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EVALUATION OF THE ROTATING WAVE APPROXIMATION INFLUENCE ON POLARIZATION SPECTRA OF A TWO-LEVEL SYSTEM IN A POLYCHROMATIC FIELD

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Abstract. Polarization spectra of a two-level system in a polychromatic field were obtained in two cases: using the rotating wave approximation and without using this approximation. The obtained spectra were compared using two indicators: the average deviation across the entire frequency range and the deviation at the transition frequency. Both indicators allow quantitative assessment of the distortion in polarization spectra introduced by the application of the rotating wave approximation. The dependencies of the above indicators on key model parameters were obtained – on the central frequency, detuning, and spectral width of the applied polychromatic field. The obtained dependencies allow evaluating the applicability limits of the rotating wave approximation for a given level of acceptable distortions in the polarization spectrum.

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1. INTRODUCTION

The rotating wave approximation (RWA) is a method of simplifying systems of differential equations describing a physical model, used in quantum optics and quantum magnetic phenomena. In the system of equations, components containing high-frequency operators are discarded, and when solving the system, only low-frequency processes that occur slowly over time are taken into account. Typically, the possibility of separating the processes existing in the model into high-frequency and low-frequency components is related to the presence of close frequencies, such as the transition frequency between atomic energy levels and the frequency of the acting field in quantum optics. The difference between these closely spaced frequencies corresponds to the low-frequency component, while their sum represents the high-frequency component.

The work of Bloch and Siegert [3] is considered [1, 2] the first successful application of the rotating wave approximation, which examines the Schrödinger equation for a particle with spin 1/2 in an alternating magnetic field with strong perpendicular constant bias magnetization. In this model, the Larmor frequency of the bias field and the frequency of the acting alternating field serve as close frequencies. Magnetic resonance occurs when these frequencies coincide, where the probability of transition between states with different spin projections on the direction of the bias field increases significantly. In work [3], the difference between the two frequencies is indeed assumed to be small compared to the frequencies themselves; however, in addition to this limit, two other important assumptions are used in deriving the approximate solution of the Schrödinger equation – the small deviation of the acting field's polarization from circular and the small amplitude of the acting field compared to the magnitude of the bias field. In a certain sense, work [3] can be considered not only as an example of successful application of the rotating wave approximation but also as the first attempt to circumvent it, since in deriving the correction to the resonant frequency value, later called the Bloch-Siegert shift, small quantities inversely proportional to the frequency of the acting field are taken into account.

The authors of work [3], neither in it nor in their subsequent works, use the term "rotating wave approximation" to denote the method used to find an approximate solution to the equation under consideration. However, the roots of the term's origin can be traced precisely to [3]: if the acting field has circular polarization, i.e., rotates in a plane perpendicular to the direction of the magnetizing field, the Schrödinger equation admits an exact analytical solution, previously obtained by Rabi [4]. If there is a deviation from circular polarization, then an exact solution becomes impossible and, to find an approximate solution, it becomes necessary to resort to additional assumptions, in particular – the smallness of the deviation of the acting field frequency from the Larmor frequency of the magnetizing field. Thus, Rabi's solution is a zero-order solution in the rotating wave approximation for the problem considered in [3], while Bloch and Siegert investigated first-order corrections in the said approximation. Rabi in [4], of course, did not consider any rotating wave approximation, since he initially solved a narrower problem with circular polarization of the acting field.

Subsequently, beyond the realm of quantum magnetic phenomena, the rotating wave approximation began to be applied in quantum optics as well. The possibility of such a methodological transfer was due to the identity of equations mathematically describing seemingly completely different physical processes (see [5], Sect. III.6). In quantum optics, the close frequencies became the frequency of the incident electromagnetic radiation and the transition frequency between atomic energy levels. However, for a long time, there was no consensus on what to call this frequently used approximation. Some researchers used the term "resonant approximation" [6]. Others designated the approach as rotating field approximation, which seems quite justified when dealing with quantum magnetic phenomena (sometimes the phrase "rotating field approximation" appears in modern articles [7, 8], but in these cases it can probably be considered a terminological error). Often, researchers did not designate the used approximation at all, limiting themselves to the mathematical formulation of the small frequency difference limit [9]. Lamb can be considered one of the first proponents of the term in its modern form, he used the term "rotating wave approximation" in his 1957 paper [10] on microwave spectroscopy of the helium atom. Gradually, especially after the publication of Lamb's "Theory of Optical Masers" [11] and Haken's handbook [5], the term "rotating wave approximation" began to replace all other variants and became generally accepted in the 1970s.

Currently, the rotating wave approximation is actively used in calculations of models in quantum optics and quantum magnetic phenomena. For example, when working with nanophotonics models [12] such as quantum dots [13, 14] and quantum wires [15]; in describing processes occurring in optoelectronic devices [16]; in studying transitions in Rydberg atoms in external fields [18], etc. However, in the vast majority of works, quantitative assessments of the impact of the rotating wave approximation on the final result are not provided. This is quite understandable, as it implies performing calculations without using the rotating wave approximation, which in most situations can be very difficult due to the absence of an exact analytical solution and the large volume of necessary computations when implementing numerical methods for solving the problem.

In this work, we consider a two-level atomic system in a polychromatic field. This model allows for an analytical solution only in the rotating wave approximation and at zero detuning of the central frequency of the acting field from the transition frequency [17]; in other cases, only a numerical solution is available. A distinctive feature of this model is that the spectral range of the acting field can be very wide, and the limits of applicability of the rotating wave approximation are significantly affected not only by the magnitude of detuning of the central frequency of the acting field from the transition frequency but also by the number of harmonics in the polychromatic field.

We evaluate the disturbance in polarization spectra arising from the use of the rotating wave approximation using two indicators: the spectral amplitude deviation averaged over the entire frequency range and the spectral amplitude deviation at the transition frequency. Dependencies of both indicators on key model parameters, such as the central frequency of the acting field, detuning, and number of polychromatic components, have been obtained. These dependencies allow determining whether the rotating wave approximation is applicable or not for a specific set of model parameters, given an acceptable deviation value. Through extrapolation, specific conclusions can also be drawn for parameter sets where direct calculations were not performed. We propose that the presented methodology for evaluating the impact of the rotating wave approximation can also be applied to other quantum optics models.

This paper is organized as follows. Section 2 discusses the density matrix equation for a multilevel atomic system in a polychromatic field, as well as a simplified version of the equation arising in the rotating wave approximation. Section 3 presents details of the numerical calculations of the original and simplified equations and introduces criteria for comparing polarization spectra obtained from solving these equations. Results of calculations, particularly the dependencies of spectrum distortion magnitudes arising from the use of the rotating wave approximation on key model parameters, are discussed in Section 4. Conclusions are presented in Section 5.

