-Wigner pole $\hat{u}$ (which lies on the lower Riemann sheet: number -1) and the corresponding error $\Delta_u=|\hat{u}-u_1|$ read as

$$u_1=\omega_0+\frac{11\lambda\omega_0}{24\pi}-\frac{5\lambda\Omega}{64}-\frac{\lambda\omega_0}{2\pi}\ln\left[\frac{\Omega}{\omega_0}\right]-i\frac{\omega_0\lambda}{2}\ , \tag{2.9}$$

$$\left|\frac{\Delta_u}{\hat{u}}\right|<4.1\times10^{-13}\ . \tag{2.10}$$

From this and the theory of residue calculus it follows that

$$\mathrm{Res}(e^{i\omega_0 t}e^{-iut}\hat{B}_1(u),\hat{u})\approx R_1(t)\ , \tag{2.11}$$

where R_1 is the approximate value of the residue (cf. Appendix B):

$$R_1(t)=b_1(0)\exp\left\{-\frac{\lambda\omega_0 t}{2}-i\left[-\frac{5}{64}\lambda\Omega+\frac{11}{24\pi}\lambda\omega_0+\frac{\lambda\omega_0}{2\pi}\ln\left[\frac{\Omega}{\omega_0}\right]\right]t\right\}\ , \tag{2.12}$$

$$||\mathrm{Res}(e^{i\omega_0 t}e^{-iut}\hat{B}_1(u),\hat{u})|-|R_1(t)||<10\lambda\exp(-\lambda\omega_0 t/2)|b_1(0)|\ . \tag{2.13}$$

Further, it holds that

$$b_1(t)=\mathrm{Res}(e^{i\omega_0 t}e^{-iut}\hat{B}_1(u),\hat{u})+D_1(t)\ , \tag{2.14}$$

where

$$D_1(t)=\frac{e^{i\omega_0 t}}{2\pi i}\int_K \hat{B}_1(u)e^{-iut}du \tag{2.15}$$

describes the deviation from the exponential decay. So altogether Eqs. (2.14) and (2.15) give us the solution of our basic equation, Eq. (2.1). Since the integral of Eq. (2.15) cannot be exactly evaluated, we next deal with approximations of $D_1(t)$. It should be noted that Robiscoe[6] has given similar approximations for finite-time deviations from the exponential decay by using a different method without error estimations. In contrast to this, we would like to stress that all our approximations are augmented by rigorous estimates of the respective errors. Here, we outline our method by giving a few steps (for more details see Appendix D).

(1) We write down the integral in Eq. (2.15) by using a concrete parametrization of the path K. This gives us

$$D_1(t)=\frac{1}{2\pi}b_1(0)e^{i\omega_0 t}(1-i)\int_0^\infty \frac{\lambda f(u)e^{-iut}\Omega\, dx}{N_0(u)N_{-1}(u)}\ . \tag{2.16}$$

Here $u=(1-i)\Omega x$ and $f(u)$ is as in Eq. (2.2). Furthermore, for the denominator we have chosen the following notation:

$$N_0(u)=u-\omega_0+\frac{\lambda}{2\pi}I_0(u),\quad N_{-1}(u)=N_0(u)+i\lambda f(u)\ , \tag{2.17}$$

where the subscripts 0 and -1 denote different branches of the functions $N(u)$ and $I(u)$ [cf. Eqs. (2.4) and (2.5)] on the Riemann surface of $\log(u)$.

(2) We restrict ourselves to times $t\geq 10^{-14}$ s.

(3) In order to estimate the integral representation of $D_1(t)$ in Eq. (2.16), we choose a suitable real number $\delta=1.69\times10^{-4}$ and divide the interval of integration: $[0,\infty)=[0,\delta]\cup[\delta,\infty)$. This turns out to be practical for the next steps.

(4) According to Appendix D we may "neglect" the contribution of the integrand in the interval $[\delta,\infty)$. More precisely, we show that

$$\Delta_1(t)=\frac{\sqrt{2}}{2\pi}|b_1(0)|\left|\int_\delta^\infty\cdots\right| \leq\frac{\lambda}{2\pi}|b_1(0)|\frac{\sqrt{2}}{(1-10^{-4})\delta_0^2}\frac{e^{-\delta\Omega t}}{\Omega t}$$

$$\text{with } \delta_0=\omega_0/\Omega\ . \tag{2.18}$$

(5) Now we look at the "remaining" part of our integral and, since δ is reasonably small, we may approximate the integrand in the small interval $[0,\delta]$ by making use of Eqs. (D7)–(D10) in Appendix D,

$$\Delta_f(x)=\left|\frac{\lambda f(u)}{N_0(u)N_{-1}(u)}-\frac{\lambda u}{\omega_0^2}\right| <\frac{\sqrt{2}\lambda^2\Omega^2}{\omega_0^3}x+\frac{5.6\lambda\Omega^2}{\omega_0^3}x^2\ , \tag{2.19}$$

where $u=(1-i)\Omega x$. By integrating this inequality we may estimate the error which arises if the complicated integrand of Eq. (2.16) is replaced by the simple function $\lambda u/\omega_0^2$,

$$\Delta_2(t)=\frac{\sqrt{2}}{2\pi}|b_1(0)|\left|\int_0^\delta \Delta_f(x)e^{-\Omega x t}\Omega\, dx\right| <\frac{\lambda^2}{\pi\delta_0\omega_0^2t^2}|b_1(0)|+15.84\frac{\lambda}{2\pi}\frac{1}{\omega_0^3t^3}|b_1(0)|\ . \tag{2.20}$$

(6) We finally integrate the simple function $\lambda u/\omega_0^2$ over the interval $[0,\delta]$ in order to approximate $D_1(t)$ in Eq. (2.16),

$$\frac{1}{2\pi}b_1(0)e^{i\omega_0 t}(1-i)\int_0^\delta\frac{\lambda u}{\omega_0^2}e^{-iut}\Omega\, dx=M(t)+\Delta_3(t)\ , \tag{2.21}$$

with the asymptotic main term

$$M(t)=-\frac{\lambda}{2\pi\omega_0^2t^2}b_1(0)e^{i\omega_0 t} \tag{2.22}$$

and the correction

$$\Delta_3(t)=[1+(1+i)\Omega\delta t]e^{-(1+i)\Omega\delta t}M(t)\ . \tag{2.23}$$

(7) The last step consists of collecting the various error estimates for different parts of $D_1(t)$ and comparing their magnitudes with that of the main term

$$\sum_{i=1}^{3}\left|\frac{\Delta_i(t)}{M(t)}\right|<16.6\times10^{-2},\quad t\geq10^{-14}\ \mathrm{s}\ . \tag{2.24}$$

In this way the major result of this section is derived and we summarize as follows.

Theorem 2.1. Let $b_1(t)$ denote the solution of the initial-value problem, Eq. (2.1), then the following holds: (i) According to Eq. (2.14) $b_1(t)$ can be written as a sum of the "classical" Weisskopf-Wigner pole contribution and a certain "correction" $D_1(t)$. (ii) The approximation for the Weisskopf-Wigner term reads as

$$\mathrm{Res}(e^{it(\omega_0-u)}\hat{B}_1(u),\hat{u})=(1+\Delta_{\mathrm{res}})b_1(0)\exp\left\{-\frac{\lambda\omega_0}{2}t-i\left[-\frac{5\lambda\Omega}{64}+\frac{11\lambda\omega_0}{24\pi}-\frac{\lambda\omega_0}{2\pi}\ln\left[\frac{\Omega}{\omega_0}\right]\right]t-\Delta_u t\right\}\ , \tag{2.25}$$

where the error terms Δ_{res} and Δ_u obey the following estimates:

$$\Delta_{\mathrm{res}}<10\lambda\approx10^{-7},\quad |\Delta_u/\hat{u}|<4.1\times10^{-13}\ . \tag{2.26}$$

(iii) For the deviation from the exponential decay $D_1(t)$ a reasonable approximation can be found for times $t\geq t_0=10^{-14}$ s:

$$D_1(t)=M(t)+\Delta(t)=-\frac{\lambda}{2\pi\omega_0^2}\frac{1}{t^2}b_1(0)e^{i\omega_0 t}+\Delta(t)\ , \tag{2.27}$$

with $M(t)$ as the asymptotic main term and $|\Delta(t)/M(t)|<16.6\times10^{-2}$.

III. DERIVATION OF EQUATIONS OF MOTION FOR DIPOLE-MOMENT EXPECTATION VALUES WITHOUT RWA

In Sec. II we have calculated the probability amplitude $b_1(t)$ for finding the atom in the excited state. Since the ground state $|2\rangle\otimes|V\rangle$ is a stationary state in the RWA, an incorrect frequency shift for the oscillation frequency of the dipole-moment EV $\langle S^-\rangle_t^{\rm RWA}=b_2^*(0)b_1(t)e^{-i\omega_0 t}$ follows. Namely, according to Eq. (2.25) the frequency shift contains the term $-5\lambda\Omega/64$. However, this term gives no contribution if the counter-rotating terms are taken into account. Moreover, the remaining term $-(\lambda\omega_0/2\pi)\ln(\Omega/\omega_0)$ is just half of the familiar Lamb shift, since it includes only the energy shift of the excited state, while that of the ground state is missing.

