DOI 10.1007/s10812-020-00935-1
Journal of Applied Spectroscopy, Vol. 86, No. 6, January, 2020 (Russian Original Vol. 86, No. 6, November–December, 2019)

A UNIFORMLY SUITABLE APPROXIMATION FOR THE CHARACTERISTICS OF THE ELECTROMAGNETIC FIELD IN THE RABI QUANTUM MODEL

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UDC 535.14

A systematic study is made of the efficiency of a uniformly suitable approximation for describing the Rabi quantum model beyond the rotating wave model. The correlation characteristics of the electromagnetic field in a resonator are calculated and the physical effects owing to the counter-rotating terms in the Hamiltonian are examined.

Keywords: *Rabi model, two-level system, quantum field, operator method.*

Introduction. The Rabi quantum model (RQM) describes the interaction of a two-level system (TLS) with a single-mode quantum field in a resonator [1, 2]. It is one of the basic models used to describe the interaction of radiation with matter and is of fundamental significance for many problems in quantum optics [3], quantum information [4], and the physics of condensed matter [5]. Various applications of this model and its generalizations are extremely important even now (see [6–8] and the literature cited there). It has been shown [9] that the RQM is an exactly integrable system and the spectrum of its stationary states is found in terms of solutions of polynomial recurrence relations. This is a fundamental result, but the eigenfunctions and characteristic values do not appear in a closed analytic form, which makes it very difficult to use them for specific applications describing the evolution of RQM, which involve summing over the entire spectrum of the stationary states of the system. Thus, the dynamics of RQM is often studied using simple analytic solutions for the stationary states based on using a rotating wave approximation (RWA) that are exact eigenfunctions for the Hamiltonian of the Jaynes–Cummings model (JCM) [10]. The range of applicability of the JCM is, however limited to small deviations from resonance and in the interaction constants of a TLS with a field. There is great interest in studies of systems corresponding to a strong coupling regime for a RQM and the physical effects arising in this regime [11–14]. There are a large number of realizations of two-level systems and resonators (superconducting cubit, polariton) corresponding to RQM with a large coupling constant [15] which can vary continuously over an interval on the order of unit [16]. Thus, developing methods for fairly simple description of RQM beyond the RWA is still an important task [7, 15, 17, 18].

An operator method (OM) has been used [19] to construct the uniformly suitable approximation (USA) for stationary states of RQM, which in the zeroth approximation provides a highly accurate approximation of the eigenvalues of the Hamiltonian of the RQM over the entire range of the deviation and coupling constant, and can be used to construct an iteration scheme for numerical diagonalization of the Hamiltonian of the RQM that converges rapidly with an optimum choice of the variational parameter [20]. An analogous approximation has been constructed [21, 22] by generalizing the rotating wave approximation. This approach has recently been improved through the choice of the variational parameter (see [7] and the references therein).

The resulting approximate solutions have a simple analytic form that is not much more complicated than in the case of the RWA, so the sum can be taken over the entire set of quantum numbers of the system when calculating these quantities. It has been shown [20, 23] that the USA makes it possible to describe the evolution of a TLS and relaxation processes in it over the entire range of variation in the field amplitude and of the deviation from resonance. At the same time, the important applied significance of the RQM in quantum optics and information theory is related both to the description of the evolution of an atom (a cubit) and to analyzing the correlation characteristics of an electric field in terms of this model.

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This paper is a systematic comparison of calculations of these characteristics based on the RWA and USA and shows that using the USA greatly expands the capabilities of the RQM for studying and optimizing the parameters of these systems and makes it possible to describe effects that do not show up in terms of the RWA, in particular the formation of a "dressed" TLS as a bound state of an atom and photons arising from the vacuum state of an electromagnetic field.