2. ROTATING WAVE APPROXIMATION IN THE CASE OF A TWO-LEVEL SYSTEM IN A POLYCHROMATIC FIELD

Let us consider the density matrix equation describing a two-level system – a stationary atom in a polychromatic field in the dipole approximation:

$$i\hbar \frac{d\rho}{dt} = \left[H, \rho\right] - i\hbar\Gamma \cdot \rho + i\hbar L, \tag{1}$$

where the interaction Hamiltonian

$$H = E + V = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} + \begin{pmatrix} 0 & V_{12} \\ V_{12}^* & 0 \end{pmatrix}$$

contains time-dependent off-diagonal elements

$$\begin{aligned} V_{12} &= \hbar\tilde{V}_{12} e^{iw_{12}t} + \hbar\tilde{V}_{12}^* e^{-iw_{12}t}, \\ \tilde{V}_{12}(t) &= \frac{\Omega_{120}}{2} + \sum_{m=1}^{M_{12}} \Omega_{12m} \cos(m\Delta_{12}t), \end{aligned} \tag{2}$$

of the matrix

$$\Gamma = \begin{pmatrix} \gamma_1 & \Gamma_{12} \\ \Gamma_{12}^* & \gamma_2 \end{pmatrix}, \quad L = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$$

respectively relaxation and pumping matrices, and the symbol “·” corresponds to element-wise multiplication of matrices. In (2) Δ_{12} denotes the spectral interval between components of the polychromatic field at the transition between levels with indices 1 and 2; M_{12} determines the number of spectral field components; Ω_{12m}, $m = 0, 1, \ldots, M_{12}$ – their amplitudes.

Let's perform a transformation that shifts the spectrum of off-diagonal elements of the density matrix by a frequency determined by the difference of the corresponding energy levels:

$$\rho = \tilde{\rho} \cdot e^{i\omega t}, \tag{3}$$

where the transformation matrix has the following form:

$$e^{i\omega t} = \begin{pmatrix} 1 & e^{i\omega_{12}t} \\ e^{i\omega_{21}t} & 1 \end{pmatrix},$$

$$\omega = \begin{pmatrix} 0 & \omega_{12} \\ \omega_{21} & 0 \end{pmatrix},$$

$$\omega_{12} = \frac{E_2 - E_1}{\hbar}.$$

After substituting (3) into (1) and element-wise multiplication of both sides of the equation by $e^{-i\omega t}$ taking into account the value of the commutator of the diagonal matrix E with the density matrix,

$$\left[E, \rho\right] = -\hbar\omega \cdot \rho,$$

and the equality

$$L \cdot e^{-i\omega t} = L$$

leads us to the following equation:

$$i\hbar \frac{d\tilde{\rho}}{dt} = \left[V, \tilde{\rho} \cdot e^{i\omega t}\right] \cdot e^{-i\omega t} - i\hbar\Gamma \cdot \tilde{\rho} + i\hbar L.$$

Since the elements of the matrix ω are determined by the difference in energy levels, for any three indices $1 \le j, k, l$: we have

$$\omega_{jk} + \omega_{kl} + \omega_{lj} = 0.$$

This allows us to put the exponential under the commutator sign:

$$\frac{d\tilde{\rho}}{dt} = -\frac{i}{\hbar}\left[V \cdot e^{-i\omega t}, \tilde{\rho}\right] - \Gamma \cdot \tilde{\rho} + L,$$

and, substituting (2), we obtain

$$\frac{d\tilde{\rho}}{dt} = -i\left[\tilde{V} \cdot e^{i(w-\omega)t}, \tilde{\rho}\right] - i\left[\tilde{V}^* \cdot e^{-i(w+\omega)t}, \tilde{\rho}\right] - \\ - \Gamma \cdot \tilde{\rho} + L. \tag{4}$$

In the resulting expression, there are two commutators with different frequency characteristics. The first commutator contains a slowly varying operator over time – the characteristic frequencies are determined by the differences between the frequencies of the acting field w and transition frequencies ω. In the second commutator, conversely, there is a rapidly oscillating operator, whose characteristic frequencies are determined by the sum of frequencies w and ω.

The rotating wave approximation consists in dropping the second, high-frequency commutator in the density matrix equation (4), resulting in a simplified equation that describes exclusively low-frequency, slowly time-dependent processes.

As a justification for such simplification, the following considerations can be presented. Let's consider the limit such that $w+\omega \to \infty$

$$|w-\omega| \ll w+\omega, \tag{5}$$

$$M \cdot \Delta \ll w+\omega, \tag{6}$$

where matrices M, Δ, characterizing the polychromatic field, for a two-level system have the form

$$M = \begin{pmatrix} 0 & M_{12} \\ M_{12} & 0 \end{pmatrix}, \quad \Delta = \begin{pmatrix} 0 & \Delta_{12} \\ -\Delta_{12} & 0 \end{pmatrix}.$$

Matrix inequalities (5), (6) imply that any non-diagonal element of the matrix from the left side is much smaller in modulus than any non-diagonal element of the matrix on the right side. For matrices of size everything reduces to relationships between the single non-diagonal elements

$$|w_{12}-\omega_{12}| \ll w_{12}+\omega_{12},$$
$$M_{12}\Delta_{12} \ll w_{12}+\omega_{12}.$$

Requirement (5) is universal and applicable, including for monochromatic field; requirement (6) is specific for polychromatic field. In the considered limit, the solution of equation (4) can be represented as a sum of components, each of which relates to one of the non-overlapping spectral domains with centers at frequencies

$$(w_{12}+\omega_{12})s, \quad s = 0, \pm 1, \pm 2, \ldots, \tag{7}$$

where the interaction between components of adjacent domains occurs exclusively due to the second, high-frequency commutator. Indeed, the remaining components of equation (4) at sufficiently large values $w+\omega$ of perform mapping only within individual spectral domains: multiplication by $e^{i(w-\omega)t}$ does not significantly change the spectrum $\tilde{\rho}$ due to (5), multiplication by $\tilde{V}$ – due to (6), differentiation does not generate new spectral components, G and are not time-dependent at all.

Let's consider the asymptotic expansion of the solution of equation (4) in the limit $w+\omega \to \infty$

$$\tilde{\rho} = \rho^{(RWA)} + \rho^{(1)} + \rho^{(2)} + \ldots, \tag{8}$$

where $\rho^{(l)}$, $l = 1,2,\ldots$ – terms of different orders of smallness in the considered limit,

$$\rho^{(l)} \propto (w+\omega)^{-l}$$

or, for individual matrix elements,

$$\rho_{jk}^{(l)} \propto \|w+\omega\|^{-l} \propto (w_{12}+\omega_{12})^{-l}, 1 \le j,k \le 2.$$

It can be stated that the first term in the asymptotic expansion (8), which does not vanish at $w+\omega \to \infty$ and denoted as $\rho^{(RWA)}$, relates exclusively to the lowest-frequency spectral domain (with index $s = 0$); in other words, its spectrum has only frequencies within the range

$$-(w_{12}+\omega_{12})/2 \ldots + (w_{12}+\omega_{12})/2.$$

Indeed, if this were not the case, then, considering the presence of time differentiation in (4), when examining any other spectral domain, we would obtain an infinitely growing left side at $w+\omega \to \infty$ which cannot be compensated by a finite right side.

