

The above approach can be extended, by renormalization of the formulas, to the case of "destruction" of order atoms or small-charge ions colliding with multiply charged ions.

¹Here, v is the relative velocity of colliding particles; we shall use the atomic system of units; $\hbar = m = e = 1$.

²We shall not consider the relationship between the exchange matrix element and the quasiclassical barrier permeability. This relationship is analyzed in Chibisov's thesis.²⁷

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Characteristics of electron and photon spectra associated with interaction between quasistationary terms

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An analysis is made of the energy spectra of electrons or photons emitted as a result of decay of two quasistationary terms which interact with one another in accordance with the Demkov or Nikitin models. General expressions are obtained for describing the lines of isolated atoms and of the background corresponding to decay of a quasimolecular state. The profiles of atomic lines, their satellites, far wings, etc., are investigated. The general problem of the interaction of discrete states with degenerate continua, corresponding to different directions of electron or photon emission and different decay channels, is considered. The interaction of discrete levels via a continuum is related to interference in the final states. It is shown that each model of the interaction of quasidiscrete levels predicts a variety of spectra which differ in respect of the nature of interference.

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§1. INTRODUCTION

Ionization in $A + B \rightarrow A + B^+ + e$ atomic collisions at velocities lower than the characteristic electron value can

conveniently be described in terms of formation and decay of the corresponding autoionizing states of a quasimolecule. In contrast to the usual discrete levels, such states are characterized not only by the dependences,

on the internuclear distance R , of their energy $E(R)$ but also of their width $\Gamma(R)$ which describes the feasibility of ionization of a given state. Similar description can also be used for the noncharacteristic radiation emitted in collisions of atoms. Detailed information on the process and on the characteristics of quasistationary states is contained in the energy spectra of the resultant electrons and photons, which have recently been attracting the attention of experimentalists and theoreticians.^{1,2}

In earlier papers^{3,4} we formulated the theory of interaction of several quasistationary states with one (non-degenerate) continuum and we considered the characteristics of the spectra which appear in a number of physically interesting cases, when only one quasistationary term is present^{4,5} and also when there are two terms forming a Landau-Zener pseudocrossing.⁶ In the present paper we shall study systematically another important (in atomic physics) case of the interaction between two states when the terms are parallel over large internuclear distances and become strongly repulsive on reduction of R . In this case, nonadiabatic transitions are usually described by the Demkov model⁷ or the more general Nikitin model.^{8,9}

The Demkov model was first suggested to describe charge exchange in the case of a small resonance defect and has subsequently found numerous applications in the theory of nonadiabatic transitions between quasimolecular terms in collisions. In particular, Meyerhof¹⁰ applied it to describe a redistribution of vacancies between the orbitals of a quasimolecule when a vacancy forms on close approach to one of the orbitals and this vacancy is then transferred to other orbitals during the subsequent motion of the colliding atomic particles. This mechanism frequently predominates in the formation of vacancies in deep internal atomic shells. The states of a quasimolecule with vacancies are unstable (quasistationary) and may decay in the course of collisions so that the vacancies become filled with electrons from outer shells, and electrons and photons are emitted, as found experimentally.^{2,11} Therefore, a calculation of the relevant energy spectra is a pressing problem.

One of the reasons for the popularity of the Demkov model is the fact that the exponential repulsion of the terms allowed in the model has a clear physical origin because it is associated with the exchange interaction of the states of a particle in potential wells which approach one another. The magnitude of this interaction can be determined from the asymptotic theory only on the basis of information on isolated atoms.¹² The Nikitin model,^{8,9} one of whose special cases is the Demkov model, has an additional free parameter which provides, in principle, a greater flexibility in reproducing the real quasimolecular terms. However, the choice of the parameters is no longer as clear and meaningful. Interesting results have been obtained recently on applying the Nikitin model to the problem of a redistribution of vacancies^{13,14} and the parameters have been selected by fitting to the known quasimolecular terms. An important advantage of the Nikitin model is the ability to

tackle also the case of crossing diabatic terms when, in contrast to the Landau-Zener model, the terms tend to constant limiting (atomic) values as atoms move apart. In investigations of the spectra this is particularly important because it makes it possible to consider in an unified manner both the atomic lines and the quasimolecular background. In view of this, we thought it would be useful to consider separately the simple Demkov model (§ 3) and the mathematically more complex Nikitin model (§ 4), and to study the relationship between them.

In the case of some interacting quasistationary terms it is exceptionally important to allow for the possibility of decay to several (degenerate) continua, which correspond either to different directions of electron emission or to different final states of a quasimolecular ion AB^+ formed by decay of a quasimolecule AB . Therefore, in § 2 we shall refine the type of interaction via a continuous spectrum and consider interference phenomena in such cases.

§2. INTERACTION OF QUASISTATIONARY STATES THROUGH DEGENERATE CONTINUUM

Let us assume that there are N discrete states $|\zeta_j\rangle$ ($j=1, 2, \dots, N$) with energies $E_{0j}(t)$ which appear against a background of continua with wave functions $|k\alpha\rangle$, where k is the momentum of the emitted particle and the index α ($\alpha=1, 2, \dots, M$) indicates the decay channel, i.e., the state in which the system remains after emergence of a particle; we shall denote the energy of this state by $\mathcal{E}_\alpha(t)$. The Hamiltonian of the system is represented in the form $H=H_0+\hat{V}$, in which the operator H_0 is diagonal in the selected basis:

$$\left. \begin{aligned} \langle \zeta_j | H_0 | \zeta_k \rangle &= E_{0j}(t) \delta_{jk}, & \langle k\alpha | H_0 | k'\beta \rangle &= (\omega + \mathcal{E}_\alpha(t)) \delta(k-k') \delta_{\alpha\beta}, \\ \langle \zeta_j | H_0 | k\alpha \rangle &= 0, & \langle k\alpha | H_0 | k'\beta \rangle &= \delta(\omega - \omega') \delta(n-n'), \\ \langle \zeta_j | k\alpha \rangle &= 0, & \langle \zeta_j | \zeta_k \rangle &= \delta_{jk}, \end{aligned} \right\} (2.1)$$

where $\omega = k^2/2$ and $n = k/|k|$ represent, respectively, the energy and direction of the emitted particle. Only the following matrix elements of the operator \hat{V} differ from zero,

$$V_{jk}(t) = \langle \zeta_j | \hat{V}(t) | \zeta_k \rangle, \quad V_{j\alpha}(k, t) = \langle \zeta_j | \hat{V}(t) | k\alpha \rangle, \quad (2.2)$$

and they describe the interaction of discrete states with one another and with continua.

