Quasienergy of a two-level system in an intense monochromatic field

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A two-level system in an intense field is considered by taking into account nonresonance processes by the Hill method. An equation is obtained which expresses in an explicit manner the quasienergy as a function of the parameters of the problem. The convergence of the expansion of the Hill determinant residue in powers of the ratio of the interaction energy to the energy of a field quantum is investigated. Approximate expressions for the quasienergy spectrum are derived and are valid with a large degree of accuracy even when the expansion parameter approaches unity. In particular, a formula is obtained for the quasienergy in the case of n-photon resonance. The relation to the results of the adiabatic approximation is discussed. In the case of extremely small values of the expansion parameter, the familiar results of perturbation theory and of the resonance approximation are obtained.

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A two-level system is the simplest model for the investigation of the various phenomena of the interaction of electromagnetic radiation with atoms, spins, and nuclei. However, the most exhaustive results concerning the behavior of a two-level system in a strong field are obtained either in the resonance approximation (this is sometimes called the "spinning wave" approximation) [1] or in the adiabatic approximation. [2] Allowance for the non-resonant members greatly complicates the problem mathematically. Although by means of numerical methods one can find the quasi-energy of a two-level system as a function of the problem parameters, satisfactory analytic results, where non-resonant processes would be taken into account, are missing from the literature. In this paper the behavior of a two-level system in an intense monochromatic field is studied by the Hill method. [3] The region of applicability of the formulas obtained for the quasi-energy extends far beyond the limits of perturbation theory and the resonance approximation.

The initial equations describing the two-level system in a classical electromagnetic field and of the form

$$i\dot{a}=2Vb\cos\omega t,\quad i\dot{b}=\omega_0 b+2Va\cos\omega t. \tag{1}$$

where a and b are correspondingly the amplitudes of the ground and excited states of the system, $\hbar\omega_0$ is the distance between the levels, the quantity $-2\hbar V$ (the multiplier $2\hbar$ is inserted for convenience) represents the matrix element of the transition of the operator of the electric-dipole or magnetic-dipole interaction. From the system (1) we can obtain for a or b, a second-order equation whose coefficients are periodic functions of time but have singular points. The latter situation indicates that the Hill method must be applied directly to system (1). We represent the amplitudes in the form [4]

$$a=e^{-iEt}\sum_{n=-\infty}^{\infty}e^{in\omega t}a_n,\quad b=e^{-iEt}\sum_{n=-\infty}^{\infty}e^{in\omega t}b_n, \tag{2}$$

where $\hbar E$ is the quasi-energy. [5] Substituting (2) in (1) we obtain

$$a_n=\frac{V}{E-n\omega}(b_{n+1}+b_{n-1}),\quad b_n=\frac{V}{E-n\omega-\omega_0}(a_{n+1}+a_{n-1}). \tag{3}$$

We note first that system (3) breaks down into two systems. In the first, the a_n with even numbers combine with the b_n with odd numbers. The second subsystem is obtained from the first by replacing E with $E-\omega$. It is therefore sufficient to consider only one of them, say the first. We write down the corresponding determinant

$$\begin{gathered}D(E)=\det|\delta_{m,n}-(\delta_{m,n+1}+\delta_{m,n-1})\beta_m|,\\ \beta_m=V/(E-m\omega)\text{ for } m=0,\pm2,\pm4,\ldots,\\ \beta_m=V/(E-m\omega-\omega_0)\text{ for } m=\pm1,\pm3,\pm5,\ldots\end{gathered} \tag{4}$$

The basic analytic properties of the determinant, proven in the Appendix, are:

1) periodicity, i.e., $D(E+2\omega)=D(E)$;

2) a series of simple poles at the points $E=2\omega$, where n = 0, ±1, ±2, ..., with a residue R′, and a series of simple poles the points $E=2n\omega-\omega+\omega_0$, n = 0, ±1, ±2, ..., with residue R; it will be shown below that $R'=-R$;

3) $|D(E)|$ is bounded in the vicinity of an infinitely distant point, apart from the poles;

4) $D(E)\to1$ as $\operatorname{Im}(E)\to\infty$.