The equation defining function $\rho^{(RWA)}$ is equation (4), considered closed in the low-frequency domain – spectral domain with index $s = 0$. This means that the high-frequency commutator is removed from equation (4), as it transfers $\rho^{(RWA)}$ to adjacent spectral domains with indices $s = \pm 1$, where the result of the high-frequency commutator action on $\rho^{(RWA)}$ equals the time derivative of $\rho^{(1)}$ in the corresponding domain – a value of the same order of smallness in $w+\omega$ (zero), as $\rho^{(RWA)}$:

$$\frac{d\rho_{s=\pm 1}^{(1)}}{dt} = -i\left[\tilde{V}^{*} \cdot e^{-i(w+\omega)t}, \rho^{(RWA)}\right]. \tag{9}$$

Thus, in the equation defining $\rho^{(RWA)}$, the dependence on the sum of the transition frequency ω and the central frequency of the acting field w completely disappears, leaving only the dependence on their difference. Introducing the detuning

$$\delta = w-\omega = \begin{pmatrix} 0 & w_{12}-\omega_{12} \\ \omega_{12}-w_{12} & 0 \end{pmatrix},$$

we finally obtain the equation for the density matrix in the rotating wave approximation:

$$\frac{d\rho^{(RWA)}}{dt} = -i\left[\tilde{V}\cdot e^{i\delta t},\rho^{(RWA)}\right] - \Gamma\cdot\rho^{(RWA)} + L. \quad (10)$$

Compared to the original equation (4), equation (10) turns out to be significantly simpler, allowing in some cases to present the solution in analytical form [17]. From the perspective of performing numerical calculations, equation (10) is also more preferable than (4). In numerical calculations, the time step size is determined by the maximum frequency at which the density matrix elements fluctuate. Therefore, when working with equation (10), which describes low-frequency processes, one can take a smaller time step compared to the time step required when numerically solving equation (4). In cases where the ratios of maximum frequencies and, consequently, time steps are large, the volume of necessary calculations can differ by orders of magnitude. This is why the rotating wave approximation is so popular in numerical solutions of density matrix equations.

After making the substitution

$$\rho^{(RWA)} = \tilde{\rho}^{(RWA)}\cdot e^{i\delta t},$$

it's possible to shift the zero frequency of the spectrum to the detuning frequency, thereby replacing the oscillating factor in the commutator with a purely imaginary addition to the relaxation matrix

$$\frac{d\tilde{\rho}^{(RWA)}}{dt} = -i\left[\tilde{V},\tilde{\rho}^{(RWA)}\right] - \left(\Gamma + i\delta\right)\cdot\tilde{\rho}^{(RWA)} + L.$$

3. PERFORMED CALCULATIONS

We studied the influence of the rotating wave approximation on the spectra of polarization

$$P_j = -\frac{1}{2}\langle\rho_{12}e^{ij\Delta_{12}t}\rangle_t,$$

of a two-level system, which determine the dispersion and absorption of the medium. For this purpose, equation (4) for the density matrix was solved numerically, and the obtained spectra of off-diagonal elements of the density matrix were compared with similar spectra obtained from solving equation (10) for the density matrix in the rotating wave approximation.

For the numerical solution of the density matrix equations, the second-order Runge-Kutta method was used. An initial value of the density matrix was set

$$\rho_0 = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix},$$

after which a sequence of matrices was recursively constructed $\rho_k = \rho(k\Delta t)$, $k = 1,2,\ldots,$ reflecting the discrete evolution of the density matrix over time with a step Δt:

$$\rho_k = \rho_{k-1} + \frac{\Delta t}{2}\left[f((k-1)\Delta t,\rho_{k-1}) + \right.$$
$$\left. + f(k\Delta t,\rho_{k-1} + \Delta t f((k-1)\Delta t,\rho_{k-1}))\right], \quad (11)$$

where matrix

$$f(t,\rho) = -i\left[\tilde{V}\cdot e^{i\delta t},\rho\right] - i\left[\tilde{V}^{*}\cdot e^{-i(2\omega+\delta)t},\rho\right] - \Gamma\cdot\rho + L$$

was used in solving the exact equation,

$$f(t,\rho) = -i\left[\tilde{V}\cdot e^{i\delta t},\rho\right] - \Gamma\cdot\rho + L$$

was used in solving the equation in the rotating wave approximation. For time-independent relaxation and pumping matrices to the levels, the following matrices were taken

$$\Gamma = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad L = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}.$$

For the two-level system in matrices M, Δ, Γ, w, ω, δ there is only one off-diagonal element (M_{12}, Δ_{12}, ...). In the further exposition, the lower indices of these quantities will be omitted.

The time step value Δt was chosen so that for the period of maximum frequency of the spectral domain (7) with index $s = 1$, i.e. $(4\pi/3)/(w + \omega)$, required 50 steps. When using the rotating wave approximation, in most situations, such a step size is excessive; however, to keep the calculation procedure as identical as possible in both cases, the value $\Delta t = (4\pi/150)/(w + \omega)$ was taken in calculations both using the exact formula and in the rotating wave approximation. The number of steps required for calculation is determined by the duration of transient processes, which ultimately lead to the density matrix elements becoming periodic functions with a period equal to the period of $2\pi/\Delta$ intercomponent shift frequency of the polychromatic field. The Δ intercomponent shift frequency becomes the minimum base frequency of the established processes in the system. The duration of transient processes, expressed in periods of the base frequency, is determined by the ratio of Δ to the averaged value of relaxation matrix elements Γ, and with the parameters under consideration, it was sufficient to calculate several periods of the base frequency to eliminate the influence of transient processes on calculation results. Taking into account the chosen time step size Δt, the number of required steps was approximately $10^5 - 10^6$.

After obtaining two sequences of matrices (11), matrices corresponding to the last period of the $2\pi/\Delta$ base frequency of the polychromatic field were selected, and the spectra of off- diagonal elements ρ_{12} at frequencies 0, $\pm\Delta$, $\pm2\Delta$... were calculated using discrete Fourier transform. In the obtained spectra, which represent the polarization spectra of the two-level system up to a coefficient, real and imaginary components were considered separately.