A Uniformly Suitable Approximation for Stationary States of the RQM. Here we recall the basic equations for solving problems regarding the stationary states of the RQM obtained in the framework of the RWA and USA. The dimensionless form of the Hamiltonian of the RQM in natural units ($\hbar = c = 1$) is given by the well known expression [24]

$$\hat{H} = \frac{1}{2}\Delta\hat{\sigma}_3 + \hat{a}^+\hat{a} + f(\hat{\sigma}_+ + \hat{\sigma}_-)(\hat{a} + \hat{a}^+) \ , \tag{1}$$

where $\hat{a}$ and $\hat{a}^+$ are the creation and annihilation operators for photons at a resonance mode of the field; the field frequency $\omega = 1$ determines the scale of a measurement of the system energy; Δ is the difference in energy between the resonance states of the atom in units of ω; f is the dimensionless coupling constant of the TLS and the field ,which is proportional to the dipole matrix element of the transition between these states; and, $\hat{\sigma}_i$ is the Pauli matrix.

An integral of motion exists in this system that can be treated as a "combined" parity:

$$\hat{P} = \hat{\sigma}_3\hat{S} = \hat{\sigma}_3 e^{i\pi\hat{a}^+\hat{a}} \ , \quad [\hat{H}, \hat{P}] = 0 \ . \tag{2}$$

In terms of the RWA the terms $\hat{\sigma}_+\hat{a}^+$ and $\hat{\sigma}_-\hat{a}$ in the Hamiltonian (1) are neglected, which also changes the integral of motion of the system, which in this approximation corresponds to conservation of the total number of excitations of the atom and field:

$$\hat{H}_{\mathrm{RWA}} = \frac{1}{2}\Delta\hat{\sigma}_3 + \hat{a}^+\hat{a} + f(\hat{\sigma}_+\hat{a} + \hat{\sigma}_-\hat{a}^+) \ ,$$

$$\hat{J} = \frac{1}{2}\hat{\sigma}_3 + \hat{a}^+\hat{a} \ , \ [\hat{H}_{\mathrm{RWA}}, \hat{J}] = 0 \ . \tag{3}$$

In this case, the stationary Schroedinger equation $\hat{H}_{\mathrm{RWA}}\left|\psi_n^{(\pm)}\right\rangle = E_n^{(\pm)}\left|\psi_n^{(\pm)}\right\rangle$ has simple analytic solutions, for both the energy eigenvalues and the eigenvectors:

$$E_n^{(\pm)} = n + \frac{1}{2} \pm \frac{1}{2}\sqrt{(\Delta - 1)^2 + 4f^2(n+1)} \ ,$$

$$|\ \psi_n^{(\pm)}\rangle = a_n^{(\pm)}\chi_\uparrow\ |\ n\rangle + b_n^{(\pm)}\chi_\downarrow\ |\ n+1\rangle \ , \quad n = 1, 2, \ldots \ , \tag{4}$$

$$E_0^{(-)} = -\frac{\Delta}{2} \ , \quad E_0^{(+)} = \frac{1}{2} + \frac{1}{2}\mathrm{Sign}(\Delta - 1)\sqrt{(\Delta - 1)^2 + 4f^2} \ ,$$

$$|\ \psi_0^{(-)}\rangle = \chi_\downarrow\ |\ 0\rangle \ , \quad |\ \psi_0^{(+)}\rangle = a_0^{(+)}\chi_\uparrow\ |\ 0\rangle + b_0^{(+)}\chi_\downarrow\ |\ 1\rangle \ , \tag{5}$$

where

$$a_n^{(\pm)} = \frac{1}{\sqrt{1 + (\lambda_n^{(\pm)})^2}} \ , \quad b_n^{(\pm)} = -\frac{\lambda_n^{(\pm)}}{\sqrt{1 + (\lambda_n^{(\pm)})^2}} \ , \tag{6}$$

$$\lambda_n^{(\pm)} \equiv \frac{(\Delta - 1) \mp \sqrt{(\Delta - 1)^2 + 4f^2(n+1)}}{2f\sqrt{n+1}} \ . \tag{7}$$

At the same time, the exact stationary states of the RQM are determined by the system of equations

$$\hat{H}\left|\psi_{np}\right\rangle = E_{np}\left|\psi_{np}\right\rangle, \quad \hat{P}\left|\psi_{np}\right\rangle = p\left|\psi_{np}\right\rangle, \tag{8}$$

where the quantum number $p = \pm 1$ determines the parity of the state and $n = 0, 1, \ldots$ is the level of excitation of the field.