Repeating in this case the procedure adopted in our earlier papers^{3,4} and using similar assumptions, we find that in the adiabatic approximation the amplitudes of populations of the discrete states $a_j(t)$ are described by the system

$$i \frac{\partial a_j(t)}{\partial t} = \sum_k (H_{eff})_{jk} a_k \quad (2.3)$$

with the effective Hamiltonian

$$(H_{eff})_{jk} = E_{0j}(t) \delta_{jk} + V_{jk}(t) - i\pi \sum_{\alpha=1}^M \int d\mathbf{n} V_{j\alpha} V_{\alpha k}. \quad (2.4)$$

The last term describes the interaction of states via a degenerate continuum; we shall represent this later in a different form. The amplitude $b_\alpha(k)$ of the population density of states in a continuum $|k\alpha\rangle$ is calculated from

$$b_\alpha(\mathbf{k}) = -i \sum_{j=1}^N \int_{t_0}^{\infty} V_{\alpha j}(\mathbf{k}, t) a_j(t) \exp \left[i\omega t - i \int \mathcal{E}_\alpha(t') dt' \right] dt, \quad (2.5)$$

where t_0 is the moment at which the initial condition is specified. Equations (2.1)–(2.5) generalize directly the results obtained earlier in Refs. 3 and 4.

For each discrete state $|\xi_j\rangle$ and a given decay channel α we shall find the “proper continuum” $|1j\omega\alpha\rangle$, i.e., such a linear combination of the functions of the continuum with a given electron energy ω that, in the absence of other discrete states, the state $|\xi_j\rangle$ decays only to this continuum. We have to assume that

$$|1j\omega\alpha\rangle = \frac{1}{c_{ij}} \int d\mathbf{n} V_{\alpha j} |k\alpha\rangle, \quad c_{ij} = \left[\int d\mathbf{n} V_{\alpha j}^* V_{\alpha j} \right]^{-1/2}, \quad (2.6)$$

where c_{ij} is the normalization coefficient. The other states of this set $|Aj\omega\alpha\rangle$ will be found by the usual orthogonalization procedure taking the state $|1j\omega\alpha\rangle$ as the first. The index A and the wave functions $|Aj\omega\alpha\rangle$ generalize, respectively, the concept of the orbital momentum and of a partial wave in the spherically symmetric case.

We thus obtain

$$\langle Aj\omega'\alpha | 1j\omega\alpha \rangle = \delta_{A1} \delta(\omega - \omega'), \quad (2.7)$$

and, on the other hand, we have

$$\begin{aligned} \langle Aj\omega'\alpha | 1j\omega\alpha \rangle &= \frac{1}{c_{ij}} \int d\mathbf{n} \langle Aj\omega'\alpha | k\alpha \rangle \langle k\alpha | \hat{V} | \xi_j \rangle \\ &= \frac{1}{c_{ij}} \langle Aj\omega'\alpha | \hat{P}_{\alpha\alpha} \hat{V} | \xi_j \rangle = \frac{1}{c_{ij}} \langle Aj\omega\alpha | \hat{V} | \xi_j \rangle \delta(\omega - \omega'), \end{aligned} \quad (2.8)$$

where $\hat{P}_{\omega\alpha}$ is the operator of the projection on the subspace of states in the continuum with an energy ω and an index α . Comparing Eqs. (2.7) and (2.8) we obtain

$$\langle Aj\omega\alpha | \mathcal{P} | \xi_j \rangle = c_{ij} \delta_{A1}, \quad (2.9)$$

which indicates that direct decay of a state $|\xi_j\rangle$ in a channel α occurs only to the proper continuum. It also follows from Eq. (2.9) that the partial width of decay of the state $|\xi_j\rangle$ in the channel α , associated with the diagonal element in the matrix of the interaction via a continuum [see Eq. (2.4)], is

$$\Gamma_{j\alpha} = 2\pi c_{ij}^2 = 2\pi |\langle 1j\omega\alpha | \mathcal{P} | \xi_j \rangle|^2 |_{\omega=E_j(t) - \mathcal{E}_\alpha(t)}. \quad (2.10)$$

Calculations similar to those given above make it possible to represent the nondiagonal elements of the interaction matrix of states $|\xi_j\rangle$ and $|\xi_k\rangle$ via a continuum:

$$\int d\mathbf{n} V_{j\alpha} V_{k\alpha}^* = \frac{1}{2\pi} (\Gamma_{j\alpha} \Gamma_{k\alpha})^{1/2} S_{jk}^{(\alpha)}, \quad (2.11)$$

where $S_{jk}^{(\alpha)}$ is found from

$$\langle 1j\omega\alpha | 1k\omega'\beta \rangle = S_{jk}^{(\alpha)} \delta_{\alpha\beta} \delta(\omega - \omega') \quad (2.12)$$

and it describes the degree of overlap of the proper continua for the two discrete states under consideration.

The energy spectrum $W(\omega)$ of electrons or photons is found by summing over all the decay channels:

$$W(\omega) = \sum_{\alpha=1}^M \int d\mathbf{n} |b_\alpha(\mathbf{k})|^2, \quad \omega = k^2/2. \quad (2.13)$$

If we can ignore the time dependence of $S_{jk}^{(\alpha)}$, we can represent the quantity $W(\omega)$ in a particularly clear form:

$$W(\omega) = \sum_{\alpha=1}^M \sum_{j,k=1}^N S_{jk}^{(\alpha)} b_{j\alpha}(\omega) b_{k\alpha}^*(\omega), \quad (2.14)$$

where

$$b_{j\alpha} = -i \int_{t_0}^{\infty} \left[\frac{\Gamma_{j\alpha}}{2\pi} \right]^{1/2} a_j(t) \exp \left[i\omega t - i \int \mathcal{E}_\alpha(t') dt' \right] dt. \quad (2.15)$$

Thus, the degree of overlap $S_{jk}^{(\alpha)}$ governs the interaction via a continuous spectrum and interference in the final state. If each state decays to its own proper continuum ($S_{jk}^{(\alpha)} = \delta_{jk}$), the energy spectrum is found by simple addition of the spectra $|b_{j\alpha}(\omega)|^2$ corresponding to the decay of each of the interacting quasistationary terms. If the proper continua overlap, then interference occurs in accordance with Eq. (2.14).