Therefore, the RWA does not give correct results for the EV's $\langle S^\pm\rangle_t$ of the dipole-moment operators. For this reason, in this section we derive EM's for $\langle S^\pm\rangle_t$ without using the RWA in the interaction Hamiltonian. The projection-operator technique developed years ago by one of the present authors seems to be a suitable method for this task.[10]

We now generalize the initial condition for the pure states of Sec. II,

$$|\psi(0)\rangle=[b_1(0)|1\rangle+b_2(0)|2\rangle]\otimes|V\rangle\ ,\quad [|b_1(0)|^2+|b_2(0)|^2=1]\ , \tag{3.1}$$

to quite general initial conditions for statistical density operators:

$$\rho(0)=\rho_A(0)\otimes\rho_R(0)\ , \tag{3.2}$$

$$\rho_A(0)=\tfrac{1}{2}I_A+2S^z\langle S^z\rangle_0+S^+\langle S^-\rangle_0+S^-\langle S^+\rangle_0\ , \tag{3.3}$$

$$\rho_R(0)=|V\rangle\langle V|\ , \tag{3.4}$$

where $\rho(t)$ is the statistical density operator (which satisfies the Liouville equation) and $\rho_A(t),\rho_R(t)$ are the reduced density operators defined by

$$\rho_A(t)={\rm Tr}_R\rho(t),\quad \rho_R(t)={\rm Tr}_A\rho(t)\ . \tag{3.5}$$

For the derivation of the EM's for the EV's $\langle S^\pm\rangle_t$, we use a generalized canonical density operator[10]

$$\sigma_A(t)=\tfrac{1}{2}I_A+S^+\langle S^-\rangle_t+S^-\langle S^+\rangle_t\ , \tag{3.6}$$

where

$$\sigma_A(t)\otimes\rho_R(0)=P\rho(t)+\tfrac{1}{2}I_A\otimes\rho_R(0)\ , \tag{3.7}$$

with the projection operator

$$P(\cdots)=\rho_R(0)\otimes\{S^+{\rm Tr}_{AR}[S^-(\cdots)]+S^-{\rm Tr}_{AR}[S^+(\cdots)]\}\ . \tag{3.8}$$

By using the modified Robertson projection-operator technique,[11] i.e., by differentiating and transforming Eq. (3.7), and afterwards integrating it by applying an integrating operator $T(t,t')$, we obtain a connecting equation between $\rho(t)$ and $\sigma_A(t)\otimes\rho_R(0)$:

$$\rho(t)-\sigma_A(t)\otimes\rho_R(0)=-i\int_0^t dt'T(t,t')(I-P)\times(L_0+L_{AR})\sigma_A(t')\otimes\rho_R(0) \tag{3.9}$$

with

$$T(t,t')=e^{-i(t-t')(I-P)(L_0+L_{AR})} \tag{3.10}$$

and $I=I_A\otimes I_R$, $L_0=[H_0,\ldots]$, and $L_{AR}=[H_{AR},\ldots]$ [cf. Eqs. (1.1)–(1.3)].

We now let the operator $iS^\pm(L_0+L_{AR})$ act upon Eq. (3.9) and afterwards take the trace over it which gives us *exact closed* EM's for the EV's $\langle S^\pm\rangle_t$:

$$\frac{d\langle S^\pm\rangle_t}{dt}=\pm i\omega\langle S^\pm\rangle_t+I^\pm(t)-\int_0^t d\tau[K_1^\pm+K_2^\pm(\tau)\langle S^\pm\rangle_{t-\tau}+K_3^\pm(\tau)\langle S^\mp\rangle_{t-\tau}]\ , \tag{3.11}$$

where

$$I^\pm(t)=i\,{\rm Tr}_{AR}\{(L_{AR}S^\pm)U(t,0)e^{-itL_0}\times[\rho_A(0)-\sigma_A(0)]\otimes\rho_R(0)\}\ , \tag{3.12}$$

$$K_1^\pm(\tau)={\rm Tr}_{AR}[S^\pm L_{AR}U(\tau,0)e^{-itL_0}L_{AR}\tfrac{1}{2}I\otimes\rho_R(0)]\ , \tag{3.13}$$

$$K_2^\pm(\tau)={\rm Tr}_{AR}[S^\pm L_{AR}U(\tau,0)e^{-itL_0}L_{AR}S^\mp\otimes\rho_R(0)]\ , \tag{3.14}$$

$$K_3^\pm(\tau)={\rm Tr}_{AR}[S^\pm L_{AR}U(\tau,0)e^{-itL_0}L_{AR}S^\pm\otimes\rho_R(0)]\ , \tag{3.15}$$

$$U(\tau,0)=\mathcal{T}\exp\left[-i\int_0^\tau dt'(I-P)e^{-it'L_0}L_{AR}e^{it'L_0}\right]\ , \tag{3.16}$$

($\mathcal{T}$ is the Dyson time-ordering operator). Now we can make some simplifications in Eq. (3.11). Since

$$\rho_A(0)-\sigma_A(0)=2S^z\langle S^z\rangle_0\ , \tag{3.17}$$

and

$${\rm Tr}_R[L_{AR}^{2l+1}\rho_R(0)\otimes S^z]=0,\quad l=0,1,2,\ldots \tag{3.18}$$

$${\rm Tr}_A[S^\pm L_{AR}^{2l}S^z\otimes\rho_R(0)]=0,\quad l=0,1,2,\ldots \tag{3.19}$$

it follows that

$$I^\pm(t)=0\ . \tag{3.20}$$

Further,

$$K_1^\pm(\tau)=0 \tag{3.21}$$

because

$$\mathrm{Tr}_R[L_{AR}^{2l+1}\rho_R(0)\otimes I_A]=0, \quad l=0,1,2,\ldots \tag{3.22}$$

$$\mathrm{Tr}_A[S^{\pm}L_{AR}^{2l}I_A\otimes\rho_R(0)]=0, \quad l=0,1,2,\ldots . \tag{3.23}$$

Moreover, since

$$L_{AR}S^{+}=L_{AR}S^{-}=2S^{z}\otimes\int_0^\infty d\omega[g(\omega)a^{-}(\omega)-g^{*}(\omega)a^{+}(\omega)] , \tag{3.24}$$

it holds that

$$K_3^{\pm}(\tau)=K_2^{\mp}(\tau) . \tag{3.25}$$

Equations (3.20), (3.21), and (3.25) simplify the exact EM's, Eq. (3.11), significantly, and only the coefficients $K_2^{\mp}(\tau)$ remain:

$$K_2^{\mp}(\tau)=-\mathrm{Tr}_{AR}[A^{\pm}U(\tau,0)e^{i\tau L_0}B^{\mp}] , \tag{3.26}$$

where

$$A^{\pm}\equiv L_{AR}S^{\pm}=A , \tag{3.27}$$

$$B^{\pm}\equiv L_{AR}S^{\pm}\otimes\rho_R(0)=\pm\tfrac{1}{2}I_A\otimes\int_0^\infty d\omega[g^{*}(\omega)a^{+}(\omega)\rho_R(0)+g(\omega)\rho_R(0)a^{-}(\omega)]-S^{z}\otimes\int_0^\infty d\omega[g^{*}(\omega)a^{+}(\omega)\rho_R(0)-g(\omega)\rho_R(0)a^{-}(\omega)] . \tag{3.28}$$

A very important fact, which has not been shown in the literature as yet, is that the time-evolution operator $U(\tau,0)$ [cf. Eq. (3.16)] acts as a *unit operator* in the expression for $K_2^{\pm}(\tau)$ if the RWA is applied to L_{AR} appearing in $U(\tau,0)$. This holds only because the interaction Liouvillian L_{AR}^{RWA}, contained to all orders in $U^{\mathrm{RWA}}(\tau,0)$, does not give any contribution:

$$\mathrm{Tr}_{AR}\{A[(I-P)L_{AR}^{\mathrm{RWA}}]^{l}B^{\mp}\}=0, \quad l=0,1,2,\ldots \tag{3.29}$$

and, therefore,

$$\begin{aligned}K_{2(\mathrm{RWA})}^{\pm}(\tau)&=-\mathrm{Tr}_{AR}[AU^{\mathrm{RWA}}(\tau,0)e^{-i\tau L_0}B^{\mp}]\\&=-\mathrm{Tr}_{AR}(Ae^{-i\tau L_0}B^{\mp})\\&=\int_0^\infty d\omega|g(\omega)|^2(e^{i\tau\omega}+e^{-i\tau\omega}) .\end{aligned} \tag{3.30}$$

This means that both the RWA applied to $U(\tau,0)$ in the expression for $K_2^{\pm}(\tau)$ as well as the BA applied to $K_2^{\pm}(\tau)$ lead to the same result. But one *significant qualitative difference* still remains, namely, the RWA takes into account all orders of the interaction Hamiltonian H_{AR}^{RWA}, whereas the BA neglects any kind of interaction which is of higher than second order. A consistent comparison of the present results with those of Sec. II (obtained by the Weisskopf-Wigner method) is now possible, since in both cases we use only one approximation: the RWA. In other words, if the present results had been obtained in the BA (as is generally accepted in the literature), no consistent comparison with the results of Sec. II, where no such approximation is made, would be possible. Unfortunately, until now no one has become aware of this inconsistency. Thus, for the first time, we were able to show that taking into account the counter-rotating terms does not make the application of the BA necessary.