To solve these equations outside the framework of the RWA, in [19] and [21] it is noted that the coupling of an atom with a field leads to a shift in the equilibrium position of the field oscillators. This shift can be described using a canonical operator transformation:

$$\hat{b} = \hat{a} + u\,, \quad \hat{b}^+ = \hat{a}^+ + u\,, \quad \hat{b} = \hat{R}^{-1}\hat{a}\hat{R}\,, \quad \hat{R} = e^{u\left(\hat{a}^+ - \hat{a}\right)} = e^{-u^2/2} e^{u\hat{a}^+} e^{-u\hat{a}}\,,$$

$$|\, n,u\rangle = \frac{(\hat{a}^+ + u)^n}{\sqrt{n!}} \sum_{k=0}^{\infty} \frac{u^k}{k!} (\hat{a}^+)^k \,|\, 0\rangle e^{-u^2/2}\,. \tag{9}$$

Using u as the variational parameter, it is possible to find a closed analytic formula for E_{np} and $|\,\psi_{np}\rangle$, which approximates the exact solutions with high accuracy over the entire range of variation of f, Δ, and the quantum number n. These solutions determine the RWA for describing the states of this system and are given by

$$E_{np} = n + \frac{1}{2}q - f^2 + \frac{1}{4}p\Delta(S_{n+q,n+q} + S_{nn}) - \frac{1}{2}qM\,, \quad n = 1, 2, \ldots\,.$$

$$M = \sqrt{\left[1 + \frac{1}{2}\Delta(-1)^n (S_{n+q,n+q} - S_{nn})\right]^2 + \Delta^2 S_{n,n+q}^2}\,, \quad q = p(-1)^n\,,$$

$$S_{km} = (-1)^m \sqrt{\frac{m!}{k!}} (2f)^{k-m} L_m^{k-m}(4f^2) e^{-2f^2}\,, \quad k \geq m; \quad S_{km} = S_{mk}\,, \tag{10}$$

where $L_m^k(x)$ are the generalized Laguerre polynomials and

$$|\,\psi_{np}\rangle = B_{np}\{\gamma \,|\, n,\, f\rangle + |\, n+q,\, f\rangle\}\chi_+ + pB_{np}\{(\gamma S_{nn} + S_{n,n+q}) \,|\, n,\, f\rangle + (\gamma S_{n+q,n} + S_{n+q,n+q}) \,|\, n+q,\, f\rangle\}\chi_-\,,$$

$$B_{np}^2 = \{(\gamma^2 + 1) + (\gamma S_{nn} + S_{n,n+q})^2 + (\gamma S_{n+q,n} + S_{n+q,n+q})^2\}^{-1}\,,$$

$$\gamma = -\frac{p\Delta S_{n,n+q}}{2n + 2f^2 + p\Delta S_{nn} - 2E_{np}}\,, \quad \chi_\pm = \frac{1}{\sqrt{2}}(\chi_\uparrow \pm \chi_\downarrow)\,. \tag{11}$$

For the ground state (0, –), we find

$$E_{0,-} = -f^2 - \frac{1}{2}\Delta S_{00}(f) = -f^2 - \frac{1}{2}\Delta e^{-2f^2}\,, \quad |\,\psi_{0-}\rangle = \frac{1}{\sqrt{2}}\left(|\, 0,\, f\rangle\,\chi_+ - \sum_{k=0}^{\infty} S_{0k}(f)\,|\, k,\, f\rangle\,\chi_-\right). \tag{12}$$

An effective iteration scheme for numerical solution of Eqs. (8) has been constructed in [19]; it makes it possible to find the stationary states of the RQM with any needed accuracy. This means it is possible to compare the results of analytic approximations for the RWA and USA with the exact solution and to determine the boundaries of applicability of the two approximations.