The distortions of spectra arising from the use of the rotating wave approximation were quantitatively evaluated using two characteristics. First, the quadratic deviation across the entire polarization spectrum, normalized to the total energy of the exact spectrum, was calculated,

$$d_{avg} = \sqrt{\frac{\sum_j \left(P_j^{(RWA)} - P_j\right)^2}{\sum_j P_j^{\,2}}}, \tag{12}$$

and this deviation can be calculated separately for both the real part of the polarization spectrum and the imaginary part. The deviation d_{avg}, calculated using formula (12) for the real part of the polarization spectrum, provides a quantitative assessment of the frequency- averaged distortion of the dispersion spectrum caused by the use of the rotating wave approximation, while calculated for the imaginary part of the spectrum – a similar assessment of the averaged distortion of the absorption spectrum.

Second, in some situations, it is also reasonable to use the spectrum deviation at the transition frequency to assess polarization spectrum distortions $j = 0$:

$$d_{peak} = \left|\frac{P_0^{(RWA)} - P_0}{P_0}\right|. \tag{13}$$

Often, it is at the transition frequency in the imaginary part of the polarization spectrum that a pronounced peak is observed, which makes it possible to evaluate the influence of the rotating wave approximation in this part of the absorption spectrum. For the real part of the polarization spectrum, the assessment using formula (13) is generally of little use, since the dispersion value at the transition frequency turns out to be close to zero. Thus, at zero detuning, the real part of the polarization spectrum in the rotating wave approximation equals zero at the transition frequency, while using the exact formula (4) yields a small but non-zero value. Consequently, the assessment of the real part of the spectrum performed using formula (13) gives exactly one, which does not adequately reflect the situation.

Obviously, the magnitude of spectrum perturbations arising from the use of the approximation depends on several parameters, such as the transition frequency, detuning value, and spectral width of the polychromatic field. The dependencies calculated and presented below allow evaluating the correctness of applying the rotating wave approximation in various cases.

4. CALCULATION RESULTS

Fig. 1 shows polarization spectra obtained using the rotating wave approximation and without using this approximation, for a two-level system under the influence of a polychromatic field consisting of 101 components with equal amplitudes ($M = 50$, $\Omega = 0.2\Gamma$). This case in the rotating wave approximation was considered in works [19, 20] and is distinguished by the presence of radiation at the transition frequency (negative pulse in the spectrum ImP at $j = 0$).

Two clear differences are notable between the spectra in the rotating wave approximation (shown by dotted line) and the exact spectra. First, the spectrum in the rotating wave approximation possesses certain parity with respect to the transition frequency $j \to -j$, while the exact spectrum does not demonstrate such parity. This is related to the fact that in a two-level system with zero tuning in the rotating wave approximation, there is no real part of the off-diagonal density matrix elements [17]. As a result, the polarization spectrum is characterized by certain parity – the real part turns out to be odd, and the imaginary part is even. If the rotating wave approximation is not used, the real part of the off-diagonal elements becomes non-zero and the spectrum parity is violated. Secondly, in the

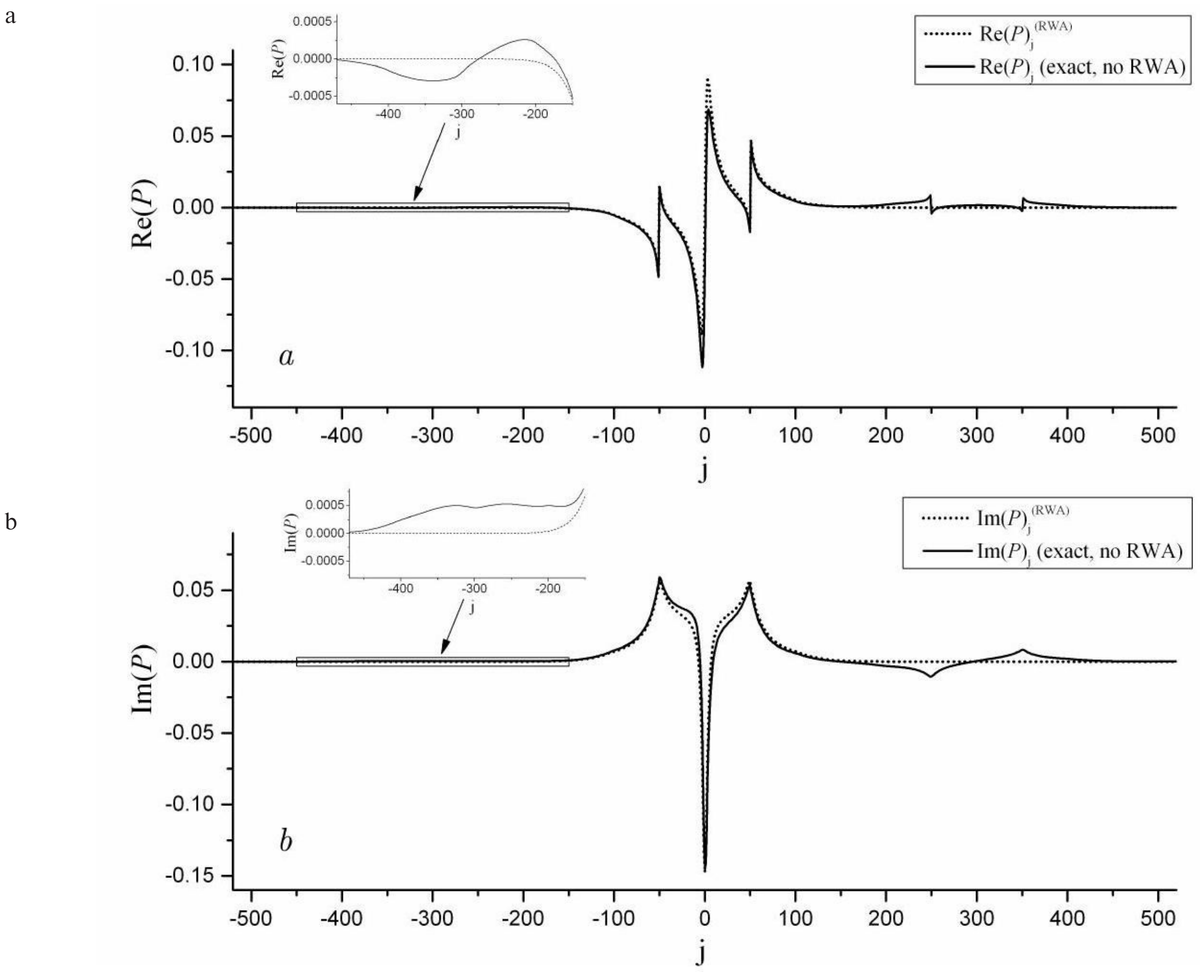

Fig. 1. Polarization spectra obtained using the rotating wave approximation and without using this approximation: *a* – real part of polarization; *b* – imaginary part of polarization. $M = 50$, $\Omega = 0.2\Gamma$, $\Delta = 0.3\Gamma$, $\delta = 0$, $w = 150\Delta$

