High-precision quasienergies for a driven two-level atom at the two-photon preresonance

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A computation with unprecedented precision is presented for quasienergies of a two-level atom in a monochromatic radiation on the basis of a recently obtained exact expression [D.-S. Guo *et al.*, Phys. Rev. A **73**, 023419 (2006)]. We start with the proof of an expression theorem. With this theorem the quasienergies for any two-level atom can be expressed in terms of the quasienergies for only those with the original energy spacing (per field photon energy) being an integer (preresonances). Then we carry out a numerical evaluation of the quasienergies at the two-photon preresonance, which involves computing an infinite determinant, up to the 18th power of the coupling strength. The theoretical prediction presents an experimental challenge for high-precision tests of quantum mechanics and could be exploited for precise calibration of high laser intensities.

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In a recent paper [1], a closed expression for quasienergies exhibiting explicit Floquet periodicity, together with the corresponding wave functions, is derived for a two-level atom in a monochromatic radiation field without any restriction on the range of the parameters. The study of the two-level atom [2] in a radiation field has occupied a central position in quantum optics (see, e.g., [3–6]). The ultimate goal of quantum optics is to achieve a complete understanding of atoms interacting with radiation fields. To reach this goal, the most important thing is to obtain accurate wave functions with corresponding accurate quasienergies for an arbitrary atom (or ion) interacting with a radiation field. A real atom (or ion) has an infinite number of energy levels, which may include a finite number of bound-state energy levels (occupied or nonoccupied ground states), an enumerable infinite number of excited states (occupied or nonoccupied Rydberg states), and a nonenumerable infinite number of states in its continuous spectrum. With present computing techniques, all continuous quantities are discretized to sets of finite numbers. Thus the N-level atom model with an arbitrarily large N number is an appropriate way to describe a real atom.

The importance of the model of a two-level atom in a radiation field is in the following two aspects. (i) The model can apply to many physical systems directly—e.g., atoms in a laser field when the laser frequency is near a transition frequency between two levels of a real atom and a two-level system of magnetic resonances. (ii) The model is the first step in the development of an accurate theory for the N-level atom in radiation fields: Analytic or numerical techniques for solving a driven two-level system may be generalized to the driven N-level system; and as a necessary condition, the analytical and numerical solutions for a driven two-level atom will provide strong checks for the correctness of the solutions for a driven N-level atom. Now, obtaining accurate analytic and numerical solutions for an arbitrary N-level atom is in our short-term plan. Thus an accurate numerical solution for a two-level atom plays a key role in our current and future researches.

There is a vast literature on the two-level atom in a monochromatic classical field described by the Bloch equation [7]. Analytic methods with various approximations have been used (see, e.g., [3–6]), while numerically accurate, direct integration of the Bloch equation in strong radiation fields still remains elusive, because the pertinent time-dependent differential equations involve discrete quasienergies and discrete boundary conditions to be determined.

The closed expression for quasienergies obtained in Ref. [1] involves infinite determinants. Numerical evaluations of these infinite determinants involve some complicated algebraic manipulations, such as multiple infinite series and infinite products, which cannot be found in any mathematics textbook. One of the main purposes of the present paper is to demonstrate, with physically interesting examples, how to evaluate these infinite determinants in a numerically satisfactory fashion. Moreover, the precise numerical values of quasienergies provide theoretical predictions which can be put to precise experimental tests and exploited to calibrate laser intensities. The techniques developed here are useful for evaluating quasienergies and wave functions at any preresonance. The special case we are presenting here is when the level spacing 2Δ is twice the photon energy ω of the radiation. We call this the two-photon *preresonance*, which has been proven [1] to be not a true resonance. (The true resonances occur only when the radiation-*shifted* level spacing is an integral multiple of the laser-photon energy, such as Freeman resonances in above-threshold photoelectron spectra [8].) However, as shown below, the preresonance cases play a very important role in calculating quasienergies for a generic value of $2\Delta/\omega \neq n$, since those quasienergies can be expressed in terms of all quasienergies only at the preresonances.

Theorem 1. The quasienergies of a driven two-level atom whose original spacing (before interacting with the driving radiation field) is a nonintegral multiple of the photon energy of the driving field can be expressed in terms of the quasienergies of all two-level atoms with an integral original spacing interacting with the same radiation field.