Finally, by using Eqs. (3.20), (3.21), (3.25), and (3.30), Eq. (3.11) takes the following form:

$$\frac{d\langle S^{\pm}\rangle_t}{dt}=\pm i\omega_0\langle S^{\pm}\rangle_t-\int_0^t d\tau(\langle S^{\pm}\rangle_{t-\tau}+\langle S^{\mp}\rangle_{t-\tau})\times\int_0^\infty d\omega|g(\omega)|^2(e^{i\tau\omega}+e^{-i\tau\omega}) . \tag{3.31}$$

In the sequel we will use the following notation:

$$S(t)=\langle S^{-}\rangle_t, \quad S^{*}(t)=\langle S^{+}\rangle_t . \tag{3.32}$$

IV. ANALYTIC TREATMENT OF EQ. (3.31)

By applying the Laplace transformation to Eq. (3.31) and using the notation (3.32), we obtain two coupled algebraic equations for the Laplace transforms $\tilde{S}(z)=\int_0^\infty S(t)e^{-tz}dt$ and $(S^{*})\tilde{}(z)$:

$$\tilde{S}(z)=\frac{S(0)-(S^{*})\tilde{}(z)\Sigma(z)}{z+i\omega_0+\Sigma(z)} , \tag{4.1}$$

$$(S^{*})\tilde{}(z)=\frac{S^{*}(0)-\tilde{S}(z)\Sigma(z)}{z-i\omega_0+\Sigma(z)} , \tag{4.2}$$

where $\Sigma(z)$ may be expressed by $I(u)$, defined in Eq. (2.5),

$$\Sigma(z)=i\frac{\lambda}{2\pi}[I(-iz)-I(iz)] . \tag{4.3}$$

The solution for $\tilde{S}(z)$ reads as

$$\tilde{S}(z)=\frac{[z-i\omega_0+\Sigma(z)]S(0)-\Sigma(z)S^{*}(0)}{z^2+2z\Sigma(z)+\omega_0^2} . \tag{4.4}$$

Next we observe that making use of the Laplace inverse[16] we may represent the solution of Eq. (3.31) by means of a path integral

$$S(t)=\int_C\tilde{S}(z)e^{zt}dz , \tag{4.5}$$

where C denotes usually a vertical straight line in the z plane, so that no singularities of $\tilde{S}(z)$ appear on C or in the semiplane on the right-hand side of C. Basically, Eq. (4.5) gives the complete solution, and this equation will be used for derivation of all further results. Since in $\Sigma(z)$ [see Eq. (2.5)] $\log(iz)$ appears, it is clear that the integrand in Eq. (4.5) is meromorphic in the semiplane $\mathrm{Im}(z)>0$. Therefore, we look for an analytic continuation of $\tilde{S}(z)$ into the rest of the complex plane. Since $\log(iz)$ has a vertical cut going downwards from $z=0$, we find that $\tilde{S}(z)$ "lives" exactly on the Riemann surface of $\log(iz)$. Thus by labeling the "branches" of the log function with respect to the sheet of the Riemann surface on which it is defined, we have

$$\log_l(iz)=\log(iz)+2l\pi i, \quad l\in Z \; . \tag{4.6}$$

Analogously, we involve the labels for the branches in the definitions of $\Sigma(z)$ and $\tilde{S}(z)$. By using Eqs. (2.5)–(2.7), (4.3), and (4.6) we obtain

$$\Sigma_0(z)=-\frac{\lambda}{\pi}\frac{\Omega^8 z}{(\Omega^2-z^2)^4} \times\left[\frac{1}{12\Omega^6}(11\Omega^6-18\Omega^4z^2+9\Omega^2z^4-2z^6)+\log\left[\frac{iz}{\Omega}\right]-\frac{i\pi}{2}\right], \tag{4.7}$$

$$\Sigma_{-1}(z)=\Sigma_0(z)+\frac{2\lambda i\Omega^8 z}{(\Omega^2-z^2)^4} =\Sigma_0(z)+2\lambda f(iz) \; . \tag{4.8}$$

The function $f(iz)$ is precisely the natural cutoff function defined in Eq. (2.2). Before getting involved with approximations, we apply the theory of complex variables and deform the contour of integration in Sec. V.

V. EXPONENTIAL-DECAY CONTRIBUTIONS STEMMING FROM POLES

Our starting point is now Eq. (4.5). We note that the integrand is defined as a multivalued function in the complex plane, or more conveniently, as a single-valued function on the Riemann surface of $\log(iz)$. We now deform the contour of integration C according to Fig. 2, so that it becomes a contour K, which consists of two horizontal rays emanating from 0 to $-\infty$. Here one of the rays runs on the sheet number 0, whereas the other one runs on the (lower) sheet number -1. During the process of deformation we might cross poles of the integrand in Eq. (4.5), so that the residue theorem (see Ref. 17) yields

$$S(t)=\sum_{\hat{z}}\mathrm{Res}(e^{tz}\tilde{S}(z),\hat{z})+D(t) \; , \tag{5.1}$$

where

$$D(t)=\frac{1}{2\pi i}\int_K e^{tz}\tilde{S}(z)dz \tag{5.2}$$

is the deviation from the exponential decay, as will be shown in the following. The summation is taken over all poles $\hat{z}$ of the integrand in Eq. (4.5) which are crossed in the process of the deformation.

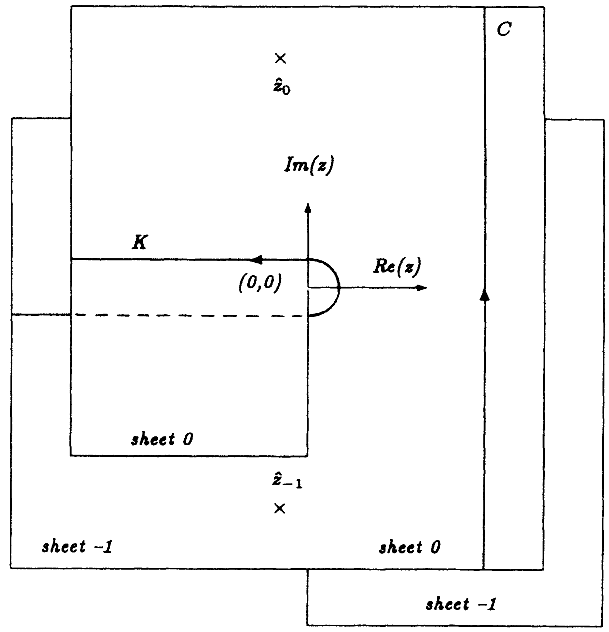

FIG. 2. Path of integration C used in Eq. (4.5) and the deformed path K on the Riemann sheets 0 and -1 used in Eq. (5.1). The relevant poles crossed in the process of deformation are $\hat{z}_{-1}$ (Weisskopf-Wigner pole) on sheet -1 and $\hat{z}_0$ on sheet 0.

Before turning to the problem of calculating the poles and residues appearing in Eq. (5.1), we observe that we may reduce Eq. (5.2) to a simple form by using a parametrization of the path K $[z(x)=-x, dz(x)=-dx, \ldots]$:

$$D(t)=\frac{1}{2\pi i}\int_0^\infty e^{-tx}[\tilde{S}_{-1}(-x)-\tilde{S}_0(-x)]dx \; . \tag{5.3}$$

We shall make use of this equation in Sec. VI.

We now turn to the sum in Eq. (5.1). Our first task is to find all the poles appearing there. If one takes a close look at Eq. (4.4), one recognizes that the poles of the integrand in Eq. (4.5) must be zeros of the respective denominator in Eq. (4.4). Here we write down the denominator of $\tilde{S}_l(z)$:

$$N_l(z)=z^2+2z\Sigma_l(z)+\omega_0^2, \quad l=0,-1 \; . \tag{5.4}$$

Intuitively, one might expect zeros of $N_l(z)$ close to $(-1)^l i\omega_0$, since in this area $z\Sigma_l(z)$ is comparatively small. In fact, in Appendix B we find the following.

Theorem 5.1. There are zeros $\hat{z}_l$ of $N_l(z)$ on the respective Riemann sheets, which read as

$$\hat{z}_l\approx\tilde{z}_l=-\frac{\lambda\omega_0}{2}+(-1)^l i\left[\omega_0+\frac{11\lambda\omega_0}{12\pi}-\frac{\lambda\omega_0}{\pi}\ln\left[\frac{\Omega}{\omega_0}\right]\right], \quad l=0,-1 \tag{5.5}$$

with the estimates for the corresponding errors

$$\left|\frac{\hat{z}_l-\tilde{z}_l}{\hat{z}_l}\right|<1.4\times10^{-13},\quad l=0,-1\ . \tag{5.6}$$

The term $(11/12\pi)\lambda\omega_0-(\lambda\omega_0/\pi)\ln(\Omega/\omega_0)$ in Eq. (5.5) represents the frequency shift (Lamb shift).

As will be shown in the following, the main contribution stems from the so-called Weisskopf-Wigner pole: $\hat{z}_{-1}$. The essential tool for computing the zeros $\hat{z}_0$ and $\hat{z}_{-1}$ is a fixed-point theorem, described in Appendix B. In Appendix B we also outline the method for finding the approximate values of the corresponding residues and give estimates for the errors. The results are summarized as follows.