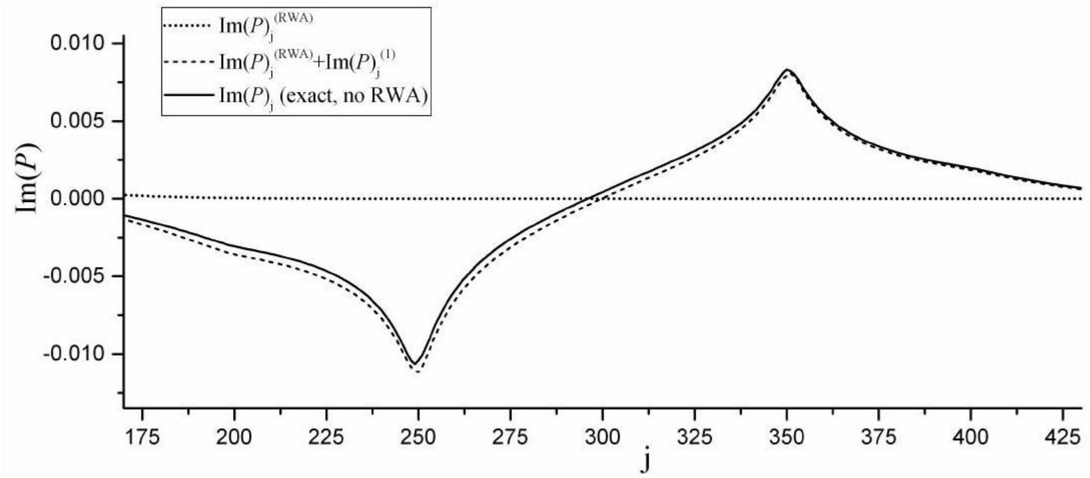

Fig. 2. Absorption spectrum in the high-frequency spectral region $M = 50$, $\Omega = 0.2\Gamma$, $\Delta = 0.3\Gamma$, $\delta = 0$, $w = 150\Delta$

polarization spectra calculated using the rotating wave approximation, there are no perturbations near twice the transition frequency ($j \approx (w + \omega)/\Delta = 2w/\Delta$), i.e., in the spectral domain with index $s = 1$ (see (7)).

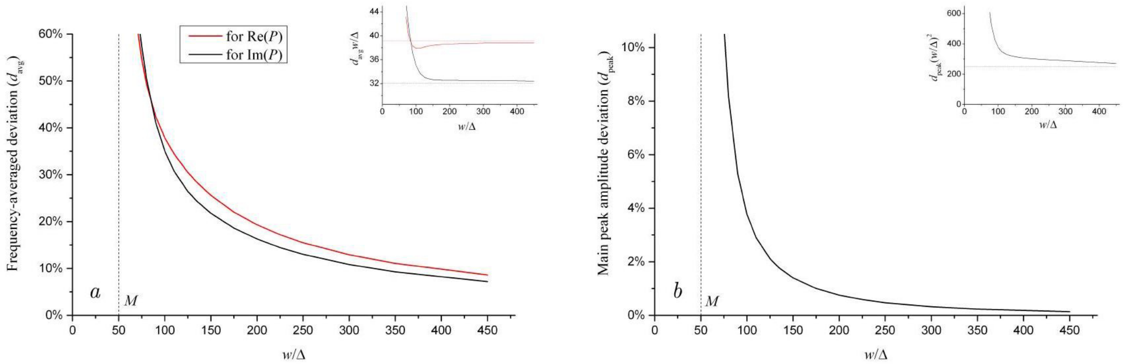

Fig. 3. (Color online) The magnitude of polarization spectra distortions arising from the use of rotating wave approximation, depending on the central frequency of the acting field w: a – spectrum-averaged distortion (d_{avg}) for both parts of polarization; b – pulse amplitude distortion at the transition frequency (d_{peak}) of the imaginary part of polarization spectrum. $M = 50$, $\Omega = 0.2\Gamma$, $\Delta = 0.3\Gamma$, $\delta = 0$

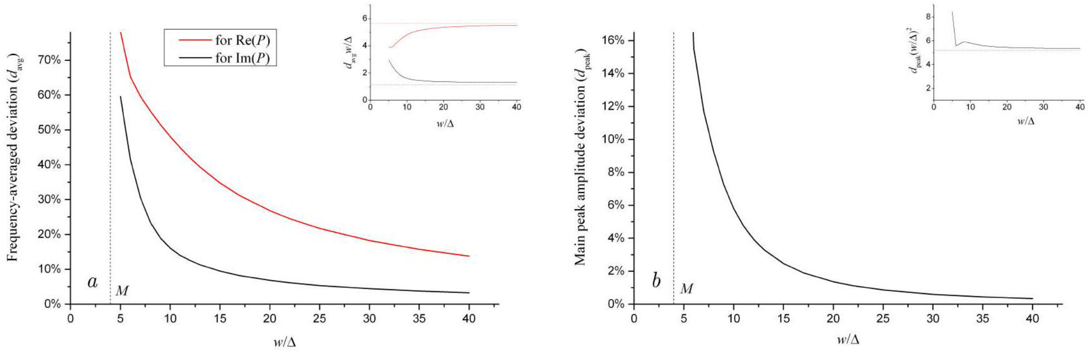

Fig. 4. (Color online) Same as in Fig. 3, but for 9-component polychromatic field ($M = 4$)

The latter is not surprising since, as noted earlier, in solution $\rho^{(RWA)}$ of equation (10), only low-frequency components in the spectral domain with index $s = 0$ play a significant role. Fig. 2 shows the high-frequency spectral region in more detail $s = 1$. To achieve better approximation to the exact solution in this spectral region, it is necessary to consider the next correction after $\rho^{(RWA)}$ in the asymptotic expansion (8), calculated using formula (9) and shown in Fig. 2 by dashed line.

A less obvious difference in the spectra in Fig. 1 lies in the distortions near the transition frequency ($j \approx 0$), in the low-frequency spectral domain (7) with index $s = 0$. The amplitude of the negative peak in the imaginary part of polarization spectrum at the transition frequency in the rotating wave approximation turns out to be approximately 1.4% larger than calculated using the exact formula (4). Furthermore, more precise calculations show a rightward shift of the peak, while the rotating wave approximation predicts emission exactly at the transition frequency $j = 0$. The amplitude and shape of the lateral positive pulses in the imaginary part of polarization spectrum also differ. Similar distortions are observed in the real part of polarization spectrum.