Figure 1 shows the dependence of the energy levels of the system on the coupling constant and deviation from the resonance for different quantum numbers. It is clear that the USA interpolates the exact solutions with fairly high accuracy for arbitrary coupling constants and quantum numbers, while the structure of the levels in terms of the RWA differs qualitatively from the exact solutions for $f\sqrt{n} > 1$. It has been shown [25] that this difference in the behavior of the levels is caused by quasiprecession of the energy terms of the system in the RWA for a coupling constant and quantum number n subject to the conditions

$$E_n^{(+)}(f) = E_{(n+2)}^{(-)}(f)\,. \tag{13}$$

For an exact resonance, solutions of Eqs. (13) exist for

$$f(\sqrt{n+1} + \sqrt{n+3}) > 2\,, \quad f\sqrt{n} \geq 1\,, \tag{14}$$

which also specifies the boundaries of the system parameters where the RWA can be used.

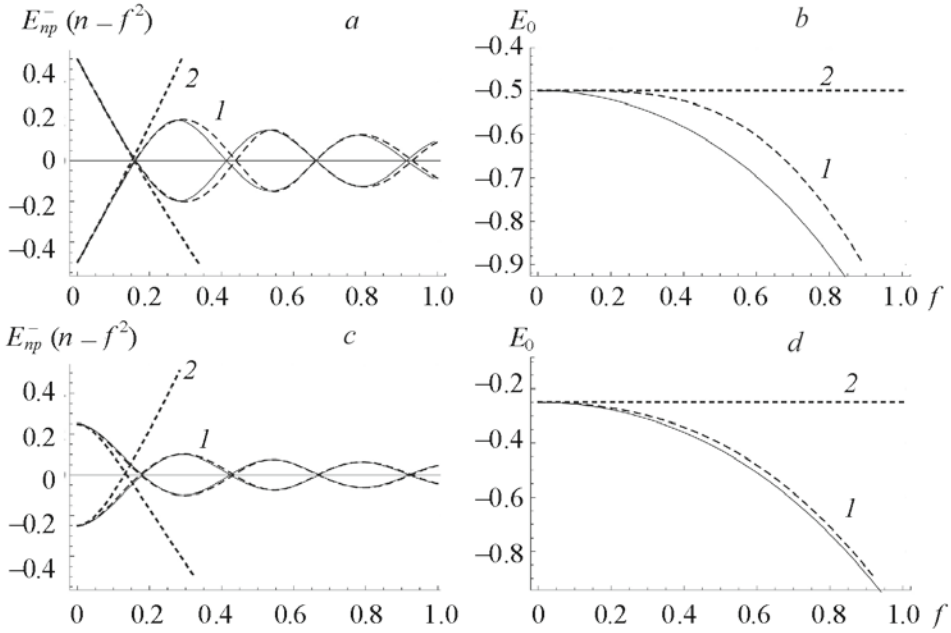

Fig. 1. The energy levels as a function of coupling constant: (a) excited states for $n = 10, p = \pm 1$, and $\Delta = 1.0$; (b) ground state ($n = 0, p = -1$) for $\Delta = 1.0$; (c) excited states for $n = 10$, $p = \pm 1$, and $\Delta = 0.5$; (d) ground state ($n = 0$, $p = -1$), for $\Delta = 0.5$; numerical solution — smooth curves; (1) USA; (2) RWA.