On the basis of the theorem on the partial-fraction expansion of a function [3] we can now write

$$D(E)=D(E_0)+R'\Sigma\left(\frac{1}{E-2n\omega}-\frac{1}{E_0-2n\omega}\right)+R\Sigma\left(\frac{1}{E-\omega_0+\omega-2n\omega}-\frac{1}{E_0-\omega_0+\omega-2n\omega}\right), \tag{5}$$

where E is an arbitrary point at which D(E) is analytic. Recalling the expansion of the cotangent

$$\operatorname{ctg}z=\frac{1}{z}+\sum_{n=1}\frac{2z}{z^2-\pi^2n^2} \tag{6}$$

the expression (5) can be rewritten in the form

$$D(E)=D(E_0)+\frac{\pi R'}{2\omega}\left(\operatorname{ctg}\frac{\pi E}{2\omega}-\operatorname{ctg}\frac{\pi E_0}{2\omega}\right)+\frac{\pi R}{2\omega}\left[\operatorname{ctg}\frac{\pi(E+\omega-\omega_0)}{2\omega}-\operatorname{ctg}\frac{\pi(E_0+\omega-\omega_0)}{2\omega}\right]. \tag{7}$$

If we now fix $\operatorname{Re}(E_0)$ and let $\operatorname{Im}(E_0)$ go to infinity, we get on the basis of the property 4)

$$D(E)=1+\frac{\pi}{2\omega}\left[R\operatorname{ctg}\frac{\pi(E+\omega-\omega_0)}{2\omega}+R'\operatorname{ctg}\frac{\pi E}{2\omega}\right]+\frac{i\pi}{2\omega}(R+R'). \tag{8}$$

Since D(E), R, and R′ are real, we conclude from (8) that $R'=-R$. Finally, we get for D the expression

$$D(E)=1+\frac{\pi R}{\omega}\frac{\sin\delta}{\cos(2\lambda+\delta)-\cos\delta}, \tag{9}$$

where

$$\delta=\frac{\pi}{2\omega}(\omega-\omega_0),\quad \lambda=\frac{\pi E}{2\omega}. \tag{10}$$

From the condition that the determinant vanish we obtain the spectrum of the quasi-energies

$$\cos(2\lambda+\delta)=\cos\delta-\frac{\pi R}{\omega}\sin\delta, \tag{11}$$

or, omitting the term $2n\omega$ in the right-hand side,

$$E=-\frac{1}{2}(\omega-\omega_0)\pm\frac{\omega}{\pi}\arccos\left(\cos\delta-\frac{\pi R}{\omega}\sin\delta\right). \tag{11'}$$

We will show how to obtain from (11) the result of perturbation theory. Let us suppose that all of the denominators in R are large compared to V; then in the first-order approximation in V/ω we have

$$R\approx 2\omega_0V^2/(\omega^2-\omega_0^2),$$
$$\cos(2\lambda+\delta)\approx\cos\delta-2\pi\frac{\omega_0}{\omega}\frac{V^2}{\omega^2-\omega_0^2}\sin\delta. \tag{12}$$

We are interested in that branch of the quasi-energy which goes to zero upon disappearance of the interaction. This denotes that $\lambda\ll 1$, and from (12) it follows that

$$E=2\omega_0V^2/(\omega^2-\omega_0^2). \tag{13}$$

Formula (13) can be obtained by applying standard perturbation theory to the system (3), where in the zeroth approximation $a_0 = 1$ and the remaining amplitudes are equal to zero.[6]