Theorem 5.2. For the residue $\mathrm{Res}(e^{tz}\tilde{S}(z),\hat{z}_{-1})$ (which is usually referred to as the Weisskopf-Wigner contribution) and $\mathrm{Res}(e^{tz}\tilde{S}(z),\hat{z}_0)$, it holds that

$$\mathrm{Res}(e^{tz}\tilde{S}(z),\tilde{z}_l)\approx A_l e^{i\tilde{z}_l t}\quad (l=0,-1)\ . \tag{5.7}$$

Here $\hat{z}_{-1}$ and $\hat{z}_0$ are given by the Theorem 5.1; furthermore, A_{-1} and A_0 are defined by

$$A_{-1}=S(0)\left[1+\frac{3i\lambda}{4}-\frac{3\lambda}{2\pi}\left[\frac{11}{12}+\ln\frac{\omega_0}{\Omega}+\frac{\lambda}{\pi}\right]\right] -\mathrm{Im}[S(0)]\left[\frac{\lambda}{2}+\frac{i\lambda}{\pi}\left[\frac{11}{12}+\ln\frac{\omega_0}{\Omega}\right]\right]\ , \tag{5.8}$$

$$A_0=S(0)\left[\frac{i\lambda}{4}+\frac{\lambda}{2\pi}\left[\frac{11}{12}+\ln\frac{\omega_0}{\Omega}\right]\right] +\mathrm{Im}[S(0)]\left[\frac{\lambda}{2}-\frac{i\lambda}{\pi}\left[\frac{11}{12}+\ln\frac{\omega_0}{\Omega}\right]\right]\ . \tag{5.9}$$

Since the "phases," $e^{it\,\mathrm{Re}(\tilde{z}_l)}$, $l=0,\,-1$, are already contaminated with some error (cf. Theorem 5.1), the absolute value of the residues should be considered in the error estimation

$$||e^{tz}\mathrm{Res}(\tilde{S}(z),\hat{z}_l)|-|A_l e^{i\tilde{z}_l t}||<72\lambda\left[\frac{\omega_0}{\Omega}\right]^2\approx7.2\times10^{-13}\quad (l=0,-1)\ . \tag{5.10}$$

It should be noted that the contribution of the Weisskopf-Wigner pole, with the amplitude $A_{-1}\approx1$, yields the largest contribution to $S(t)$ for $t<10^{-8}$. Still we do not know all the other poles. In Appendix C we show how to estimate their position and the values of the corresponding residues. It turns out that all of them are close to $-\Omega$, but their contribution can be ignored.

Theorem 5.3. Let ζ denote any of the poles except the ones already mentioned in Theorem 5.1. Then the following holds:

$$\frac{\Omega\sqrt[4]{\lambda}}{2}<|\zeta-(-\Omega)|<\Omega\sqrt[4]{\lambda}\ , \tag{5.11}$$

$$\left|\sum_{\zeta}\mathrm{Res}(e^{tz}\tilde{S}(z),\zeta)\right|<\exp(-10^5),\quad t>10^{-13}\ . \tag{5.12}$$

VI. ESTIMATION OF DEVIATIONS FROM EXPONENTIAL DECAY IN THE CASE OF DIPOLE-MOMENT EV's

In Sec. IV we found the integral representation (4.5) of the solution of the basic equation, Eq. (4.1), and we used the theory of complex variables in order to deform the contour of integration. The residue theorem, finally, led us to Eqs. (5.1) and (5.2). We now turn to the discussion of Eq. (5.2). As will be shown below, the asymptotic main term of $S(t)$ reads as

$$M(t)=-\frac{\lambda}{2\pi}\frac{4i\,\mathrm{Im}[S(0)]}{\omega_0^2t^2}\ . \tag{6.1}$$

In contrast to I, in the present paper we shall not need Abel's asymptote. The task to be accomplished now consists of giving an approximate evaluation of $D(t)$ for times $t\geq10^{-13}$ s, including estimates of the errors. So we start from the integral representation of $D(t)$, Eq. (5.3). We find it convenient to change the variable of integration, i.e., to put

$$x=\Omega y,\quad dx=\Omega dx\ , \tag{6.2}$$

$$\phi(x)=\tilde{S}_{-1}(-x)-\tilde{S}_0(-x)\ . \tag{6.3}$$

Thus the integral representation of $D(t)$ reads as

$$D(t)=\frac{1}{2\pi i}\int_0^\infty\Omega\phi(-\Omega y)e^{-\Omega yt}dy\ . \tag{6.4}$$

The next step consists of having a close look at the integrand ϕ in Eq. (6.4). A tedious elementary calculation yields

$$\Omega\phi(-\Omega y)=\frac{-4\lambda i\nu(y)y(y+i\delta_0)\{-y\,\mathrm{Re}[S(0)]+\delta_0\,\mathrm{Im}[S(0)]\}}{\psi^2(y)+4\lambda^2y^4}\ , \tag{6.5}$$

where the following functions are used:

$$\nu(y)=(1-y^2)^4\ , \tag{6.6}$$

$$P(y)=\tfrac{11}{12}-\tfrac{18}{12}y^2+\tfrac{9}{12}y^4-\tfrac{2}{12}y^6\ , \tag{6.7}$$

$$\tau(y)=\frac{\lambda y}{\pi}[P(y)+\ln(y)+i\pi]\ , \tag{6.8}$$

$$\psi(y)=(y^2+\delta_0^2)\nu(y)-\frac{2\lambda y^2}{\pi}[P(y)+\ln(y)],\quad \delta_0=\frac{\omega_0}{\Omega}\ . \tag{6.9}$$

The essential idea is now to divide the interval of integration in Eq. (6.4), $[0,\infty)$ into three subintervals. The reason for performing this subdivision is the different behavior of the integrand $\phi\exp(-\Omega t y)$ of Eq. (6.4) in each of these subintervals. As we show in Appendix D the following theorem is valid.

Theorem 6.1. The function $\phi(-\Omega y)$ satisfies the following inequalities: (i) For $y\in I_1=[0,\eta],\eta=\delta_0/10 \approx 10^{-4}$, it holds that

$$\Omega\left|\phi(-\Omega y)-\frac{4\lambda y\,\mathrm{Im}[S(0)]}{\delta_0^2}\right|<2\lambda y^2\left[\frac{15\eta^{0.85}}{\delta_0^4}+\frac{5}{\delta_0^3}\right]. \tag{6.10}$$

(ii) For $y\in I_2=[\eta,1+2/\sqrt[4]{\kappa}]$, $\kappa=\exp(10^3)$, it holds that

$$|\Omega\phi(-\Omega y)|<\frac{4}{\lambda y^3}. \tag{6.11}$$

(iii) For $y\in I_3=[1+2/\sqrt[4]{\kappa},\infty)$, it holds that

$$|\Omega\phi(-\Omega y)|<\frac{2^6\kappa^2(1+\delta_0)^2\lambda}{y^9}. \tag{6.12}$$

Let us briefly comment on this technical result: It just means that we can replace the function $\phi(-\Omega y)$ in the integrand of Eq. (6.4) by 0 in intervals I_2 and I_3, and by $4\lambda y\,\mathrm{Im}[S(0)]/\delta_0^2$ in I_1. Thus Theorem 6.1 gives the estimates of the respective error functions.

Our next step consists of integrating the inequalities in Theorem 6.1. This is quite elementary and we get the following.

Theorem 6.2. The following final estimates hold for the integration in Eq. (6.4) over the intervals I_1, I_2, and I_3:

$$\frac{1}{2\pi i}\int_{I_1}\cdots=-\frac{\lambda}{2\pi}\frac{4i\,\mathrm{Im}[S(0)]}{\omega_0^2t^2}[1-(\Omega\eta t+1)e^{-\Omega\eta t}]+e(t), \tag{6.13}$$

with the error estimate

$$|e(t)|<\frac{\lambda}{2\pi}\left[\frac{15\eta^{0.85}}{\delta_0^4}+\frac{5}{\delta_0^3}\right]\frac{4}{\Omega^3t^3}, \tag{6.14}$$

and upper bounds

$$\left|\int_{I_2}\cdots\right|<\frac{2}{\lambda\pi}\frac{1}{\eta^3}\frac{\exp(-\Omega\eta t)}{\Omega t}, \tag{6.15}$$

$$\left|\int_{I_3}\cdots\right|<\lambda\frac{2^5\kappa^2(1+\delta_0)^2}{\pi\Omega}\frac{\exp(-\Omega t)}{t} \tag{6.16}$$

In other words, we may "neglect" the integrals over the second and third interval for $t\geq 10^{-13}$. Note that the main term $M(t)$ of Eq. (6.1) appears in Eq. (6.13). In fact, in the last step of this section we compare the values of all the contributions and errors with the value of the main term for times $t\geq 10^{-13}$ and $\mathrm{Im}[S(0)]\geq\frac{1}{10}$. It turns out that the main term is a good approximation for the expression $D(t)$ in Eqs. (5.2) and (6.4). We find the following.

Theorem 6.3. For $t\geq 10^{-13}$ s it holds that

$$D(t)=-\frac{\lambda}{2\pi}\frac{4i\,\mathrm{Im}[S(0)]}{\omega_0^2t^2}+E(t), \tag{6.17}$$

with the estimate for the "error term" $E(t)$:

$$\left|\frac{E(t)}{M(t)}\right|<\frac{1.3\times10^{-15}}{|\mathrm{Im}[S(0)]|t}. \tag{6.18}$$

VII. CONCLUSION

In this paper we have given a rigorous mathematical treatment for the spontaneous Lyman-α radiation emission from a single two-level hydrogenic atom. In our calculations no kind of ultraviolet divergency occurs, since all the retardation effects were taken into account. Further, as a very important fact, at every step of our calculations, the diverse approximations are provided with very accurate error estimates.

Finite-time deviations from the exponential decay were calculated for two different cases. In the first case we have treated the so-called Weisskopf-Wigner model (where the RWA is implied) and derived corrections to the exponential decay which are valid for times $t\geq 10^{-14}$ s.