In the case of a single nondegenerate continuum ($M = 1$, $S_{jk}^{(f)} = 1$) the interference is complete, i.e., it corresponds to the addition of the amplitudes. The degree of the overlap (2.12) is governed by the problem in question and cannot be found in its general form. Therefore, we shall calculate only the amplitudes $b_{j\alpha}(\omega)$ and, for simplicity, we shall assume that there is only one decay channel so that the index α can be omitted. This allows us also to ignore the dependence $\mathcal{E}_\alpha(t)$ in Eq. (2.15) on the assumption that the energies $E_{\alpha j}(t)$ are already measured from the lower limit of the continuum. The initial conditions are specified for the adiabatic states in the limit $t_0 \rightarrow -\infty$ and they have the form [see the discussion in Ref. 4; $E_j(t)$ is the energy of the initially populated adiabatic term, i.e., the eigenvalue of H_{eff}]

$$a_j(t) = G \exp \left[-i \int_{t_0}^t E_j(t') dt' \right] \quad (2.16)$$

in the limit $t \rightarrow -\infty$. The constant G is found from the condition of matching Eq. (2.16) to the solution of a model problem which describes the process of formation of a vacancy on close approach between the atoms. Since all the amplitudes of a transition to a continuous spectrum are proportional to G , we shall simplify further treatment by assuming that $G = 1$.

We shall conclude by noting that Dalidchik *et al.*^{15,16} considered the interaction of resonance states, including the interaction via a continuous spectrum, in a number of concrete cases. The results of these investigations and those obtained in the present paper are analogous but not completely so, because in the former case the resonances are governed by the form of the potential, whereas we are considering resonances of the Feshbach type, associated with the multichannel nature of the problem.

§3. DEMKOV MODEL WITH DECAY

The Demkov model⁷ corresponds to two parallel terms with the interaction between them depending exponentially on time, so that Eq. (2.3) becomes

$$\left. \begin{aligned} i\dot{a}_1 &= \left(e + \frac{\Delta E}{2} - \frac{i}{2} \Gamma_1 \right) a_1 + \frac{1}{2} V e^{-\alpha t} a_2, \\ i\dot{a}_2 &= \frac{1}{2} V e^{-\alpha t} a_1 + \left(e - \frac{\Delta E}{2} - \frac{i}{2} \Gamma_2 \right) a_2. \end{aligned} \right\} \quad (3.1)$$

The parameter α represents the time during which the

adiabatic basis becomes modified from the molecular ($t \rightarrow -\infty$) to the atomic ($t \rightarrow +\infty$) states,⁷ and it is governed by the exchange interaction (§ 1). In contrast to the usual Demkov model, the system (3.1) includes also the interaction of discrete states with a continuum, which is assumed approximately to be independent of time ($\Gamma_{1,2} = \text{const}$). In the limit $t \rightarrow \infty$, i.e., when the atoms fly apart, the adiabatic terms reduce to atomic levels with complex energies.

$$E_{1,2} = \varepsilon_{1,2} - i/2 \Gamma_{1,2}, \quad \varepsilon_{1,2} = \varepsilon \pm \Delta \varepsilon / 2, \quad \Delta \varepsilon > 0. \quad (3.2)$$

Allowance for the interaction via a continuum in the exactly soluble Demkov model (and also in the Nikitin model) is possible only if it is proportional to $\exp(-\alpha t)$. It follows from Eq. (2.11) that the same dependence has to be assumed for $S_{jk}(t)$, which is difficult to justify physically. Therefore, we shall not introduce this interaction in the treatment below although allowance for it is basically simple. The results obtained are then known to be applicable to the frequently considered case of small widths (for example, in the case of optical spectra), when the last term can be neglected completely in the effective Hamiltonian (2.4) and the interaction with a continuum is allowed for only in the calculation of the amplitude (2.15). In general, a calculation of this kind reproduces all the qualitative features of the spectra (for example, the positions and profiles of the atomic lines, interference structure, etc.).

Assuming initially (for $t \rightarrow -\infty$) that the upper adiabatic term is populated, i.e., that the combination of states $(|\xi_1\rangle + |\xi_2\rangle)/\sqrt{2}$ is occupied, we shall write down the solutions of the system (3.1):

$$\left. \begin{aligned} a_{1,2} &= \exp[-i\varepsilon t - i/2(\Gamma_1 + \Gamma_2)t] c_{1,2}(t), \\ c_1 &= iH_{12}^{(1)}(z) \left(\frac{\pi}{2}\right)^{1/2} \left(\frac{V}{4\alpha}\right)^{1/2 + i(\varepsilon_1 + \varepsilon_2)/2\alpha} \exp\left(-\frac{\alpha t}{2} + \frac{\pi \kappa}{2}\right), \\ c_2 &= H_{21}^{(1)}(z) \left(\frac{\pi}{2}\right)^{1/2} \left(\frac{V}{4\alpha}\right)^{1/2 + i(\varepsilon_1 + \varepsilon_2)/2\alpha} \exp\left(-\frac{\alpha t}{2} + \frac{\pi \kappa}{2}\right), \\ z &= \frac{V}{2\alpha} e^{-\alpha t}, \quad \kappa = \frac{1}{2\alpha} \left[\Delta \varepsilon - \frac{i}{2}(\Gamma_1 - \Gamma_2)\right]. \end{aligned} \right\} (3.3)$$

The spectrum of the decay products is governed by the higher amplitudes, which are exact in the Demkov model with decay:

$$b_1(\omega) = -\frac{\Gamma_1^{1/2}}{4\pi\alpha} \left(\frac{V}{4\alpha}\right)^{i\omega/\alpha} \exp\left[-\frac{\pi}{2\alpha}(\varepsilon - \omega)\right] \times \Gamma\left[\frac{1}{2} + \frac{i}{2\alpha}(\varepsilon_2 - \omega)\right] \Gamma\left[\frac{i}{2\alpha}(\varepsilon_1 - \omega)\right], \quad (3.4)$$

$$b_2(\omega) = -i\frac{\Gamma_2^{1/2}}{4\pi\alpha} \left(\frac{V}{4\alpha}\right)^{i\omega/\alpha} \exp\left[-\frac{\pi}{2\alpha}(\varepsilon - \omega)\right] \times \Gamma\left[\frac{1}{2} + \frac{i}{2\alpha}(\varepsilon_1 - \omega)\right] \Gamma\left[\frac{i}{2\alpha}(\varepsilon_2 - \omega)\right]. \quad (3.5)$$