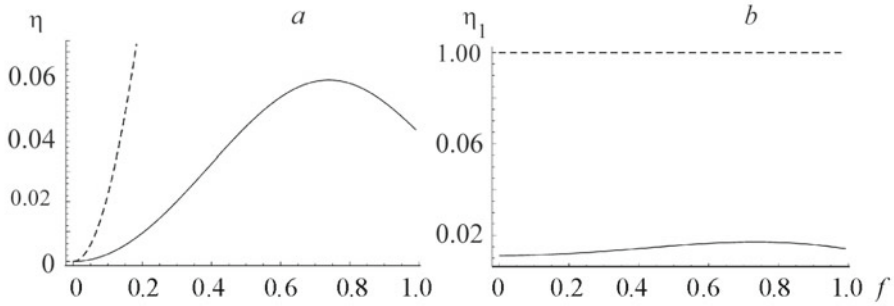

Fig. 2. The moments η_0 (a) and η_1 (b) as functions of the coupling constant for the ground state of a RQM at a resonance: USA — smooth curves; RWA, dashed curves.

We now examine the accuracy of the approximation for the state vector of the system in different approximations. We write the exact eigenfunction of the Hamiltonian of the RQM in the form of an expansion with respect to the Fock basis of the free electron field and the spin state of the unperturbed TLS:

$$| \psi_{np} \rangle = \sum_{ms} A_{ms}^{np} \mid m \rangle \chi_s \,. \tag{15}$$

The dependence of the two first moments on the coupling constant is shown in Fig. 2.

The accuracy of the approximation for the vectors of state can be characterized using the moments which determine the deviation with respect to the norm of the exact coefficients A_{ms}^{np} from their values $A_{ms}^{np}(R)$ and $A_{ms}^{np}(U)$, calculated in terms of the RWA and USA:

$$\eta_l(F)^{np} = \frac{\sum\limits_{ms} m^l \mid A_{ms}^{np} - A_{ms}^{np}(F) \mid^2}{\sum\limits_{ms} m^l \mid A_{ms}^{np} \mid^2}, \quad F = (R, U) \,. \tag{16}$$

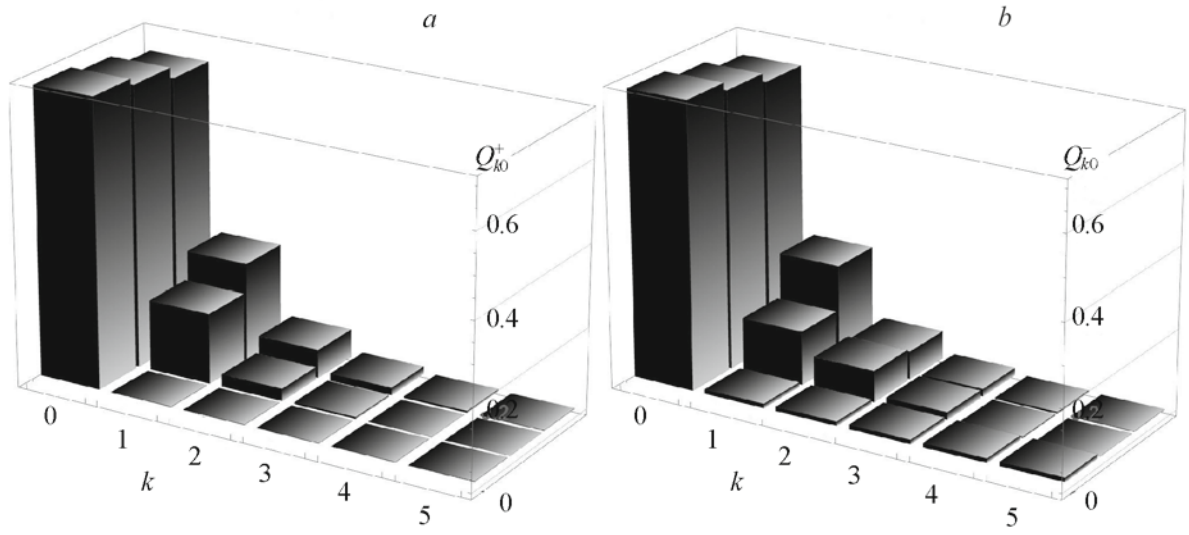

Fig. 3. Moduli of the filling factors for the ground state of a JQM at resonance and $f = 0.25$; the front row is RWA, middle row USA, and back row a numerical solution.