In the second case we have gone beyond the RWA by taking into account the counter-rotating terms. In order to obtain results superior to those of the Weisskopf-Wigner model we applied a projection-operator method, where no kind of the usual BA is made. Thus we obtained results for the dipole-moment expectation values which contain the Lamb shift $(\gamma/\pi)[\frac{11}{12}-\ln(\Omega/\omega_0)]$ differing from the familiar Lamb shift (obtained in the dipole approximation)[3,13] by a non-negligible correction $11\gamma/(12\pi)$. Further, by a complex, but very accurate, estimation method, deviations from the exponential decay valid for times $t\geq 10^{-13}$ s were obtained. It should be emphasized that the accuracy of all the results obtained in the present paper is proved by error estimates.

Finally, we would like to stress the fact that the Lamb shift as well as the deviations from exponential decay were calculated for the two-level model; however, this does not mean that the contributions of the other levels (which were neglected in our model) are negligible. The inclusion of these levels would influence the deviations from the exponential decay (see Ref. 9) as well as the value of the Lamb shift (cf. Refs. 7–9).

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APPENDIX A: EVALUATION OF SOME ELEMENTARY INTEGRALS

Here we sketch the evaluation of $I(u)$ [cf. Eq. (2.5)] which is also used for the evaluation of $\Sigma(z)$ [cf. Eq. (4.3)]. The first step consists of rewriting the integrand

$$\frac{f(\omega)}{\omega-u}=\frac{\omega\Omega^8}{(\Omega^2+\omega^2)^4(\omega-u)} \tag{A1}$$

in the following form:

$$\frac{f(\omega)}{\omega-u}=\frac{P_7(\omega)}{(\Omega^2+\omega^2)^4}+\frac{c}{\omega-u} . \tag{A2}$$

Here $P_7(\omega)$ is a polynomial of degree 7 in ω, and c is a constant. We might be able to determine $P_7(\omega)$, explicitly, using some ansatz, but we postpone this step for later. Multiplying Eq. (A2) by $\omega-u$ and putting $\omega=u$, we deduce that $c=f(u)$, where $f(u)$ is defined by Eq. (2.2). We thus complete our task if we evaluate the two integrals corresponding to the two summands in Eq. (A2). It follows from integration technique that one can find a polynomial $P_5(\omega)$ with

$$\int\frac{P_7(\omega)d\omega}{(\Omega^2+\omega^2)^4}=\frac{P_5(\omega)}{(\Omega^2+\omega^2)^3}+\int\frac{(A_6\omega+A_7)d\omega}{\Omega^2+\omega^2} . \tag{A3}$$

So altogether we find the following integration formula:

$$\int\frac{f(\omega)d\omega}{\omega-u}=\frac{P_5(\omega)}{(\Omega^2+\omega^2)^3}+\int\frac{(A_6\omega+A_7)d\omega}{\Omega^2+\omega^2}+\int\frac{f(u)d\omega}{\omega-u} . \tag{A4}$$

Next we put $P_5(\omega)=A_0+\cdots A_5\omega^5$ with unknown coefficients A_i, where $i=0,\ldots,5$. Differentiating both sides of Eq. (A4), one finds a linear system of equations for all the unknown coefficients in the integral. Tedious calculation yields the following:

$$A_0=\frac{f(u)}{12}(11\Omega^6+18\Omega^4u^2+9\Omega^2u^4+2u^6) , \tag{A5}$$

$$A_1=\frac{f(u)}{16u}(11\Omega^6+15\Omega^4u^2+5\Omega^2u^4+u^6) , \tag{A6}$$

$$A_2=\frac{f(u)}{4}(5\Omega^4+6\Omega^2u^2+u^4) , \tag{A7}$$

$$A_3=\frac{f(u)}{6\Omega^2u}(5\Omega^6+3\Omega^4u^2-3\Omega^2u^4-u^6) , \tag{A8}$$

$$A_4=\frac{f(u)}{2}(\Omega^2+u^2) , \tag{A9}$$

$$A_5=\frac{f(u)}{16\Omega^4u}(5\Omega^6+\Omega^4u^2-5\Omega^2u^4-u^6) , \tag{A10}$$

$$A_6=-f(u) , \tag{A11}$$

$$A_7=\frac{f(u)}{16\Omega^4u}(5\Omega^6-15\Omega^4u^2-5\Omega^2u^4-u^6) . \tag{A12}$$

Finally, we evaluate the integral between 0 and ∞. This now can be done in a completely elementary way and after changing the notation $C_1(u)=A_0(u)$ and $C_2(u)=A_7(u)$, Eq. (2.5) can be deduced.

APPENDIX B: APPROXIMATIONS FOR THE POLES AND RESIDUES

Lemma B.1 (fixed-point theorem). Let $\Phi(z)$ denote a complex function analytic in $G:=\{z|\,|z-z_{(0)}|<R\}$ and continuous on the closure $\bar{G}=\{z|\,|z-z_{(0)}|\le R\}$. Assume that there is some real non-negative number $\kappa<1$, so that for all $z\in G$ the inequality $|\Phi'(z)|=|d\Phi(z)/dz|\le\kappa$ holds. Assume furthermore that $|\Phi(z_{(0)})-z_{(0)}|\le(1-\kappa)R$. Then the following statements hold: (i) The sequence starting with $z_{(0)}\in G$ and defined by

$$z_{(n+1)}=\Phi(z_{(n)}) \tag{B1}$$

converges to the unique fixed-point $z_{(\infty)}$ in $\bar{G}$, i.e., $z_{(\infty)}=\Phi(z_{(\infty)})$. (ii) For the rate of convergence, one has

$$|z_{(n)}-z_{(\infty)}|\le\kappa^nR , \tag{B2}$$

and

$$|z_{(n)}-z_{(\infty)}|\le\frac{\kappa^n|z_{(1)}-z_{(0)}|}{1-\kappa} . \tag{B3}$$

Note for the proof. This is a summary of Theorems 6.12a and 6.12b on pages 524 and 525 in Ref. 18, together with some standard statements as stated in the exercises *ibidem*.

Our first application of this fixed-point theorem is finding zeros of the denominator $N_{-1}(u)=u-\omega_0+(\lambda/2\pi)I_{-1}(u)$ in Eq. (2.4) $[I_{-1}=I_0+2\pi if(u)]$. If we rewrite our problem as $u=\omega_0-(\lambda/2\pi)I_{-1}(u)$, it becomes clear that we may apply the fixed-point theorem to the function $\Phi(u)=\omega_0-(\lambda/2\pi)I_{-1}(u)$. Since the term $(\lambda/2\pi)I_{-1}(u)$ is comparatively small for u close enough to $u=\omega_0$, we expect a fixed point close to $u=\omega_0$. Thus, with $u_{(0)}=\omega_0-i0$, we start an iteration for approximating this fixed point.

Lemma B.2. In the fixed-point theorem for $\Phi(u)=\omega_0-(\lambda/2\pi)I_{-1}(u)$, $u_{(0)}=\omega_0$, $R=\lambda\Omega$, and $\kappa=4\lambda$, the following statements hold true:

$$u_{(1)}=\omega_0+\frac{11\lambda\omega_0}{24\pi}-\frac{5\lambda\Omega}{64}-\frac{\lambda\omega_0}{2\pi}\ln\left|\frac{\Omega}{\omega_0}\right|-i\frac{\omega_0\lambda}{2} , \tag{B4}$$

$$\left|\frac{\Delta_u}{u_{(\infty)}}\right|<4.1\times10^{-13} . \tag{B5}$$

Proof. By inserting $u=\omega_0-i0$ (we start on the lower sheet) into the equation $u_{(1)}=\Phi(u_{(0)})$, we immediately obtain Eq. (B4), where

$$|u_{(1)}-u_{(0)}|=\frac{\lambda}{2\pi}|I_{-1}(\omega_0-i0)|<0.76\lambda\Omega \tag{B6}$$

as can be seen from Eqs. (D1) and (D2). Further, by making use of Eqs. (2.5)–(2.7), it is easy to show that

$$|\Phi'(u)|=\frac{\lambda}{2\pi}|I'_{-1}(u)|<\kappa , \tag{B7}$$

where $|u-\omega_0|<\omega_0/10$, and the estimations $|f(u)|<1.01|u|$, $|f'(u)|<1.01$, $|C_1'(u)|<1.01\Omega^6$, $|C_2'(u)|<10|u|/\pi$, and $|\log_{-1}(\Omega/u)+i\pi|<17$ are taken into account. Therefore, from Theorem B.1 we deduce that $\Delta_u=|u_{(1)}-u_{(\infty)}|<4\lambda^2\Omega$ holds, so that Eq. (B5) follows. Our next task is an approximate evaluation of the residue.

Remark. If $f(z)=M(z)/N(z)$, so that $N(z)$ has a simple zero at $z=z_0$ and $M(z)$ is analytic in a (small) neighborhood of z_0, then it holds for the residue that

$$\mathrm{Res}(f(z),z_0)=\frac{M(z_0)}{N'(z_0)} . \tag{B8}$$

Lemma B.3. For $\hat{B}_1(u)$ in Eq. (2.4) we find

$$\mathrm{Res}(\hat{B}_1(u),\hat{u})\approx b_1(0) , \tag{B9}$$

$$\Delta_{\mathrm{res}}=|\mathrm{Res}(\hat{B}_1(u),\hat{u})-b_1(0)|<10\lambda|b_1(0)| . \tag{B10}$$

Proof. Since $\hat{u}$ is a simple pole of $N_{-1}(u)=u-\Phi(u)$, it follows from the above Remark that

$$\mathrm{Res}(\hat{B}(u),\hat{u})=\frac{b_1(0)}{1-\Phi'(\hat{u})} . \tag{B11}$$

Then Eq. (B7) leads directly to Eqs. (B9) and (B10).