We shall next consider the case of practical interest when the characteristic decay time of the states ($\sim 1/\Gamma$) is much greater than the characteristic time of the non-adiabatic interaction of the terms ($\sim 1/\alpha$), i.e.,

$$\Gamma/\alpha \ll 1. \quad (3.6)$$

In this approximation we can separate (in this energy spectrum) the atomic lines near which the probability density has a Lorentzian maximum:

$$|b_1(\omega)|^2 = \frac{1}{2\pi} \frac{\Gamma_1}{(\varepsilon_1 - \omega)^2 + (\Gamma_1/2)^2} (1 - P), \quad (3.7)$$

$$|b_2(\omega)|^2 = \frac{1}{2\pi} \frac{\Gamma_2}{(\varepsilon_2 - \omega)^2 + (\Gamma_2/2)^2} P. \quad (3.8)$$

Thus, the positions and widths of the lines correspond to free atoms and their relative intensity is governed by the probability $P = [1 + \exp(\pi\alpha^{-1}\Delta\varepsilon)]^{-1}$ of a nonadiabatic transition in the Demkov model.^{7,10} Hence, it follows that in the case of sufficiently small widths when the integrals of the densities $|b_i(\omega)|^2$ over all the energies are governed primarily by the regions where Eqs. (3.7) and (3.8) are valid, we have the relationship

$$\int |b_2(\omega)|^2 d\omega / \int |b_1(\omega)|^2 d\omega = P/(1 - P), \quad (3.9)$$

which extends in a natural manner the concept of the transition probability to the case under consideration. We note that, in general, introduction of the transition probability concept is not a trivial matter because of the need to separate it from the effects of decay of the adiabatic terms.³ This has encouraged some authors^{17,18} to consider only the populations of quasistationary terms, but this makes it difficult to interpret the results and to use them in the adiabatic approximation calculations.

Equations (3.4) and (3.5) easily yield also approximate expressions for the line wings: subject to the condition (3.6) and if $|\varepsilon_{1,2} - \omega| \gg \Gamma_{1,2}$, we have

$$|b_1(\omega)|^2 = \frac{\Gamma_1}{8\alpha} \frac{e^{-\pi(\varepsilon - \omega)/\alpha}}{(\varepsilon_1 - \omega) \text{sh}[\pi(\varepsilon_1 - \omega)/2\alpha] \text{ch}[\pi(\varepsilon_2 - \omega)/2\alpha]}, \quad (3.10)$$

$$|b_2(\omega)|^2 = \frac{\Gamma_2}{8\alpha} \frac{e^{-\pi(\varepsilon - \omega)/\alpha}}{(\varepsilon_2 - \omega) \text{sh}[\pi(\varepsilon_2 - \omega)/2\alpha] \text{ch}[\pi(\varepsilon_1 - \omega)/2\alpha]}. \quad (3.11)$$

It follows from Eqs. (3.4) and (3.5) that both amplitudes $b_{1,2}$ have the same phase in the region of far wings of the lines $|\varepsilon_{1,2} - \omega| \gg \alpha$. Therefore, even in the case of decay to the same channel there are not interference effects in this part of the spectrum. The reduced distributions of the spectral intensities $|b_{1,2}|^2/\Gamma_{1,2}$ are also the same in the far wings of the lines:

$$\frac{|b_1|^2}{\Gamma_1} = \frac{|b_2|^2}{\Gamma_2} \approx \frac{\pi}{4\alpha} \frac{1}{(\varepsilon - \omega) \text{sh}[\pi(\varepsilon - \omega)/\alpha]} \exp\left[-\frac{\pi}{\alpha}(\varepsilon - \omega)\right], \quad (3.12)$$

which is obtained quite simply from Eqs. (3.10) and (3.11). These features of the spectra are due to the fact that the far wings of the lines are due to decay at $t < 0$, when both atomic states are strongly coupled and the initial condition is such that they decay as a single quasimolecular state. Naturally, the part of the spectrum formed in this way should be identical with the spectrum as a result of decay of a single exponential term¹⁾:

$$E(t) = E_1 + C e^{-\alpha t}, \quad (3.13)$$

$$b_{\text{exp}}(\omega) = \frac{1}{\alpha} \left(\frac{\Gamma}{2\pi}\right)^{1/2} \left(\frac{i\alpha}{C}\right)^{i(\varepsilon_1 - \omega)/\alpha} \Gamma\left[\frac{i}{\alpha}(\varepsilon_1 - \omega)\right], \quad (3.14)$$

where the parameters have the values $\alpha = \alpha$ and $C = V$.

The behavior of the terms is described approximately by the exponential function (3.13) also in the other case corresponding to $t > 0$, when the profile is formed in the direct vicinity of atomic lines. In this case, we have $\alpha = 2\alpha$, $C = V^2/4\Delta\varepsilon$, and the characteristic dependence on ω in the form of the gamma function, corres-

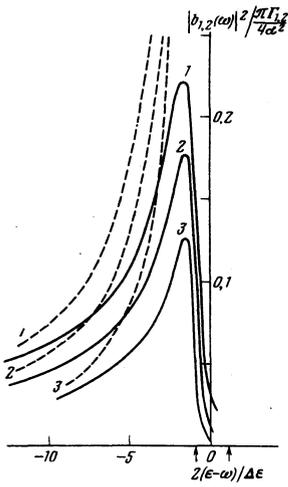


FIG. 1. Dependences of the quasimolecular background in the Demkov model [Eqs. (3.10) and (3.11)] for various values of the parameter $\xi = \pi \Delta \epsilon / 4\alpha$. The continuous curves represent $|b_2(\omega)|^2$ and the dashed curves correspond to $|b_1(\omega)|^2$; 1) $\xi = 1.5$; 2) $\xi = 2$; 3) $\xi = 3$. The centers of the Lorentzian parts of the spectra for $|b_{1,2}|^2$ are located at $2(\epsilon - \omega) / \Delta \epsilon = \pm 1$. A change in ξ by unity reduces the transition probability P by two orders of magnitude.

ponding to Eq. (3.14), is separated in a natural manner also in the exact amplitude (3.4) for $|\epsilon_1 - \omega| \ll \Delta \epsilon$.