Figure 3 shows the dependence of the filling factors of the Fock states of the electromagnetic field in the resonator in the stationary states of the system on the coupling constant:

$$Q^{s}_{kn} = \sum_{p} |\chi_s \langle k \mid \psi_{np} \rangle|^2 \ . \tag{17}$$

These coefficients are important for describing the evolution of a RQM and their behavior is closely related to the difference in the integrals of motion of the system for both approximations. The populations of only two neighboring Fock states are nonzero in terms of the RWA, while in the exact solutions and the USA, the populations of these states "spread out" over an interval of $|k-n| \sim f\sqrt{n}$.

The structure of the ground state of the system differs qualitatively in terms of the RWA from the exact solution and from the USA for the RQM. In fact, the state $|0\rangle \chi_{\downarrow}$ corresponding to the vacuum electromagnetic field is an exact eigenvector of the Hamiltonian (3). At the same time, the ground state of the RQM corresponds to a "dressed" TLS, a bound state of a qubit and a coherent state of the electromagnetic field, corresponding to a nonzero value of the number of photons in the Fock basis. The formation of a state of this kind can be regarded as a manifestation of a "polaron" effect, typical for arbitrary systems corresponding to the interaction of a particle with quantum field [26]. The binding energy of the ground state of the "dressed" TLS in terms of the USA is given by

$$E_B = E_{0,-} - (-\Delta/2) = -f^2 + \frac{1}{2}\Delta(1 - e^{-2f^2}) \ , \tag{18}$$

while the wave function (12) describes an "entangled" state of a TLS and a quantum field. The simple formula (18) is a good approximation to the exact dependence of the ground state energy on the coupling constant (Fig. 1).

Characteristics of the Electromagnetic Field in a RQM. As pointed out above, the domain of applicability of the RWA is determined by the parameter $f\sqrt{n}$. Recall that the RQM arises as the result of approximating the interaction operator of an atomic system with a resonance mode of an electromagnetic field. The original Hamiltonian for a nonrelativistic atom has the form ($\hbar = c = 1$)

$$\hat{H} = \hat{H}_{\rm a} + \hat{H}_{\rm int} + \sum_{\mathbf{k}} \omega_{\mathbf{k}} a^{+}_{\mathbf{k}} a_{\mathbf{k}} \ , \quad \hat{H}_{\rm int} = -\frac{e_0(\mathbf{pA})}{m_0} + \frac{e_0^2(\mathbf{A})^2}{2m_0} \ , \quad \mathbf{A}(\mathbf{r}) = \sum_{\mathbf{k},s} \sqrt{\frac{2\pi}{\omega_{\mathbf{k}} V}} \mathbf{e}_s(\mathbf{k}) [a_{\mathbf{k}} e^{i\mathbf{kr}} + a^{+}_{\mathbf{k}} e^{-i\mathbf{kr}}] \ , \tag{19}$$

where $\mathbf{A}(\mathbf{r})$ is a potential of the electromagnetic field; e_0 and m_0 are the electronic charge and mass ($e_0^2 \approx 1/137$); $a^{+}_{\mathbf{k}}$ and $a_{\mathbf{k}}$ are the creation and annihilation operators for a photon with wave vector $\mathbf{k}$, frequency $\omega_{\mathbf{k}}$, and polarization $\mathbf{e}_s(\mathbf{k})$; and V is the volume of the resonator.