Our second application is the calculation of the zeros in Theorem 5.1. In order to find zeros of N_l in Eq. (5.4) we apply the fixed-point theorem to

$$z=(-1)^l i\omega_0\left[1+2\frac{\Sigma_l(z)}{z}\right]^{-1/2} .$$

We state this more formally.

Lemma B.4. Put

$$\sigma_l(z)=\Sigma_l(z)/z,\quad l=0,-1$$
$$\Phi_l(z)=(-1)^l i\omega_0[1+2\sigma_l(z)]^{-1/2} . \tag{B12}$$

Here the branch of the root has to be taken in such a way that it becomes analytic in a neighborhood of $\pm i\omega_0$. Put $R=\omega_0\times 10^{-5}$ and $z_{l(0)}=(-1)^l i\omega_0$. Then for $\kappa=7\lambda^2$ the hypothesis of the fixed-point theorem is satisfied.

Proof. The first thing to show is that $|\Phi_l'(z)|\le\kappa$ holds. Note that

$$\Phi_l'(z)=(-1)^{l+1}i\omega_0\frac{\sigma_l(z)\sigma_l'(z)}{[1+2\sigma_l(z)]^{3/2}} .$$

Now, after some elementary calculations, the following estimates can be shown:

$$|\sigma_l(z)|<6\lambda,\quad |\sigma_l'(z)|<\frac{\lambda}{\omega_0} . \tag{B13}$$

With this result we easily derive

$$|\Phi_l'(z)|<\frac{6\lambda^2}{(1-12\lambda)^{3/2}}<7\lambda^2 . \tag{B14}$$

Thus we proved that we may put $\kappa=7\lambda^2$. Next we show that $|z_{l(1)}-z_{l(0)}|\le(1-\kappa)R$. Note that

$$|z_{l(1)}-z_{l(0)}|=\omega_0|[1+2\sigma_l(z_{l(0)})]^{-1/2}-1|$$
$$\le 2\omega_0|\sigma_l(z_{l(0)})|\le 12\omega_0\lambda . \tag{B15}$$

This is evidently much smaller than $(1-\kappa)R=10^{-5}(1-7\lambda^2)\omega_0$, so that the estimate holds true.

This allows the application of the fixed-point theorem; after having performed the first step of the fixed-point algorithm and making use of Eq. (B15), we find

$$z_{l(1)}=\Phi_l(z_{l(0)}) ,$$
$$|z_{l(\infty)}-z_{l(1)}|<12\frac{\lambda\omega_0\kappa}{1-\kappa}\le 85\lambda^3\omega_0 . \tag{B16}$$

From this we see that $z_{l(\infty)}\approx(-1)^l i\omega_0$ and thus the error is extremely small, i.e., the convergence is pretty good. We are, however, interested in a simpler expression for $\Phi_l(z_{l(0)})$, which can be obtained by means of a power series: If we put $\Phi_l(z_{l(0)})\approx\bar{z}_l=(-1)^l i\omega_0[1-\sigma_l(z_{l(0)})]$, then the error amounts to

$$|z_{l(1)}-\bar{z}_l|<109\lambda^2\omega_0 . \tag{B17}$$

Another simplification concerns $\Sigma_l(z_{l(0)})$ [cf. Eq. (4.3)]. If we put

$$\Sigma_l(z_{l(0)})\approx\bar{\Sigma}_l=\frac{\lambda\omega_0}{2}+(-1)^{l+1}i\frac{\lambda\omega_0}{\pi}\left[\frac{11}{12}+\ln\frac{\omega_0}{\Omega}\right] , \tag{B18}$$

then the following estimate is valid:

$$|\Sigma_l(z_{l(0)})-\bar{\Sigma}_l|<11\lambda\omega_0\left[\frac{\omega_0}{\Omega}\right]^2 , \tag{B19}$$

where we made use of elementary estimates with a power series. Further, we put

$$\bar{z}_l=-\frac{\lambda\omega_0}{2}+(-1)^l i\left[\omega_0+\frac{11\lambda\omega_0}{12\pi}-\frac{\lambda\omega_0}{\pi}\ln\left[\frac{\Omega}{\omega_0}\right]\right] . \tag{B20}$$

By collecting the three estimates of Eqs. (B16), (B17), and (B19) and denoting the zeros $z_{l(\infty)}$ (according to their localization on the lth Riemann sheet) by

$$\hat{z}_l=z_{l(\infty)},\quad l=0,-1 \tag{B21}$$

one finally obtains the results in Theorem 5.2.

Our next task is to sketch the approximate evaluation of the residues of the poles as stated in Theorem 5.1. According to Eq. (4.4) it follows that

$$M(z)=(z-i\omega_0)[S(0)]+2i\Sigma(z)\,\mathrm{Im}[S(0)] , \tag{B22}$$

$$N(z)=z^2+2z\Sigma(z)+\omega_0^2 , \tag{B23}$$

and from the above Remark we have

$$\mathrm{Res}(\tilde{S}_l(z),z_{l(\infty)})=\frac{M_l(z_{l(\infty)})}{N_l'(z_{l(\infty)})} . \tag{B24}$$

By making use of Eqs. (B17), (B19), and (B20), one finds the following estimates:

$$|\Sigma_l(z_{l(\infty)})-\bar{\Sigma}_l|<11\lambda\omega_0\left[\frac{\omega_0}{\Omega}\right]^2 , \tag{B25}$$

$$|z_{l(\infty)}\Sigma_l'(z_{l(\infty)})-[\bar{\Sigma}_l+(-1)^{l+1}i\omega_0\lambda/\pi]|$$
$$<31\lambda\omega_0\left[\frac{\omega_0}{\Omega}\right]^2 . \tag{B26}$$

Again one has to perform some estimates with a power series. Next we give approximations for M and N', respectively,

$$\bar{M}_l=(\bar{z}_l-i\omega_0)S(0)+2i\bar{\Sigma}_l\,\mathrm{Im}[S(0)]\ , \tag{B27}$$

$$\bar{N}'_l=2[\bar{z}_l+2\bar{\Sigma}_l+(-1)^{l+1}i\omega_0(\lambda/\pi)]\ . \tag{B28}$$

For the errors one finds, in a tedious but elementary way, the following estimates:

$$|M_l-\bar{M}_l|<35\lambda\omega_0\left[\frac{\omega_0}{\Omega}\right]^2 , \tag{B29}$$

$$|N'_l-\bar{N}'_l|<110\lambda\omega_0\left[\frac{\omega_0}{\Omega}\right]^2 , \tag{B30}$$

$$|M_0|<6\lambda\omega_0,\quad |M_{-1}|<2\omega_0,\quad |N'_l|>2\omega_0\ . \tag{B31}$$

These inequalities lead to

$$|M_l(z_{l(\infty)})/N'_l(z_{l(\infty)})-\bar{M}_l/\bar{N}'_l|<71\lambda\left[\frac{\omega_0}{\Omega}\right]^2 . \tag{B32}$$

Finally, we remark that the expression $\bar{N}'_l$ [cf. Eq. (B28)] can be approximated by

$$\bar{N}'_l\approx\tilde{N}'_l=2(-1)^l i\omega_0\ , \tag{B33}$$

so that

$$|\tilde{N}'_l-\bar{N}'_l|<3.4\lambda\omega_0\ . \tag{B34}$$

We thus remark that $\tilde{N}'_l$ and $\bar{M}_l$ are approximations for M and N [cf. Eqs. (B22) and (B23)] on the respective sheets of the Riemann surface (i.e., $l=0,-1$). The various estimates, finally, yield Eq. (5.10) of Theorem 5.2.

APPENDIX C: ARGUMENT PRINCIPLE

The argument principle reads as follows.

Lemma C.1. Let $f(z)$ denote a complex function meromorphic in some simply connected open subset G of a Riemann surface. Let C denote a closed piecewise differentiable continuous curve in G having no double point. Assume that $f(z)$ has no poles or zeros on C. The quantity

$$\Delta_C \arg(f)=\int_C \frac{f'(z)dz}{f(z)}$$

is equal to 2π times $(Z-P)$, where Z (P) denotes the zeros (poles) of $f(z)$ in the area enclosed by C, each of them counted with their order. For a continuous parametrization $z(\theta)$ of C, $\Delta_C \arg(f)$ is equal to 2π times the length of the curve $v(\theta)=f(z(\theta))/|f(z(\theta))|$, where θ runs from 0 to 2π.

For more details we refer to Ref. 17. The second important ingredient is the Lemma of Rouché.

Lemma C.2. Assume that the meromorphic functions $f(z)$ and $g(z)$ are analytic in the simply connected open subset of the Riemann surface. Let C be a curve, as in Lemma C.1, and assume that $f(z)$ has no poles or zeros on C. Furthermore, assume that $|g(z)|<|f(z)|$ holds on C. Then

$$\Delta_C \arg(f)=\Delta_C \arg(f+g)\ .$$

(For this Lemma we also refer to Ref. 17.)

Our first candidate is the function $\hat{B}_1(u)$ in Eq. (2.4). We choose C to be "composed" by a finite part of K and the circular part C^* with radius R as is shown in Fig. 3. With $f(u)=u-\omega_0$, $g(u)=(\lambda/2\pi)I_l(u)$ ($l=0,-1$), and R large enough (cf. Fig. 3), the hypothesis of the Lemma of Rouché is satisfied along the circular part C^*.