An even less obvious difference in the spectra is found near the negative doubled transition frequency ($j \approx -(w + \omega)/\Delta = -2w/\Delta$). The insets in Figs. 1$a$,$b$ with enlarged vertical scale show polarization spectra in the spectral domain with index $s = -1$. Spectra calculated using the exact formula have non-zero components in this frequency region, although, of course, the magnitude of perturbations is almost 2 orders lower than that observed in the spectral domain $s = 1$ at $2w/\Delta - M \lesssim j \lesssim\, < 2w/\Delta + M$. The dispersion of perturbation at negative frequencies is higher and affects a wider part of the spectrum. Moreover, the center of perturbation is slightly shifted towards positive frequency values, just like the spectrum near the transition frequency. As for the spectrum obtained in the rotating wave

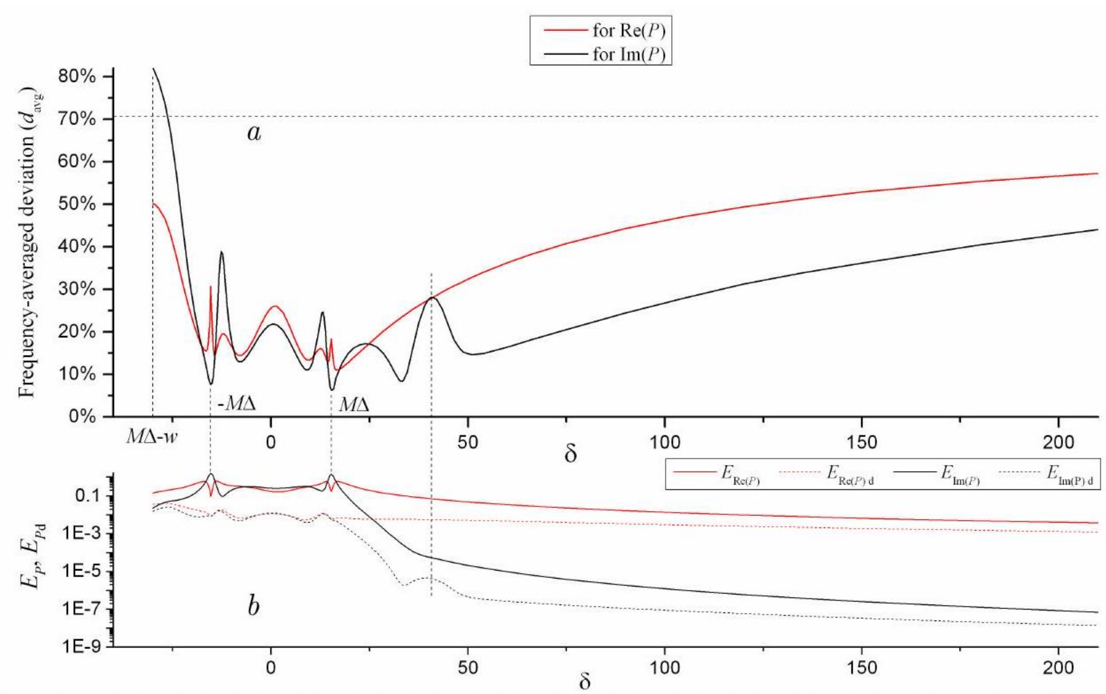

Fig. 5. (In color online) The magnitude of polarization spectra distortions arising from the use of the rotating wave approximation, depending on the detuning δ: *a* – relative distortion d_{avg}; *b* – polarization spectra energy $E_{\mathrm{Re}\,P}$, $E_{\mathrm{Im}\,P}$ without using the approximation and absolute values of distortions $E^{(d)}_{\mathrm{Re}\,P}$, $E^{(d)}_{\mathrm{Im}\,P}$. $M = 50$, $\Omega = 0.2\Gamma$, $\Delta = 0.3\Gamma$, $w = 150\Delta$

approximation, any perturbations at $j \approx -2w/\Delta$ are practically completely absent.

With increasing frequency of the acting field (and transition frequency at zero detuning), the perturbation at $j \approx 2w/\Delta$, observed in Figs. 1*a*,*b* shifts to the right, its magnitude decreases. The deviations in the spectra in the low-frequency domain $s = 0$ near the transition frequency $j \approx 0$ also become smaller. All this manifests in a monotonic decrease of the averaged spectra deviation d_{avg}, which is demonstrated in Fig. 3*a*. The magnitude d_{avg} at high frequencies of the acting field becomes inversely proportional to w (see inset in Fig. 3*a*). Similar dependencies are observed for the spectra of both real and imaginary parts of polarization.

As the frequency of the acting field decreases, the magnitude of spectrum distortions when using the rotating wave approximation increases. When approaching frequencies $w/\Delta \sim M$ condition (6) is violated, the magnitude of distortions sharply increases, making the rotating wave approximation absolutely unsuitable for calculating polarization spectra. The edges of the polychromatic field spectra regions $-M \lesssim j \lesssim M$ and $2w/\Delta - M \lesssim j \lesssim 2w/\Delta + M$ begin to overlap, resulting in significant changes in dispersion and absorption spectra. Calculations using the exact formula (4) fully reflect these changes, while calculations in the rotating wave approximation do not, as they fail to correctly describe the spectra in the frequency range $2w/\Delta - M \lesssim j \lesssim 2w/\Delta + M$. As a result, at small the rotating wave approximation for polychromatic radiation becomes inadequate not when approaching zero, but already at $w/\Delta \sim M$.

The distortion of the imaginary part of polarization at the transition frequency d_{peak} also tends to zero at high frequencies of the acting field (Fig. 3*b*). However, as shown in the inset in Fig. 3*b*, the magnitude d_{peak} turns out to be inversely proportional not to the first power of w, but to its square. The faster decrease in the error of the rotating wave approximation compared to that observed on average across the spectrum is characteristic exclusively for the component at the transition frequency ($j = 0$) and is apparently related to the special symmetry of the spectrum manifesting in the limit $w \to \infty$.