The graphs of $4\alpha^2 |b_{1,2}|^2 / \pi \Gamma_{1,2}$ based on Eqs. (3.10) and (3.11) are plotted in Fig. 1 for various values of the nonadiabaticity parameter $\xi = \pi \Delta \epsilon / 4\alpha$. An increase in the nonadiabaticity reduces the intensity of the Lorentzian part in the spectrum $|b_2|^2$ in the same way as the transition probability, but there is no significant change in the quasimolecular background. It should be noted that in the case of detuning $\Delta \epsilon \neq 0$ the spectrum of $|b_2|^2$ should have a sharp maximum in the Lorentzian part at $\omega \approx \epsilon_2$ as well as a broad maximum (satellite) at $\omega \approx \epsilon_1$, the latter being associated with the quasimolecular nature of the wings of the spectral line (see Fig. 1). A satellite is observed most conveniently for the decay of states to various continua or for the decay of states to a single continuum but subject to the condition $\Gamma_1 \ll \Gamma_2$.

§4. SPECTRA IN THE NIKITIN MODEL

The Nikitin model involves the following approximation for the matrix elements of the effective Hamiltonian:

$$\left. \begin{aligned} (H_{eff})_{11,22} &= H_{11,22} = E_{1,2} \pm \frac{1}{2} \Delta \epsilon \cos \theta e^{-\alpha t}, \\ (H_{eff})_{12} &= -\frac{1}{2} \Delta \epsilon \sin \theta e^{-\alpha t}, \\ E_{1,2} &= \epsilon_{1,2} - \frac{1}{2} i \Gamma_{1,2} \\ &= \epsilon \pm \frac{1}{2} \Delta \epsilon - \frac{1}{2} i \Gamma_{1,2}, \quad 0 \leq \theta \leq \pi. \end{aligned} \right\} \quad (4.1)$$

The parameters $\Delta \epsilon$, $\Gamma_{1,2}$ and α are the same as in the Demkov model; following § 3, we shall simplify the treatment by ignoring the interaction of terms via a continuous spectrum. The meaning of the additional parameter becomes clear if we write down the expressions for the adiabatic states $|\Psi_{I,II}\rangle$ in the limits $t \rightarrow \pm \infty$:

$$\left. \begin{aligned} |\Psi_I\rangle &= \cos \frac{\theta}{2} |\zeta_1\rangle - \sin \frac{\theta}{2} |\zeta_2\rangle, \\ |\Psi_{II}\rangle &= \sin \frac{\theta}{2} |\zeta_1\rangle + \cos \frac{\theta}{2} |\zeta_2\rangle, \quad t \rightarrow -\infty; \\ |\Psi_I\rangle &= |\zeta_1\rangle, \quad |\Psi_{II}\rangle = |\zeta_2\rangle, \quad t \rightarrow +\infty. \end{aligned} \right\} \quad (4.2)$$

The energies of the adiabatic terms are

$$\begin{aligned} E_{I,II} &= \epsilon - \frac{i}{4} (\Gamma_1 + \Gamma_2) \\ &\pm \frac{1}{2} \left\{ \left[\Delta \epsilon + \Delta \epsilon \cos \theta e^{-\alpha t} - \frac{i}{2} (\Gamma_1 - \Gamma_2) \right]^2 + \Delta \epsilon \sin^2 \theta e^{-2\alpha t} \right\}^{1/2}. \end{aligned} \quad (4.3)$$

For $\theta = \pi/2$ the problem reduces to the Demkov model, whereas for $\theta = 0$ or π we obtain two noninteracting terms dependent exponentially on time: for $\theta = 0$ they are repulsive, whereas for $\theta = \pi$ they cross.

The solution of the system (2.3) corresponding to the initial population of the upper adiabatic term (state $|\Psi\rangle$) is of the form²⁾

$$\left. \begin{aligned} a_1(t) &= \cos \frac{\theta}{2} W_{\kappa, \mu}(z) \exp \left[-\frac{i}{2} \int_0^t (H_{11} + H_{22}) dt' + i \frac{\pi}{2} \kappa \right], \\ a_2(t) &= -\sin \frac{\theta}{2} W_{\kappa, \mu+1}(z) \exp \left[-\frac{i}{2} \int_0^t (H_{11} + H_{22}) dt' + i \frac{\pi}{2} \kappa \right]; \\ z &= -\frac{i \Delta \epsilon}{\alpha} e^{-\alpha t}, \quad \kappa = i \frac{\cos \theta}{2\alpha} (\Delta \epsilon + \gamma), \\ \mu &= -\frac{1}{2} + \frac{i}{2\alpha} (\Delta \epsilon + \gamma), \quad \gamma = -\frac{i}{2} (\Gamma_1 - \Gamma_2), \end{aligned} \right\} \quad (4.4)$$

where $W_{\kappa, \mu}$ is the Whittaker function.¹⁹ In the Nikitin model the amplitudes of a transition to a continuous spectrum are expressed in terms of the hypergeometric and gamma functions:

$$\begin{aligned} b_1(\omega) &= \left(\frac{\Gamma_1}{2\pi} \right)^{1/2} \frac{\cos(\theta/2)}{\alpha} \left(\frac{2\alpha}{\Delta \epsilon} \right)^{\mu + 1/2} \frac{\Gamma(\mu + s + 1/2) \Gamma(-\mu + s + 1/2)}{\Gamma(s - \kappa + 1)} \\ &\times F(\mu + s + 1/2, \mu - \kappa + 1/2, s - \kappa + 1, -1) \exp[i'2\pi(s + \kappa)], \end{aligned} \quad (4.6)$$

$$\begin{aligned} b_2(\omega) &= -\left(\frac{\Gamma_2}{2\pi} \right)^{1/2} \frac{\sin(\theta/2)}{\alpha} \left(\frac{2\alpha}{\Delta \epsilon} \right)^{\mu + 1/2} \frac{\Gamma(\mu + s + 3/2) \Gamma(-\mu + s - 1/2)}{\Gamma(s - \kappa + 1)} \\ &\times F(\mu + s + 3/2, \mu - \kappa + 3/2, s - \kappa + 1, -1) \exp[i'2\pi(s + \kappa)], \end{aligned} \quad (4.7)$$

$$s = \frac{i}{\alpha} \left[\epsilon - \omega - \frac{i}{4} (\Gamma_1 + \Gamma_2) \right]. \quad (4.8)$$

Reduction to the Demkov model in the spectra is given in Sec. 1 of the Appendix. In the limiting case of $\theta = 0$ we can easily show on the basis of Eq. (A.2) that the amplitudes $b_1(\omega)$ are proportional to the amplitude of the exponential term (3.14) and then $b_2 = 0$; in the other limiting case of $\theta = \pi$ we have conversely $b_1 = 0$ and b_2 reduces to Eq. (3.14) by means of Eq. (A.3).