Next we observe that, from Eqs. (D1) and (D2) and the relation

$$|u-\omega_0|\geq\frac{\omega_0}{\sqrt{2}},\quad u\in K \tag{C1}$$

one easily obtains

$$\left|\frac{\lambda}{2\pi}I_l(u)\right|<|u-\omega_0|,\quad u\in K,\quad l=0,-1 \tag{C2}$$

and thus the hypothesis of Lemma C.2 is satisfied along the whole curve C. So, according to this Lemma, instead of the complicated denominator $N(u)$ of $\hat{B}_1(u)$ [cf. Eq. (2.4)], we may deal with the very simple function $f(u)=u-\omega_0$, which has exactly one zero at $u=\omega_0$ and no poles. Since $N(u)$ evidently has no poles, we infer that the function $N(u)$ has a simple zero in the area enclosed by C. We remark that we found an estimate for it in Appendix B, Eqs. (B4) and (B5).

Our next application of Rouché's Lemma and the argument principle will consist in deriving Theorem 5.3. Here we start with the denominator $N(z)$ of Eq. (4.4), which is given by Eq. (5.4). We use a path according to Fig. 4, which consists of one and a half circles of large radius R and a part of the line $\mathrm{Re}(z)=0$ denoted by K. It is immediate that $f(z)=z^2+\omega_0^2$ and $g(z)=z\Sigma(z)$ satisfy the hypothesis of Rouché's Lemma along the circular part C^* of the curve (cf. Fig. 4), since the term z^2 dominates. So we find 6π for the value of $\Delta_{C^*}\arg(f+g)$. Next

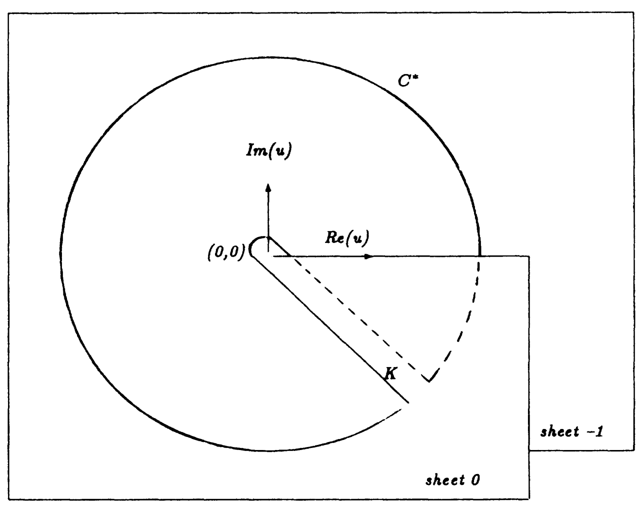

FIG. 3. Curve C, consisting of the circular part C^* and a finite part of the path of integration K [cf. Eq. (2.15)]. Curve C is used for finding the zeros and poles of the function $\hat{B}_1(u)$ [cf. Eq. (2.4)] by means of the argument principle in Appendix C.

note that $\text{Im}[N_0(-iy)]>0$ and $\text{Im}[N_{-1}(iy)]<0$ hold for $y>0$. Therefore, from $N(0+0)=\omega_0^2>0$, it follows that the contribution of $\Delta_K \arg(f)=\Delta_K \arg(f+g) =\Delta_K \arg(N)$ will be -2π. Thus altogether $\Delta_C \arg(N) =4\pi$, so that $Z-P=2$ holds (cf. Lemma C.1). So we find by Lemma C.2 that $N(z)$ has two zeros more than poles in the area enclosed by the curve C (see Fig. 4).

Next, a very elementary calculation shows that both $\Sigma_0(z)$ and $\Sigma_{-1}(z)$ [cf. Eq. (4.7)] have a pole of the fourth order at $z=-\Omega$, and $\Sigma_0(z)$ has no pole at $z=\Omega$. There are evidently no other relevant poles than these eight ones. Therefore, $N(z)$ must have exactly ten zeros in the area enclosed by C. We already found two zeros in Appendix B, so eight of them are missing. We next localize the zeros close to $z=-\Omega$.

We first start with a simple scaling

$$z(\mu)=-\Omega(1-\mu), \quad \mu\in C \tag{C3}$$

and then, in order to apply the argument principle, instead of $N[z(\mu)]$ we introduce an auxiliary function $F(\mu)=\pi N[z(\mu)]\mu^4(2-\mu)^4/\Omega^2$ which has the same zeros as $N[z(\mu)]$ but none of its poles. Further, we define the following expressions $F_1(\mu)$ and $F_2(\mu)$:

$$F_1(\mu)=\mu^4\left\{(1-\mu)^2\left[\pi(2-\mu)^4-2\lambda\left[R_4(\mu)-\frac{7}{4}+\mu-\frac{\mu^2}{6}\right]\right]+\left[\frac{\omega_0}{\Omega}\right]^2\pi(2-\mu)^4\right\}, \tag{C4}$$

$$F_2(\mu)=2i\pi\lambda(1-\mu)^2\ , \tag{C5}$$

where $R_4(\mu)$ denotes the remainder of the power-series expansion for $\log(1-\mu)/\mu^4$ (around $\mu=0$). We remark that $F(\mu)=F_1(\mu)\mp F_2(\mu)$, where the sign has to be chosen according to the sheet number 0 or -1. If one has a close look at $F(\mu)$, one can see the following.

Lemma C.3. (i) Along the circle $|\mu|=\sqrt[4]{\lambda}$ the inequality $|F_1(\mu)|>|F_2(\mu)|$ is valid. (ii) Along the circle $|\mu|=\sqrt[4]{\lambda}/2$ the inequality $|F_1(\mu)|<|F_2(\mu)|$ is valid.

Proof. We outline the proof for (i) and (ii). It is reasonable that one might simplify $F_i(\mu)$ $(i=1,2)$:

$$F_1(\mu)\approx\bar{F}_1(\mu)=16\pi\mu^4\ , \tag{C6}$$

$$F_2(\mu)\approx\bar{F}_2=2i\pi\lambda\ . \tag{C7}$$

This is certainly good if $|\mu|\le\sqrt[4]{\lambda}\approx10^{-2}$, which is much smaller than 1. In fact, using Taylor-series expansions one can show the following estimates:

$$|F_1(\mu)-\bar{F}_1(\mu)|<205|\mu|^5\ , \tag{C8}$$

$$|F_2(\mu)-\bar{F}_2|<13\lambda|\mu|\ . \tag{C9}$$

Then it is evident that the statements (i) and (ii) of the Lemma are true, when F_1 and F_2 are replaced by $\bar{F}_1$ and $\bar{F}_2$, respectively.

The statements of Lemma C.3 can be used in connection with Lemmas C.1 and C.2. Then on each Riemann sheet $(l=0,-1)$ the following holds: Along the circle $\mu=\sqrt[4]{\lambda}$ the function F_1 dominates, so that inside of the circle there must be four zeros of F according to Lemma C.1. Since along the inner circle $\mu=\sqrt[4]{\lambda}/2$ the function F_2 dominates, there can be no zero of F inside. Therefore, all eight zeros of the function $N(z)$ (four on each Riemann sheet) are contained in the annulus

$$L=\{z|\Omega\sqrt[4]{\lambda}/2<|z-(-\Omega)|<\Omega\sqrt[4]{\lambda}\}\ . \tag{C10}$$

We turn to the estimates for the residues. Using the scaling of Eq. (C3), an elementary calculation shows that

$$\tilde{S}_l(z)=\frac{M_l(z)}{N_l(z)}=\frac{E_l(\mu)}{F^l(\mu)}\ , \tag{C11}$$

where M_l and N_l are given by Eqs. (B22) and (B23), $F^l(\mu)=F_1(\mu)+(-1)^{l+1}F_2(\mu)$, and

$$E_l(\mu)=\lambda(1-\mu)\left[\mu^4\left[R_4(\mu)-\frac{7}{4}+\mu-\frac{\mu^2}{6}\right]+(-1)^l i\pi\left[2i\,\text{Im}[S(0)]\right]\right.$$
$$\left.-[(1-\mu)+i\omega_0/\Omega]S(0)\pi\mu^4(2-\mu)^4\right], \tag{C12}$$

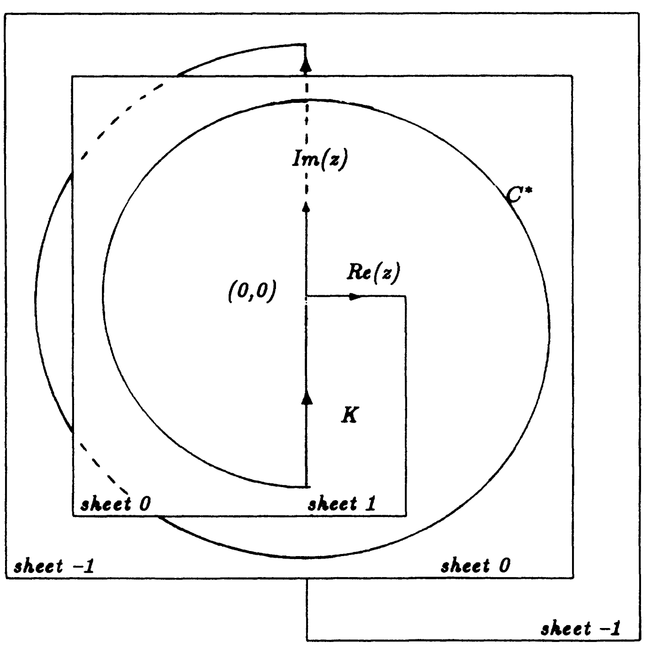

FIG. 4. Curve C consisting of the circular part C^* (one and a half circles) and a finite part of the line $\text{Re}(z)=0$ denoted by K. Curve C is used for finding the zeros and poles of the function $\tilde{S}(z)$ [cf. Eq. (4.4)] by means of the argument principle in Appendix C.