The determination of the quasi-energy spectrum has thus been reduced to a calculation of the determinant R. Since it is impossible to get a closed expression for R, we will explore the convergence of the expansion in powers of V. It is more convenient, however, to consider the determinants $R_1(\omega)$ and $R_2(\omega)$ [Eq. (A.6)]. Obviously one could write

$$R_1(\omega)=1-\Sigma\gamma_m+\sum_{m_1>m}\gamma_m\gamma_{m_1+1}+\ldots+(-1)^{k+1}\sum_{m_k>\ldots>m}\gamma_m\ldots\gamma_{m_k+k},$$
$$\gamma_m=\mu_m\mu_{m+1}. \tag{14}$$

Let us consider the relationship between two neighboring terms with sufficiently large numbers k and k + 1:

$$\left|\frac{R_{1,k+1}}{R_{1,k}}\right|=\left|\frac{\sum\gamma_m\ldots\gamma_{m_{k-1}+k-1}\gamma_{m_k+k}}{\sum\gamma_m\ldots\gamma_{m_{k-1}+k-1}}\right|\leqslant\sum_{m=2k+1}\gamma_m\approx 2\left(\frac{V}{2\omega}\right)^2\sum_{m=k}\frac{1}{m^2}$$
$$\approx\frac{2}{k}\left(\frac{V}{2\omega}\right)^2. \tag{15}$$

In deriving the inequality we made use of the positiveness of γ_{2k} for sufficiently large k. From (15) it follows that the expansion parameter is the quantity $2(V/2\omega)^2$ and the series converges at all values of this parameter. In addition, if $\omega>\omega_0$, all $\gamma_m>0$ and the series becomes sign-alternating, which allows us to obtain a better approximation if we limit ourselves to the first few terms of the series. We now calculate $R_1(\omega)$ and $R_2(\omega)$, retaining in them the lowest-order terms in V/ω:

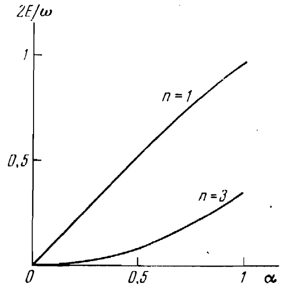
$$R_1(\omega)\approx 1-\sum_{m=1}\gamma_m,\quad R_2(\omega)\approx 1-\sum_{m=2}\gamma_m. \tag{16}$$

For $\delta\sim 1$ the discarded terms make a contribution of the order of $2(V/2\omega)^4$ to R_1 and R_2 or, introducing the parameter

$$\alpha=|2V/\omega|, \tag{17}$$

which is the ratio of the interaction energy to the energy of one quantum of the field, this contribution is of the order of $2(\alpha/4)^4$. Summing the series in (16), we obtain for R

$$\frac{1}{\omega}R=\frac{\alpha^2}{2}\frac{\omega\omega_0}{\omega^2-\omega_0^2}\left\{1+\frac{\alpha^2}{4}\frac{\omega^2}{\omega^2-\omega_0^2}\left[\frac{\pi\omega_0}{\omega}\operatorname{ctg}\delta-\frac{\omega^2+3\omega_0^2}{\omega^2-\omega_0^2}\right]\right\}. \tag{18}$$



This formula together with (11′) determines the quasi-energy spectrum. Far from resonance, when $\alpha\sim 1$, the value of R is determined accurate to $\sim 10^{-3}$. Close to the resonances, i.e., when ω approaches the values

$$\omega=\omega_0/n,\quad n=1,3,5,\ldots, \tag{19}$$

at which R has poles, the product R sin δ remains finite. In this case the value of R sin δ is determined accurate to 10^{-2}, i.e., the accuracy decreases near the resonances. Calculation of the more remote terms of the expansion R leads to rather cumbersome formulas. We note that when $\alpha\ll 1$ and $\delta\ll 1$ we obtain from (18) and (11) the usual result of the resonance approximation.[7]

If condition (19) is satisfied, the computation is significantly simplified and it is possible to retain the terms with α^6 in the expansion. Putting

$$\lim_{n\omega\to\omega_0}(n\omega-\omega_0)R=\omega^2r_n,\quad n=1,3,5,\ldots, \tag{20}$$

we get

$$E=\pm\frac{\omega}{\pi}\arccos\left(1-\frac{\pi^2}{2}r_n\right)=\pm\frac{2\omega}{\pi}\arcsin\left(\frac{\pi}{2}\sqrt{r_n}\right). \tag{21}$$