As in the Demkov model, atomic lines appear in the spectrum because of decay after a long time t . The expressions (3.7) and (3.8) are obtained, subject to the condition (3.6), by means of Eq. (A.5) in the Appendix and the approximation $\Gamma(\mu + s + \frac{1}{2}) \approx \alpha / i(E_1 - \omega)$, assuming that P is now the probability of a nonadiabatic transition in the Nikitin model without the decay:

$$P = \frac{\text{sh}[\pi \alpha^{-1} \Delta \epsilon \sin^2(\theta/2)]}{\text{sh}(\pi \Delta \epsilon / \alpha)} \exp\left(-\frac{\pi \Delta \epsilon}{\alpha} \cos^2 \frac{\theta}{2}\right). \quad (4.9)$$

We shall now consider the spectrum in the region of the line wings, which implies (for the b_1 amplitude) those energies of the emitted particles which satisfy the conditions $|\epsilon_1 - \omega| / \alpha > 1$, $|\epsilon_1 - \omega| > \Delta \epsilon$; the condition (3.6) is also assumed to be fulfilled. In Sec. 2 of the Appendix it is shown that in this case the spectrum can be described by the amplitude (A.7):

$$b_1(\omega) \approx \left(\frac{\Gamma_1}{2\pi}\right)^{1/2} \frac{\cos(\theta/2)}{\alpha} \left(\frac{\alpha}{\Delta\varepsilon}\right)^{(\varepsilon-\omega)/\alpha} 2^{i(\varepsilon_1-\omega)/\alpha} \quad (4.10)$$

$$\times \frac{\Gamma[i(\varepsilon_1-\omega)/\alpha] \Gamma[1+i(\varepsilon_2-\omega)/\alpha]}{\Gamma[1+i\alpha^{-1}(\varepsilon-\omega-1/2\Delta\varepsilon \cos\theta)]} \exp\left[-\frac{\pi}{2\alpha} \left(\varepsilon-\omega + \frac{\Delta\varepsilon}{2} \cos\theta\right)\right].$$

The form of the spectrum simplifies further in the region which is separated from the line center by more than $\Delta\varepsilon$ ($\Delta\varepsilon \ll |\varepsilon_1 - \omega|$):

$$|b_1(\omega)|^2 = \frac{\Gamma_1 \cos^2(\theta/2)}{2\alpha(\varepsilon-\omega) \text{sh}[\pi(\varepsilon-\omega)/\alpha]} \exp\left[-\frac{\pi}{\alpha}(\varepsilon-\omega)\right], \quad (4.11)$$

and, finally, in the far wings of the lines $|\varepsilon - \omega|/\alpha \gg 1$, we have

$$|b_1(\omega)|^2 = \frac{\Gamma_1 \cos^2(\theta/2)}{2\alpha(\varepsilon-\omega)} \begin{cases} 2 \exp[-2\pi(\varepsilon-\omega)/\alpha], & \varepsilon > \omega, \\ -2, & \varepsilon < \omega. \end{cases} \quad (4.12a)$$

$$(4.12b)$$

For b_2 , the wings of the spectrum $|\varepsilon_2 - \omega|/\alpha > 1$, $|\varepsilon_2 - \omega| > \Delta\varepsilon$ can be described by Eqs. (A.9), (4.11), and (4.12) replacing $\Gamma_1 \cos^2(\theta/2)$ with $\Gamma_2 \sin^2(\theta/2)$ and $\varepsilon_{1,2}$ with $\varepsilon_{2,1}$.

We note that Eq. (4.11) and the analogous expression for $|b_2|^2$ are independent of θ , with the exception of the factors $\cos^2(\theta/2)$ and $\sin^2(\theta/2)$, which we shall not consider here. Thus, in the energy ranges in question the spectra of both components have the same form, which is identical with the form of the spectrum for a single exponential term ($\theta=0$); this can be checked by direct analysis of the limit of the expression (4.6). The reason is that in the case of sufficiently large values of $|t|$ for $t < 0$ the term (4.3) behaves exponentially and is independent of θ : $E_1 \approx \varepsilon + \frac{1}{2}\Delta\varepsilon \exp(-\alpha t)$. The factor $\cos^2(\theta/2)$ is simply the square of the coefficient in the expansion of the corresponding adiabatic wave function in terms of the basis of diabatic states; for the same reason the amplitude b_2 acquires the factor $\sin^2(\theta/2)$. The regions $\varepsilon < \omega$ and $\varepsilon > \omega$ in Eq. (4.12) correspond to the classically allowed and forbidden populations of the states in the continuum, as discussed in detail in Ref. 4. We shall stress once again that these regions are the same for $|b_1|^2$ and $|b_2|^2$.

It is interesting that Eqs. (A.7), (A.8) and the analogous (in the case of b_2) Eq. (A.9) can be regarded as convenient approximate expressions for the spectrum with all values of ω in the Nikitin model. It follows from Eq. (A.2) that these formulas are valid in the region of the wings of the spectrum, as well as near the centers of atomic lines. In the latter case the expressions (A.8) and (A.9) reduce, for $\Gamma_{1,2}/\alpha \ll 1$, to Eqs. (3.7) and (3.8), respectively, in which the transition probability is now given by Eq. (4.9). If the condition $\pi\Delta\varepsilon/2\alpha \ll 1$ is satisfied, we can check that Eqs. (4.10), (A.8), and (A.9) describe correctly the spectrum for all values of ω except in regions of width of the order of $\Gamma_{1,2}$ near $\omega = \varepsilon_{1,2}$ in the case of parallel diabatic terms [Demkov model, Eqs. (3.10) and (3.11)]. In the case of a weak interaction ($\theta \approx 0$), Eq. (A.8) is also valid for all ω with the exception $|\varepsilon_1 - \omega| \leq \Gamma_1$ [see Eq. (A.2) in the Appendix]. It follows from Eq. (A.8) that the spectrum of the "strong" component associated with the decay of a state $|\xi_1\rangle$ is then

$$|b_1(\omega)|^2 = \frac{\Gamma_1}{2\pi\alpha^2 \pi\alpha^{-1}(\varepsilon_1-\omega) \text{sh}[\pi(\varepsilon_1-\omega)/\alpha]} \exp\left[-\frac{\pi}{\alpha}(\varepsilon_1-\omega)\right]. \quad (4.13)$$