one observes that for a simple zero ζ

$$\text{Res}(\tilde{S}(z),\zeta)=\text{Res}\left[\frac{E(\mu)}{F(\mu)},\hat{\mu}\right], \quad [\zeta=-\Omega(1-\hat{\mu})] \tag{C13}$$

holds true. Again, using Taylor-series expansions one finds that for $\mu\in L$ [cf. Eq. (C10)],

$$|E(\mu)|<60\lambda , \tag{C14}$$

$$|F'(\mu)|>4\pi\lambda^{3/4} . \tag{C15}$$

From Eq. (C15) we immediately conclude that all the poles of $\tilde{S}(z)$ are simple and this justifies *a posteriori* the application of Eq. (C13). From inequalities, Eqs. (C14) and (C15), it follows that

$$|\text{Res}(\tilde{S}(z),\zeta)|<5\lambda^{1/4} . \tag{C16}$$

Finally, let ζ denote any of the (simple) poles of $\tilde{S}(z)$ in the annulus defined in Eq. (C10). Taking into account

$$|\text{Res}(e^{tz}\tilde{S}(z),\zeta)|=e^{t\,\text{Re}(\zeta)}|\text{Res}(\tilde{S}(z),\zeta)| \tag{C17}$$

and $\text{Re}(\zeta)<-\Omega+\Omega\lambda^{1/4}$, Theorem 5.3 follows.

APPENDIX D: APPROXIMATIONS FOR THE INTEGRANDS OF SECS. II AND VI

In this appendix we sketch the proofs of those inequalities which are connected with integrations over the deformed paths K in Secs. II and V, respectively. We already used some of these inequalities in Appendix C on the argument principle.

Our first task is to note that for $u=(1-i)\Omega x$ with non-negative real x,

$$|f(u)|=\frac{\sqrt{2}\Omega x}{(1+4x^4)^2}<\frac{\Omega}{2} \tag{D1}$$

holds as an elementary evaluation of the maximum of this function, with respect to x shows. Our next concern is to derive the inequality

$$\left|\frac{\lambda}{2\pi}I_0(u)\right|\le 0.26\lambda\Omega . \tag{D2}$$

Starting from the definition of $I_0(u)$ [cf. Eq. (2.5)] and introducing a new variable y of integration $\omega=\Omega y$, we find

$$\left|\frac{\lambda}{2\pi}I_0(u)\right|=\frac{\lambda}{2\pi}\left|\int_0^\infty\frac{\Omega y\,dy}{(1+y^2)^4[y-(1-i)x]}\right| \le\frac{\lambda\Omega}{2\pi}\int_0^\infty\frac{\sqrt{2}dy}{(1+y^2)^4} . \tag{D3}$$

If we now replace the integrand in the last inequality by $\sqrt{2}$ in the interval [0,1], and by $\sqrt{2}/y^8$ in the rest interval $[1,\infty)$, and afterwards integrate, we find the final estimate in Eq. (D2). Equipped with these inequalities, i.e., Eqs. (D1) and (D2), it is easy to derive

$$|N_l(u)|\ge|u-\omega_0|(1-1.1\times10^{-5}) \quad l=0,-1 . \tag{D4}$$

Here u has the same meaning as above. From Eqs. (D2) and (D4) it is elementary to perform the following estimate for the integrand in Eq. (2.16):

$$\begin{aligned}\left|\frac{f(u)}{N_0(u)N_{-1}(u)}\right| &\le\frac{\Omega}{2|u-\omega_0|^2(1-1.1\times10^{-5})^2}\\ &\le\cdots\le\frac{1}{2(1-10^{-4})\Omega[(x-\delta_0)^2+x^2]}\\ &\le\frac{1}{(1-10^{-4})\Omega\delta_0^2},\quad \delta_0=\frac{\omega_0}{\Omega} .\end{aligned} \tag{D5}$$

The last estimate follows from looking at the minimum of the denominator function $[(x-\delta_0)^2+x^2]$, which is attained at $x=\delta_0/2$. This last inequality being integrated over the interval $[\delta,\infty)$ gives the estimate of Eq. (2.18) in step (4) of Sec. II.

Our next task consists in deriving the estimate in step (5) of Sec. II. Intuitively one expects in the interval $[0,\delta]$ that

$$f(u)\approx u, \quad N(u)\approx\omega_0 . \tag{D6}$$

So we find immediately that

$$\begin{aligned}&\left|\frac{i\lambda f(u)}{N_0(u)N_{-1}(u)}-\frac{i\lambda u}{\omega_0^2}\right|\\ &\le\lambda|f(u)|\left[\left|\frac{1}{N_0(u)N_{-1}(u)}-\frac{1}{N_0(u)^2}\right|\right.\\ &\qquad\left.+\left|\frac{1}{N_0(u)^2}-\frac{1}{\omega_0^2}\right|+\frac{1}{\omega_0^2}\left|1-\frac{u}{f(u)}\right|\right] .\end{aligned} \tag{D7}$$

The common factor in front is bounded by $\lambda|u|$. Thus we turn to the three summands in large parentheses. For the first one, using Eq. (D4) and the bound for the common factor in front, we get $\lambda|u||u-\omega_0|^{-3}(1-10^{-4})^{-3}$ as a suitable bound. Since $|u-\omega_0|^{-3}$ is decreasing, we finally find a good bound for this first term:

$$s_1=1.64\frac{\lambda|u|}{\omega_0^3} . \tag{D8}$$

In a similar elementary way one finds a bound for the second term:

$$s_2=\frac{2.78}{\omega_0^3}|u|+\frac{\lambda\Omega}{\omega_0^3} . \tag{D9}$$

And, finally, using power-series expansions we find a bound for the third term:

$$s_3=8.1\frac{x^2}{\omega_0^2} . \tag{D10}$$

Thus summing up these estimates we obtain the estimate of Eq. (2.19) in step (5) of Sec. II.

We now start discussing some of the technical details in Sec. VI. So we turn to an explanation for the estimates found in Theorem 6.1. We have three intervals there, and we start with I_1. The basic idea is that the following simplifications can be made for $y\in I_1$:

$$\nu(y)\approx 1 , \tag{D11}$$

$$P(y)\approx \tfrac{11}{12}\ , \tag{D12}$$

$$\tau(y)\approx \frac{\lambda y}{\pi}\left(\tfrac{11}{12}+\ln y+i\pi\right)\ . \tag{D13}$$

The $\ln y$ term is a bit subtle. We make use of the following elementary inequality:

$$-y^2\ln y \le \frac{3\ln 10}{e}y^{2-1/(3\ln 10)} < 2.55y^{1.85}\ , \tag{D14}$$

which holds for $0\le y\le \exp(-3\ln 10)=\delta_0$. In fact, with this and more care in the approximations of ν, P, τ, we find that

$$|\psi(y)-\delta_0^2| \le y^2+5\delta_0^2 y^{1.85}\ . \tag{D15}$$

Thus for the denominator $\mathcal{D}(y)$ in Eq. (6.5), after elementary tedious estimations, we find

$$\begin{aligned} &|\mathcal{D}(y)-\delta_0^4| \le 3\delta_0^2 y^{1.85}\ ,\\ &|1/\mathcal{D}(y)-1/\delta_0^4| \le 4.2y^{1.85}/\delta_0^2\ . \end{aligned} \tag{D16}$$

We next denote by $\mathcal{N}(y)$ the numerator in Eq. (6.5). Again, some elementary work leads to the estimates

$$\begin{aligned} &|\mathcal{N}(y)-4\lambda\delta_0^2 y\ \mathrm{Im}[S(0)]| \le 9.7\lambda\delta_0 y^2\ ,\\ &|\mathcal{N}(y)| \le 4.88\lambda y\delta_0^2\ . \end{aligned} \tag{D17}$$

The inequalities (D16) and (D17) yield the statement (i) in Theorem 6.1.

We next turn to interval I_2. An estimate for the lower bound of $|\mathcal{D}(u)|$ is given by $4\lambda^2y^4$. For $|\mathcal{N}(y)|$ a crude estimate yields the upper bound $16\lambda y$. This immediately leads to statement (ii) in Theorem 6.1.

So we come to the third and final interval I_3. As a rough upper bound for $|\mathcal{N}(y)|$ we may use $2^6\lambda y^{11}(1+\delta_0)^2$ [cf. Eqs. (6.5) and (6.6)]. In order to get a reasonable bound for $|\mathcal{D}(y)|$ we have to be a bit more careful. Clearly, we may estimate the lower bound $|\mathcal{D}(y)|$ by $\psi^2(y)$. Having a closer look at $\psi(y)$ we find a lower bound $(y^2+\delta_0^2)(1-y^2)^4$, which itself can be bounded by y^{10}/κ again. So this leaves us with y^{20}/κ^2 as a lower bound for $|\mathcal{D}(y)|$. A combination of the estimates for $|\mathcal{N}|$ and $|\mathcal{D}|$ leads to statement (iii) in Theorem 6.1.

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