For r_n, according to (14), (20), and (A.6), we obtain

$$r_1=\left(\frac{\alpha}{2}\right)^2\left[1-\left(\frac{\alpha}{4}\right)^2\left(\frac{\pi^2}{3}+1\right)+\left(\frac{\alpha}{4}\right)^4\left(\frac{2\pi^4}{45}+\frac{2\pi^2}{3}-3\right)\right], \tag{22}$$

$$r_n=\frac{\alpha^4}{4}\frac{n^2}{(n^2-1)^2}\left[1-\alpha^2\frac{3n^2+1}{2(n^2-1)^2}\right],\quad n=3,5,7,\ldots \tag{23}$$

The figure shows a plot of the quasi-energy against the field intensity for one-photon or three-photon resonance. In connection with these results it is interesting to note the following: When $n\gg 1$, i.e., $\omega\ll\omega_0$, Eq. (1) can be solved in the adiabatic approximation[2]

$$a=e^{-iS(t)}A(t),\quad b=e^{-iS(t)}B(t), \tag{24}$$

where

$$S(t)=\frac{\omega_0}{2}\int^t\left[1\pm\left(1+16\frac{V^2}{\omega_0^2}\cos^2\omega t'\right)^{1/2}\right]dt'; \tag{25}$$

and A(t) and B(t) are time-periodic functions with period $2\pi/\omega$. From (24) and (25) it follows that the quasi-energy in this approximation is equal to

$$E=\frac{\omega_0}{2}\left[1\pm\int_0^{2\pi}\left(1+4\alpha^2\frac{\omega^2}{\omega_0^2}\cos^2\varphi\right)^{1/2}\frac{d\varphi}{2\pi}\right]. \tag{26}$$

It is easy to verify that when $\omega_0/\omega=n\gg 1$ the first terms of the expansion of the quasi-energies given by (21) and (26) in powers of α coincide, but those terms whose numbers are commensurate with n give different results. This is natural, for since the resonant nature of the interaction is not taken into account in the adiabatic approximation, it follows that an important contribution to (21)—(23) is made precisely by the resonant pole terms.

We can also note that in a degenerate two-level system ($\omega_0 = 0$) the quasi-energy vanishes, since R is an odd function of ω_0. The degenerate case is considered in detail in [8], where various corrections at small ω_0 are also computed.

It is known that the quasi-energy determines the emission and absorption spectra of an atomic system in an intense monochromatic field, i.e., it can be directly observed experimentally. For $\alpha \sim 1$ the most fitting object for the applications of our calculations is a particle with spin $1/2$ in a magnetic field, for if the frequency ω lies in the optical region the external field becomes comparable with the atomic field and the two-level idealization no longer has meaning.

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APPENDIX

Assume that in (4) the indices m and n take on values from $-N$ to N. We designate the corresponding determinant D_N. It must be proven that as $N \to \infty$ the determinant D_N tends to a particular limit, i.e., it converges. The result is obtained by applying to D_N^2 the main attribute of the convergence of infinite determinants [3], recognizing that D_N does not change its value when V is replaced by $-V$. Actually, the product of the diagonal elements in $D_N^2 = D_N(E, V)D_N(E, -V)$

$$\prod\left[1-\frac{V^2}{(E-n\omega)(E-n\omega-\omega+\omega_0)}-\frac{V^2}{(E-n\omega)(E-n\omega+\omega+\omega_0)}\right]$$

converges by virtue of the absolute convergence of the sum

$$\sum\left|\frac{1}{(E-n\omega)(E-n\omega-\omega+\omega_0)}\right|.$$

The sum of all the non-diagonal elements also converges absolutely. A determinant that converges in the sense of this attribute has all of the properties of finite determinants.