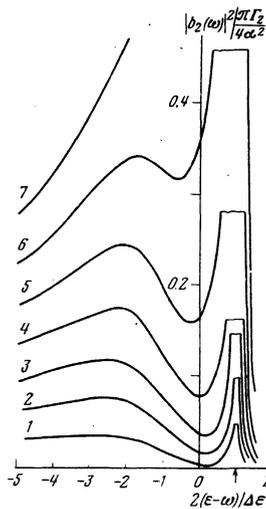


FIG. 2. Dependences of the quasimolecular background $|b_2(\omega)|^2$ in the Nikitin model [Eq. (A.8)] for various values of $\cos\theta$ and $\xi = \pi\Delta\varepsilon/4\alpha = 1$: 1) $\cos\theta = \frac{3}{4}$; 2) $\cos\theta = \frac{1}{2}$; 3) $\cos\theta = \frac{1}{4}$; 4) $\cos\theta = 0$; 5) $\cos\theta = -\frac{1}{4}$; 6) $\cos\theta = -\frac{1}{2}$; 7) $\cos\theta = -\frac{3}{4}$.

In the opposite case of term crossing ($\theta \approx \pi$), the spectrum of the "strong" component is obtained from Eq. (A.9) and has the form (4.13) where Γ_1 and ε_1 are replaced with Γ_2 and ε_2 .

The energy dependence of the reduced spectral intensity, obtained from Eq. (A.8), is plotted in Fig. 2 and can be used to study the nature of the influence of the parameter θ on the form of the spectrum. On increase of θ the intensity $|b_2|^2$ rises because of an increase in the probability of a nonadiabatic transition but the satellite is more pronounced in the case of the strongest coupling between diabatic states $\theta \approx \pi/2$.

§5. CONCLUSIONS

The usefulness of the models considered in §§ 3 and 4 is greater than suggested by the formal conditions of their validity, because they can be used to study various asymptotic parts of the spectra (atomic lines and their broadening, satellites, far wings in the spectra) and to determine how the spectra are formed as a result of decay of quasistationary states.

In the case of close approach of the atoms the interaction gives rise to a vacancy whose evolution in time can be described by an adiabatic wave function. The decay of this wave function in the region of a strong interaction of diabatic states ($t < 0$ in the models considered above) produces the line wings; in this case, the part of the spectrum formed by the classically forbidden transitions (4.12a) is proportional to the exchange interaction parameter α , and the part corresponding to classically allowed transitions is governed by the difference between the energies of vacancy transitions in coupled and separated atoms. In the range of classically allowed transitions, as pointed out in §§ 3 and 4, a satellite may form and it should be experimentally observable in the case of those states whose interaction can be described by the Demkov model and which satisfy $\Gamma_1 \ll \Gamma_2$. The strongest features of these spectra are the broadened atomic lines on a background of a quasimolecular con-

tinuum, which disappear in this continuum away from the line center.

It is worth considering separately the range of strong interaction between adiabatic terms. In the Demkov model there are no significant features associated with this interaction because adiabatic terms depend fairly smoothly on time. This is the considerable difference from the Landau-Zener case or from the Nikitin model in the $\pi/2 \leq \theta \leq \pi$ case, when adiabatic terms in the pseudocrossing region have a sharp inflection. The most easily interpreted feature appears on crossing of an initially populated diabatic term characterized by a small width and a rapidly decaying diabatic term; here, the decay is included effectively in the region of term pseudocrossing and it terminates almost immediately because of the considerable width of the second term. This gives rise to a group of monoenergetic electrons of new type in the spectrum (see a figure in Ref. 4; the captions to figures in Ref. 4 should be interchanged) and this group is retained also when summation is carried out over the impact parameters of the colliding atomic particles. Observation of a corresponding maximum in the spectrum makes it possible to determine experimentally the energy of the terms at the point of their pseudocrossing.

It follows from § 2 that each solution of the problem of determination of the amplitudes $b_j(\omega)$ gives in fact a whole class of energy spectra, depending on the nature of the overlap of the continuum eigenstates and on interference. As in Ref. 4, we are concerned here mainly with the behavior of the quantities $|b_j|^2$, whose sum represents directly the spectrum when states decay to nonoverlapping continua. In the other limiting case of decay to one common continuum the addition of the amplitudes produces a further interference structure in the range of energies between the atomic levels and rapid oscillations in the spectrum between the envelopes $(|b_1| + |b_2|)^2$ and $(|b_1| - |b_2|)^2$. A situation of this kind is considered in Ref. 4.

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APPENDIX

1. In the case of parallel diabatic terms, we have $\theta = \pi/2$, and, consequently, $\kappa = 0$. The relationship between the parameters of the hypergeometric functions in Eqs. (4.6) and (4.7) is then such that we can use one of the quadratic transformations of the hypergeometric function [see Ref. 19, §2.1.5, Eq. (25)]:

$$F\left(\mu + s + \frac{1}{2}, \mu + \frac{1}{2}, s + 1, -1\right) = \frac{2^{-\mu-s-1/2} \Gamma(1+s) \Gamma(1/2)}{\Gamma(s/2 - \mu/2 + 1/2) \Gamma(s/2 + \mu/2 + 1/2)}. \quad (\text{A.1})$$

Substitution of Eq. (A.1) into Eq. (4.6) and application of the formula for doubling of the argument of the gamma function to $\Gamma(\mu + s + \frac{1}{2})$ and $\Gamma(-\mu + s + \frac{1}{2})$ gives Eq. (3.4). We can similarly simplify Eq. (4.7).