The approximation of this Hamiltonian corresponding to the RQM involves accounting for only two states of the atom $\chi_\uparrow$ and $\chi_\downarrow$, for which the transition frequency is $\Delta = E_\uparrow - E_\downarrow$, close to the frequency of a distinct resonator for the mode, $\omega_{\mathbf{k}_0} = \omega$, $\omega_{\mathbf{k}_0} = \omega$, $a_{\mathbf{k}_0} = a$, and $a_{\mathbf{k}_0}^+ = a^+$, and using a dipole approximation in the interaction operator [17]. We assume also that the resonance mode has a certain polarization $\mathbf{e}_s(\mathbf{k}_0) = \mathbf{e}$. Then in the basis of the TLS we obtain

$$\hat{H} = \omega\left[\frac{\Delta}{2}\sigma_3 + f(a + a^+)\sigma_1 + \frac{2\pi e_0^2}{2m_0\omega^2 V}(a + a^+)^2 + a^+a\right], \quad f = -e_0 v\sqrt{\frac{2\pi}{\omega^3 V}}, \quad v = \frac{1}{m_0}\chi_\uparrow(\mathbf{pe})\chi_\downarrow. \tag{20}$$

If we neglect the "dipole" term, which is quadratic in the field, in this operator, then we obtain the Hamiltonian of the RQM; its spectrum was examined above, where it was shown that the RWA can be used for calculating it provided that

$$\xi = f\sqrt{\langle a\rangle} \approx e_0 \mid v \mid \sqrt{\frac{2\pi\bar{n}}{V\omega^3}} < 1, \tag{21}$$

where $\bar{n}$ is the average number of photons in the resonance mode of the field.

The matrix element of the velocity is expressed in terms of the dipole moment of the transition,

$$\mid v \mid = \omega\Delta \mid \langle\chi_\uparrow \mid (\mathbf{re}) \mid \chi_\downarrow\rangle \mid \approx d\Delta, \tag{22}$$

where d is the dipole matrix element of the LTS transition.

We express the average density of photons, $\bar{n}/V$, in terms of the energy density I of the electromagnetic field in the resonator as

$$\bar{n}/V\omega = I. \tag{23}$$

As a result, we obtain

$$\xi = \frac{e_0 d\Delta}{\omega}\sqrt{2\pi I}. \tag{24}$$

Thus, it is necessary to go beyond the RWA when describing the interaction of the atomic system with the field on the basis of a JQM if the energy density in the resonator

$$I > \frac{\omega^2}{2\pi e_0^2 d^2\Delta^2} \equiv I_c. \tag{25}$$

It should be pointed out that when the critical energy density after which it is necessary to go beyond the RWA is reached, the diamagnetic contribution to the operator (20) can be comparable to the term linear in the field, as noted in [15] and [27]. This circumstance can be taken into account using a canonical transformation of the field operators in the Hamiltonian (20) to reduce the quadratic form with respect to the field operators to a diagonal form. As a result, the operator (20) is reduced to a JQM Hamiltonian with renormalized parameters:

$$\hat{H} = \tilde{\omega}\left[\frac{\tilde{\Delta}}{2}\sigma_3 + \tilde{f}(a + a^+)\sigma_1 + a^+a\right],$$

$$\tilde{\omega} = \omega\sqrt{1+\lambda}, \quad \tilde{f} = \frac{f}{\sqrt{1+\lambda}}, \quad \tilde{\Delta} = \frac{\Delta}{\sqrt{1+\lambda}}, \quad \lambda = \frac{2\pi e_0^2}{m_0\omega^2 V}. \tag{26}$$

Therefore, including the diamagnetic contribution does not change the characteristic structure of the spectrum of the JQM, but the behavior of the energy levels of the system in the strong coupling limit may be substantially renormalized. As shown above, in this limit

$$E_{np} \approx \tilde{\omega}(n - \tilde{f}^2) = n\sqrt{1+\lambda} - \frac{f^2}{\sqrt{1+\lambda}} = n\sqrt{1 + \frac{2\pi e_0^2}{m_0\omega^2 V}} - \frac{\frac{2\pi e_0^2\Delta^2 d^2}{V\omega^3}}{\sqrt{1 + \frac{2\pi e_0^2}{m_0\omega^2 V}}}. \tag{27}$$

This formula can be used to estimate the radiative shift in the levels of this system.