Fig. 4 shows the dependences of polarization spectra distortions on w for the case of a nine-component ($M = 4$) polychromatic field. This case was considered in the rotating wave approximation [17] and, unlike the case with $M = 50$, has no

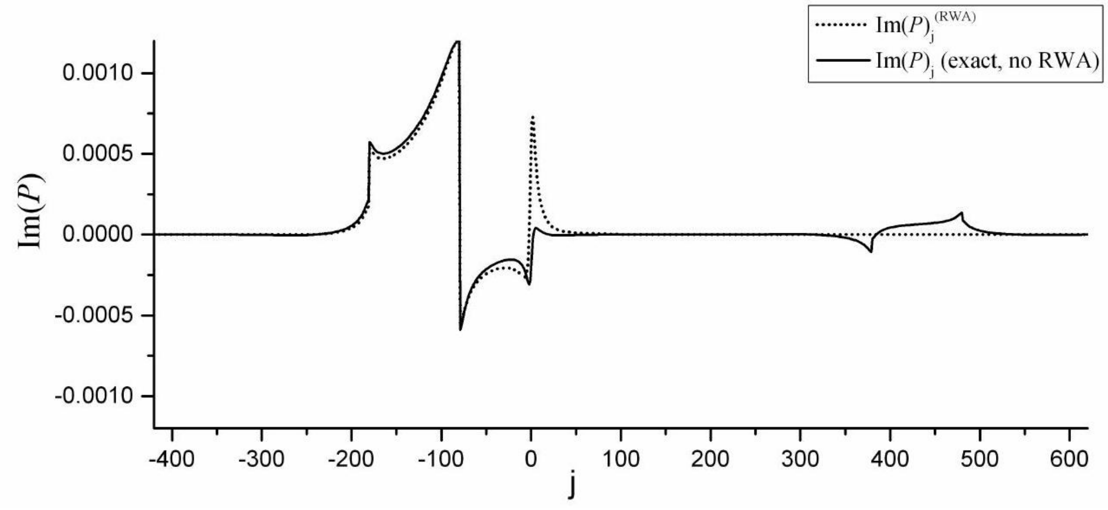

Fig. 6. The spectrum of the imaginary part of polarization, obtained using the rotating wave approximation and without using the specified approximation. $M = 50$, $\Omega = 0.2\Gamma$, $\Delta = 0.3\Gamma$, $w = 150\Delta$. The maximum deviation is observed at the transition frequency ($j = 0$)

radiation at the transition frequency. However, the nature of dependencies d_{avg}, d_{peak} remains the same as in the case of a broader spectral band of the acting field. The distortion of the component at the transition frequency (Fig. 4*b*) decreases inversely proportional to the square of w, and the average distortion across the spectrum (Fig. 4*a*) is inversely proportional to the first power of w. This indicates the fundamental nature of the error dependencies caused by the application of the rotating wave approximation in the limit of high frequencies of acting fields.

A peculiarity of the polarization spectra distortion dependencies on detuning δ (Fig. 5), compared to the dependencies on the frequency of the acting field w at zero detuning, is that the total energy of the spectra significantly depends on the variable parameter. When the detuning value δ is sufficiently large and exceeds half the width of the spectral range of the acting polychromatic field, i.e., the transition frequency goes beyond the specified range, the total energy of the polarization spectra, both calculated using the exact equation (4) and in the rotating wave approximation (10), begins to decrease exponentially. This is clearly visible in Fig. 5*b*, which shows the total energies of the polarization spectra

$$E_{\mathrm{Re}\,P} = \sum_j (\mathrm{Re}\,P_j)^2,$$

$$E_{\mathrm{Im}\,P} = \sum_j (\mathrm{Im}\,P_j)^2$$

and the total energies of spectral deviations arising from the use of the rotating wave approximation,

$$E^{(d)}_{\mathrm{Re}\,P} = \sum_j \left(\mathrm{Re}\,P_j^{(RWA)} - \mathrm{Re}\,P_j\right)^2,$$

$$E^{(d)}_{\mathrm{Im}P} = \sum_j \left(\mathrm{Im}P_j^{(RWA)} - \mathrm{Im}P_j\right)^2,$$

on a logarithmic scale along the vertical axis. At large detuning values, the decay rate of the total polarization spectrum energy slows down – at $\delta \to \infty$ the energy of the real part of the spectrum decreases inversely proportional to δ^2, and the energy of the imaginary part – inversely proportional to δ^4. If we consider a sufficiently wide range of parameter values δ, the energy of the polarization spectrum can differ by orders of magnitude. Thus, it turns out that the oscillations of the relative, averaged over the entire spectrum magnitude of distortions d_{avg}, observed in Fig. 5*a*, are the result of a combination of two factors. First, d_{avg} is directly affected by deviations caused by the use of the rotating wave approximation, which is accounted for in the numerator of expression (12). Second, part of the oscillations in the magnitude of d_{avg} is the result of changes in the total energy of polarization spectra, which enters the denominator of expression (12). Thus, the minima for the spectrum of the imaginary part of polarization, observed at $\delta = \pm M\Delta$, detunings, are consequences of the second factor – at these detuning values, the edges of the spectral range coincide with the transition frequency. This causes a sharp increase in the total energy of the imaginary part of the polarization spectrum,

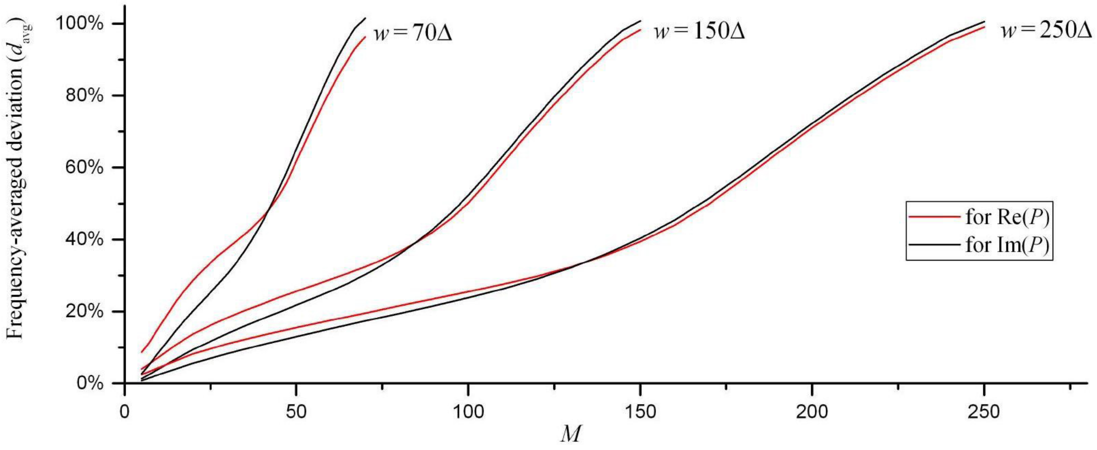

Fig. 7. (In color online) The magnitude of distortions in polarization spectra arising from the use of the rotating wave approximation, depending on the number of polychromatic field components M at three fixed values of the incident field frequency $w = 70\Delta$, 150Δ, 250Δ; $\Omega = 0.2\Gamma$, $\Delta = 0.3\Gamma$, $\delta = 0$