In the limiting case of noninteracting terms with $\theta = 0$ and π , the formulas for the amplitudes (4.6) and (4.7) can be simplified greatly if we bear in mind that $\mu - \kappa + \frac{1}{2} = 0$ for $\theta = 0$, so that

$$F(\mu + s + 1/2, \mu - \kappa + 1/2, s - \kappa + 1, -1) = 1, \quad (\text{A.2})$$

and for $\theta = \pi$ we have $\mu + s + \frac{3}{2} = s - \kappa + 1$, so that

$$F(\mu + s + 3/2, \mu - \kappa + 3/2, s - \kappa + 1, -1) = 2^{-\mu + \kappa - 3/2}. \quad (\text{A.3})$$

2. We shall now find the values of the parameters of the hypergeometric function in Eq. (4.6) by means of Eqs. (4.5) and (4.8):

$$F(\mu + s + 1/2, \mu - \kappa + 1/2, s - \kappa + 1, -1) = F\left[\frac{i}{\alpha}(E_1 - \omega), \frac{i}{\alpha}(\Delta\varepsilon + \gamma) \sin^2 \frac{\theta}{2}, 1 + \frac{i}{\alpha}(E_1 - \omega) - \frac{i}{\alpha}(\Delta\varepsilon + \gamma) \cos^2 \frac{\theta}{2}, -1\right], \quad (\text{A.4})$$

where $E_1 = \varepsilon + \frac{1}{2}\Delta\varepsilon - i\Gamma_1/2 = \varepsilon_1 - i\Gamma_1/2$. If either of the conditions $|\varepsilon_1 - \omega|/\alpha \ll 1$ (corresponding to the part of the spectrum near an atomic line) or $\theta \ll 1$ (weak coupling between the states) is satisfied, an approximate expression for the amplitude can be obtained using the formula

$$F \approx 1 + O\left(\frac{(E_1 - \omega)(\Delta\varepsilon + \gamma) \sin^2(\theta/2)}{\alpha^2}\right), \quad (\text{A.5})$$

which follows from the definition of the hypergeometric series. In the regions of the wings of the lines $|\varepsilon_1 - \omega|/\alpha \gg 1$ and $|\varepsilon_1 - \omega|/\alpha > \Delta\varepsilon$, the approximate expression for the amplitude can be obtained if we go over in Eq. (A.4) to the hypergeometric function of the argument $z/(z-1)$ [see Ref. 19, § 2.1.4, Eq. (22)]. We then obtain

$$F \approx 2^\alpha \left[1 + O\left(\frac{1}{1 + i\alpha^{-1}(E_1 - \omega) - \alpha^{-1}(\Delta\varepsilon + \gamma) \cos^2(\theta/2)}\right) \right], \quad \left. \begin{aligned} q = -\frac{i}{\alpha}(\Delta\varepsilon + \gamma) \sin^2 \frac{\theta}{2}, \end{aligned} \right\} \quad (\text{A.6})$$

and the approximate expression for the amplitude in the region of the line wings becomes

$$b_1(\omega) \approx \left(\frac{\Gamma_1}{2\pi}\right)^{1/2} \frac{\cos(\theta/2)}{\alpha} \left(\frac{\alpha}{\Delta\varepsilon}\right)^{i(\varepsilon - \omega)/\alpha} \frac{\Gamma[i(\varepsilon_1 - \omega)/\alpha] \Gamma[1 + i(\varepsilon_2 - \omega)/\alpha]}{\Gamma[1 + i\alpha^{-1}(\varepsilon - \omega - 1/2\Delta\varepsilon \cos \theta)]} \times 2^{i(\varepsilon_1 - \omega)/\alpha} \exp\left[-\frac{\pi}{2\alpha}(\varepsilon - \omega + \frac{\Delta\varepsilon}{2} \cos \theta)\right]. \quad (\text{A.7})$$

We should note specially that it follows from Eqs. (A.5) and (A.6) that when $\Gamma_{1,2}/\alpha \ll 1$ and when one of the conditions $|\varepsilon_1 - \omega|/\alpha \ll 1$ and $\theta \ll 1$ or $|\varepsilon_1 - \omega|/\alpha \gg 1$ and $|\varepsilon_1 - \omega| > \Delta\varepsilon$ is satisfied, the modulus of the first term in the expression (A.4) in terms of the small parameter $(E_1 - \omega)/\alpha$ or θ or $\alpha/(E_1 - \omega)$ is the same and equal to unity. It therefore follows from Eq. (4.6) that in these cases

$$|b_1(\omega)|^2 = \frac{\Gamma_1}{2\alpha} \frac{\cos^2(\theta/2)}{(\varepsilon_1 - \omega) \text{sh}[\pi(\varepsilon_1 - \omega)/\alpha]} \frac{\varepsilon_2 - \omega}{\text{sh}[\pi(\varepsilon_2 - \omega)/\alpha]} \times \frac{\text{sh}[\pi\alpha^{-1}(\varepsilon - \omega - 1/2\Delta\varepsilon \cos \theta)]}{\varepsilon - \omega - 1/2\Delta\varepsilon \cos \theta} \exp\left[-\frac{\pi}{\alpha}(\varepsilon - \omega + \frac{\Delta\varepsilon}{2} \cos \theta)\right]. \quad (\text{A.8})$$

Similarly, we can show that the modulus of the first term of the expansion $F(\mu + s + \frac{3}{2}, \mu - \kappa + \frac{3}{2}, s - \kappa + 1, -1)$ in terms of one of the small parameters $(E_2 - \omega)/\alpha$, $(\pi - \theta)$, $\alpha/(E_2 - \omega)$ is 2^{-1} and it then follows from Eq. (4.7) that the first term of the expansion of $|b_2|^2$ in terms of one of these small parameters is

$$|b_2(\omega)|^2 = \frac{\Gamma_2}{2\alpha} \frac{\sin^2(\theta/2)}{(\varepsilon_2 - \omega) \text{sh}[\pi(\varepsilon_2 - \omega)/\alpha]} \frac{\varepsilon_1 - \omega}{\text{sh}[\pi(\varepsilon_1 - \omega)/\alpha]} \times \frac{\text{sh}[\pi\alpha^{-1}(\varepsilon - \omega - 1/2\Delta\varepsilon \cos \theta)]}{\varepsilon - \omega - 1/2\Delta\varepsilon \cos \theta} \exp\left[-\frac{\pi}{\alpha}(\varepsilon - \omega + \frac{\Delta\varepsilon}{2} \cos \theta)\right]. \quad (\text{A.9})$$

- ¹This amplitude was given by us earlier⁴ in specifying the initial condition at a finite time t_0 .
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