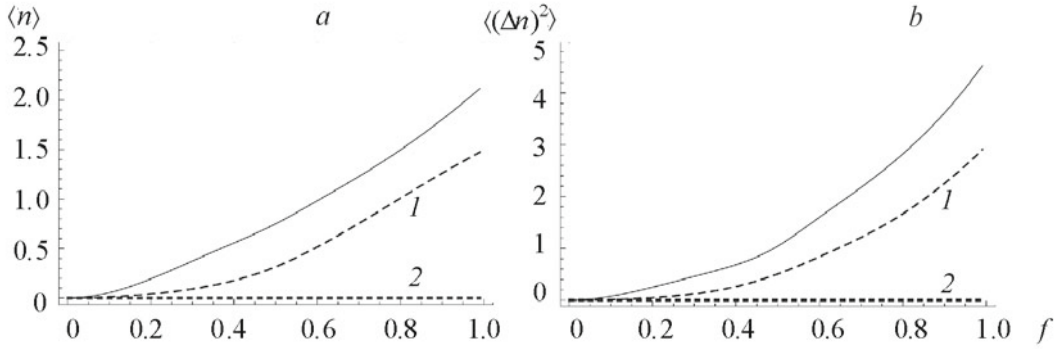

Fig. 4. Average number of photons (a) and variation in the number of photons (b) as functions of the coupling constant for the ground state of a JQM at resonance; numerical solution smooth curves; (1) USA; (2) RWA.

The change in the dynamics of a TLS in the strong coupling regime has been studied previously [20]. We now examine how including the "antirotational" terms in the JQM operator affects the statistical characteristics of an electromagnetic field in the resonator. For this we compare calculations of the following quantities based on the RWA and the USA.

The probability of detecting n quanta of the electromagnetic field at time t when the system was found in the state $\left| l, s \right\rangle \equiv \left| l \right\rangle \chi_s$ at time $t = 0$ is

$$P_n(t,f) = \sum_{s'} \left| \left\langle n, s' \mid \Psi(t) \right\rangle \right|^2 , \quad \left| \Psi(0) \right\rangle = \left| l, s \right\rangle . \tag{28}$$

In general this quantity is a rapidly oscillating function of time, but when the system is observed for a long enough time interval $T >> 1/\omega$, it approaches a constant value of

$$\left\langle P_n(f) \right\rangle = \frac{1}{T} \int_0^T P_n(t,\ f)dt \ = \ \sum_{s'mp} \left| \left\langle n,\ s' \mid \psi_{mp} \right\rangle \right|^2 \ \left| \left\langle l,\ s \mid \psi_{mp} \right\rangle \right|^2 \ . \tag{29}$$

This probability distribution can be used to find the average number of photons in the resonator

$$\left\langle n(f) \right\rangle = \sum_n n \left\langle P_n(f) \right\rangle , \tag{30}$$

and its variation [24]

$$\left\langle (\Delta n)^2 \right\rangle = \left\langle n^2(f) \right\rangle - \left\langle n(f) \right\rangle^2 \ . \tag{31}$$

Figure 4 shows the dependence of the average number of photons in the resonator and the variation in the number of photons, calculated numerically with the USA and RWA, as functions of the coupling constant. As noted above, the most substantial change in the spectrum of the state of a JQM shows up as a qualitative readjustment of the ground state of the system. In fact, when a TLS is placed in a resonator with a vacuum electromagnetic field, a nonzero electromagnetic field develops in the ground state of the resonator; this can be interpreted as the "generation" photons from the vacuum, as discussed in [28] in a numerical analysis of the states of a JQM. This effect does not exist in terms of the RWA, but is well described on the basis of the USA.

Conclusions. The efficiency of using a uniformly suitable analytic approximation of the operator method for describing stationary states and observed characteristics of the Rabi quantum model outside the rotating wave approximation is discussed. It is shown that this approximation is in good agreement with a numerical solution and describes all the qualitative features of the system being studied. A new "polaron" effect is described with formation of a bound state of the atom and field in the ground state of the system owing to the antirotational term in the original Hamiltonian.

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