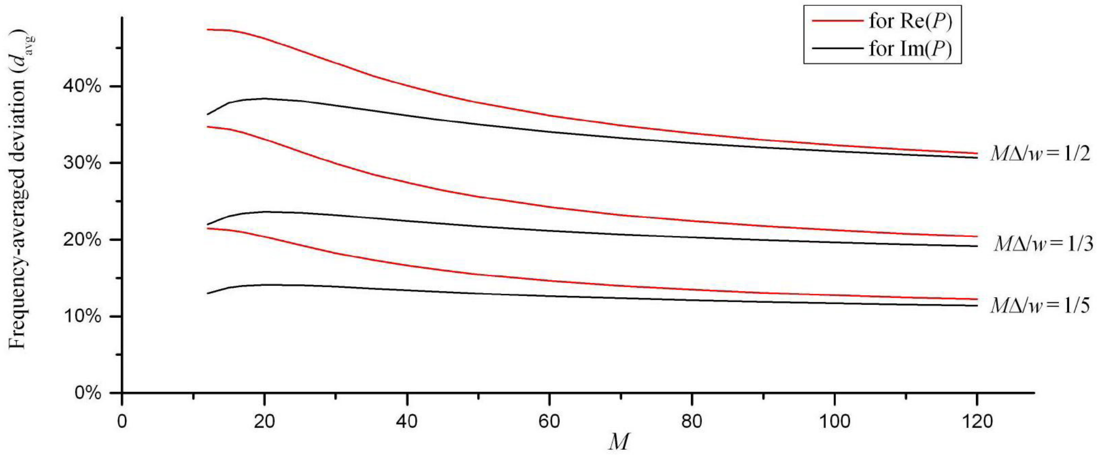

Fig. 8. (In color online) The magnitude of distortions in polarization spectra arising from the use of the rotating wave approximation, depending on the number of polychromatic field components M. The frequency of the incident field w here changes proportionally to M, thus fixing the fraction of the spectral range covered by the polychromatic field band (considered fractions 1/5, 1/3, 1/2); $\Omega = 0.2\Gamma$, $\Delta = 0.3\Gamma$, $\delta = 0$

which ultimately leads to a decrease in the relative magnitude of distortions. The maximum d_{avg}, detected at $\delta \approx 39 \pm 3$, on the contrary, is the result of the first factor – at these detuning values, there is a significant deviation of the spectrum in the rotating wave approximation from the exact one (see Fig. 6). The rotating wave approximation predicts here the existence of absorption at the transition frequency, while when using the more exact equation (4), this conclusion cannot be made.

At large detuning values, the polarization spectrum splits into two non-interacting frequency regions:

$$-\frac{\delta}{\Delta} - M < j < -\frac{\delta}{\Delta} + M,$$

$$\frac{2\omega + \delta}{\Delta} - M < j < \frac{2\omega + \delta}{\Delta} + M.$$

The spectrum in the first region is described with high accuracy by the rotating wave approximation, while the spectrum in the second region is completely absent in this approximation. The energies of the spectral regions at $\delta \gg 2\omega$ are practically equal, therefore d_{avg}, as shown in Fig. 5*a*, asymptotically approaches $1/\sqrt{2} \approx 70.7\%$ at $\delta \to \infty$. Such a high level of distortions in this limit is associated with the violation of the applicability condition for the rotating wave approximation (5). This behavior of the averaged spectrum deviation at $\delta \to \infty$ is characteristic for both the real and imaginary parts of polarization.

At negative detuning values when approaching $M\Delta - \omega$, the spectral regions begin to overlap, violating the applicability condition of the rotating wave approximation (6), resulting in this approximation becoming completely inadequate, producing spectra that strongly differ from those calculated based on the exact equation (4).

Fig. 7 shows the dependencies of relative magnitudes of polarization spectra distortions arising from the use of rotating wave approximation, d_{avg} on the number of components M of the acting polychromatic field at several values of the central frequency w. The central frequency of the acting field w determines the distance between spectral regions, and the number of components M, at a fixed value of distance between components Δ, determines the width of spectral regions. With the increase of the relative magnitudes of polarization spectra distortions monotonically increase, reaching values at $M = w/\Delta$ close to 100%. The latter means that when the edges of spectral regions begin to overlap, the energy of spectra deviation caused by the use of rotating wave approximation becomes close to the energy of the initial, exact spectrum. Obviously, condition (6) is violated here, and the rotating wave approximation in this case gives unsatisfactory results.

Similar form of dependencies $d_{avg}(M)$ at different values of w with accuracy up to stretching along the horizontal axis in Figure 7 indicates that the spectra distortions in rotating wave approximation are determined not by the number of components in the acting polychromatic field as such, but by the fraction in the spectral range between frequencies $\omega - w$ and $\omega + w$, which is occupied by the polychromatic field spectrum. This is confirmed by Fig. 8, which shows the graphs of dependency $d_{avg}(M)$ not at fixed w, but at fixed ratios $M\Delta/w$, i.e., at fixed fractions of spectral range occupied by the polychromatic field spectrum. If w changes proportionally to M, the form of polarization spectra changes weakly, as well as the magnitudes of spectra distortions caused by the use of rotating wave approximation. Note that at sufficiently large M and w the value $d_{avg}(M)$ stabilizes at a level approximately equal to two-thirds of the ratio $M\Delta/w$.

5. CONCLUSIONS

We performed a quantitative assessment of the impact that the rotating wave approximation has on the polarization spectra of a two-level system in a polychromatic field. The frequency-averaged deviation of the spectra caused by the rotating wave approximation was calculated for various system parameters, specifically – the frequency of the acting field w, the detuning value δ, and the number of components of the acting field M.

The magnitude of the averaged spectral deviation proved to be inversely proportional to the frequency of the acting field, which confirms the assumption that the first correction to the density matrix in the asymptotic expansion in the limit $w + \omega \to \infty$ has an order of $(w + \omega)^1$. However, the deviation at the transition frequency demonstrated a faster decrease with increasing acting field frequency, specifically being inversely proportional to the frequency squared.

The dependence of the averaged spectral deviation on the detuning of the central frequency of the polychromatic field w from the transition frequency ω shows no clear trends when the detuning magnitude is small relative to the sum of the transition frequency and the mean frequency of the acting field, and is largely determined by the total energy of the polarization spectrum. A local minimum of spectral deviation is observed when the transition frequency corresponds to the boundary of the acting polychromatic field. At large detunings, the applicability condition of the rotating wave approximation is violated and the spectral deviations asymptotically approach $1/\sqrt{2}$.

Regarding the influence of the number of components of the acting polychromatic field on the averaged spectral deviation, it manifests indirectly through the fraction of the frequency range occupied by the polychromatic field in the frequency range from $\omega - w$ to $\omega + w$. With an increase in the number of components at a fixed distance between them, the fraction increases, leading to increased deviations. If the fraction is fixed, for example, due to the growth of the central frequency of the acting field proportionally to the number of components, then the magnitude of deviations stabilizes at a level approximately equal to 2/3 of the fraction.

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