To prove periodicity it is sufficient to note that replacement of E by E + 2ω merely shifts the row numbers, i.e., D(E) remains unchanged. If one expands the determinant in terms of the elements of some row, it will be discovered that D(E) has simple poles at the points where convergence of the sums written out above is violated. By virtue of the inequality

$$|\det|\delta_{ik}+a_{ik}||\leqslant\prod_i\left(1+\sum_k|a_{ik}|\right)\leqslant\exp\left\{\sum_{i,k}|a_{ik}|\right\} \tag{A.1}$$

we have

$$|D^2|\leqslant e^s,$$

$$s=4V^2\sum\left(\left|\frac{1}{(E-n\omega)(E-n\omega+\omega_0-\omega)}\right|+\left|\frac{1}{(E-n\omega)(E-n\omega+\omega_0+\omega)}\right|\right) \tag{A.2}$$

from which the property 3) follows. Now let us expand D^2 in powers of V^2:

$$D^2=1+\sum_{m=1}A_m, \tag{A.3}$$

where $A_m \sim V^{2m}$, and we take into account the fact that

$$|A_m|\leqslant s^m/m!. \tag{A.4}$$

Actually, all of the terms of A_m are contained in s^m; furthermore, each of them enters m! times in s^m; besides, s^m contains additional terms that do not appear in the expansion of the determinant. Since $s \to 0$ as $\mathrm{Im}(E) \to \infty$, it follows from the inequality

$$|D^2-1|\leqslant\sum_{m=1}|A_m|\leqslant\sum_{m=1}\frac{s^m}{m!}=e^s-1 \tag{A.5}$$

that $D^2 \to 1$ as $\mathrm{Im}(E) \to \infty$. Taking into account the continuity as $V \to 0$, we find that $D(E) \to 1$.

Let us consider now the residue of D at $E = \omega_0 - \omega$. The value of R can be represented in the form

$$R=\frac{V^2}{\omega-\omega_0}R_1(-\omega)R_2(\omega)-\frac{V^2}{\omega+\omega_0}R_1(\omega)R_2(-\omega), \tag{A.6}$$

where $R_1(\omega)$ has the following structure:

$$R_1(\omega)=\det\begin{vmatrix}1 & \mu_1 & & & \\ \mu_2 & 1 & \mu_2 & & \\ & \mu_3 & 1 & \mu_3 & \\ & & \mu_4 & 1 & \mu_4 \\ & & \ldots & \ldots & \ldots\end{vmatrix}, \tag{A.7}$$

$$\mu_n=V/(\omega_0-n\omega),\quad n=1, 3, 5,\ldots,$$
$$\mu_n=(-V/n\omega),\quad n=2, 4, 6,\ldots,$$

$R_2(\omega)$ is obtained from $R_1(\omega)$ by deleting the first row and the first column.

[1] M. L. Ter-Mikaelyan, Lektsii po resonansnoĭ nelineinoĭ optike (Lectures on Resonant Nonlinear Optics), Preprint IFI-74-11, Erevan, 1970.

[2] D. F. Zaretskiĭ and V. P. Krainov, Zh. Eksp. Teor. Fiz. 66, 537, 1974 [Sov. Phys.-JETP 39, 257 (1974)].

[3] E. T. Whittaker and G. N. Watson, Modern Analysis, Cambridge, 1927.

[4] V. I. Ritus, Zh. Eksp. Teor. Fiz. 51, 1544, 1966 [Sov. Phys.-JETP 24, 1041 (1967)].

[5] Ya. B. Zel'dovich, ibid. 51, 1492, 1966 [24, 1066 (1967)].

[6] N. D. Sen Gupta, J. Phys. A., Gen. Phys. 3, 618, 1970.

[7] M. L. Ter-Mikaelyan and A. O. Melikyan, Zh. Eksp. Teor. Fiz. 58, 281, 1970 [Sov. Phys.-JETP 31, 153 (1970)].

[8] V. P. Yakovlev, ibid. 67, 921, 1974 [40, 457 (1975)].

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