Proof. In Ref. [1], the quasienergy when the original spacing $2\Delta \neq$ integer (we set $\omega=1$, as in Ref. [1]), the quasienergies can be expressed as any one of the following two expressions:

$$E=\frac{1}{\pi}\cos^{-1}\sqrt{\cos^2(\pi\Delta)+\pi R_+\sin(2\pi\Delta)}\quad(2\Delta\neq n),$$

$$E=\frac{1}{\pi}\sin^{-1}\sqrt{\sin^2(\pi\Delta)-\pi R_+\sin(2\pi\Delta)}\quad(2\Delta\neq n),\quad(1)$$

where, for notation simplification, we do not write the additive arbitrary integer explicitly. In the square root of above equations, R_+ has an expression

$$R_+=\sum_{n=1}^{\infty}\frac{4\Delta}{4\Delta^2-n^2}r_n,\quad(2)$$

where the residues r_n relate to the quasienergies of the two-level atoms with the original spacing $2\Delta=$integer as

$$E_{2k-1}=\frac{1}{\pi}\cos^{-1}(\pi\sqrt{-r_{2k-1}})\quad(2\Delta=2k-1),$$

$$E_{2k}=\frac{1}{\pi}\sin^{-1}(\pi\sqrt{-r_{2k}})\quad(2\Delta=2k)\quad(k=1,2,3,\ldots),\quad(3)$$

which can be converted to

$$r_{2k-1}=-\frac{1}{\pi^2}\cos^2(\pi E_{2k-1})\quad(2\Delta=2k-1),$$

$$r_{2k}=-\frac{1}{\pi^2}\sin^2(\pi E_{2k})\quad(2\Delta=2k)\quad(k=1,2,3,\ldots).\quad(4)$$

Thus we have

$$R_+=-\frac{1}{\pi^2}\sum_{k=1}^{\infty}\left[\frac{4\Delta}{4\Delta^2-(2k-1)^2}\cos^2(\pi E_{2k-1})+\frac{4\Delta}{4\Delta^2-(2k)^2}\sin^2(\pi E_{2k})\right].\quad(5)$$

Now, the quasienergies for any two-level atom with an arbitrary original spacing are expressed in terms of the quasienergies of all preresonance cases through Eqs. (1), (3), and (5). Q.E.D.

According to this theorem, the entire calculations of the quasienergies of two-level atoms, where the original spacing 2Δ is an arbitrary number, greatly reduce to the calculations in the preresonance cases, where $2\Delta=$integer. The application of this theorem is not limited to the exact solutions obtained in [1]. For example, one may develop other solution techniques to get the quasienergies from other methods without calculating the residues r_n, such as solving the differential equation set directly. This theorem tells us that we can just concentrate on the preresonance cases in quasienergy calculations with any kind of solution techniques.

In the following, we show the detailed evaluation process for r_2. The mathematical technique developed here should be useful for future calculations for $r_1, r_3, r_4, \ldots$.

We proceed to present details of evaluating r_2. The quasienergy at the two-photon preresonance is given by $E_2=\pm\frac{1}{\pi}\sin^{-1}(\pi\sqrt{-r_2})$, with r_2 being the following determinant infinite in the two directions along the main diagonal:

$$r_2=\begin{vmatrix}
1 & \frac{4D}{3\times5} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots\\
\frac{3D}{2\cdot4} & 1 & \frac{3D}{2\times4} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots\\
\cdots & \frac{2D}{1\times3} & 1 & \frac{2D}{1\times3} & \cdots & \cdots & \cdots & \cdots & \cdots\\
\cdots & \cdots & \frac{D}{2} & 0 & \frac{D}{2} & \cdots & \cdots & \cdots & \cdots\\
\cdots & \cdots & \cdots & 0 & 1 & 0 & \cdots & \cdots & \cdots\\
\cdots & \cdots & \cdots & \cdots & \frac{D}{2} & 0 & \frac{D}{2} & \cdots & \cdots\\
\cdots & \cdots & \cdots & \cdots & \cdots & -\frac{2D}{3\times1} & 1 & -\frac{2D}{3\times1} & \cdots\\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & -\frac{3D}{4\times2} & 1 & -\frac{3D}{4\times2}\\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & -\frac{4D}{5\times3} & 1
\end{vmatrix}.\quad(6)$$

We simplify this determinant by multiplying and dividing the row and the column crossing each main-diagonal element 1 by the same factor, respectively, and then break it into the product of two subdeterminants with equal value, resulting in $r_2=-\frac{D^4}{9}r_2'^2$, where r_2' is a half-infinite determinant (infinite in the down-right direction):

$$r_2' = \begin{vmatrix} 1 & \frac{D}{2} & \cdots & \cdots & \cdots & \cdots \\ \frac{D}{5} & 1 & \frac{D}{3} & \cdots & \cdots & \cdots \\ \cdots & \frac{D}{6} & 1 & \frac{D}{4} & \cdots & \cdots \\ \cdots & \cdots & \frac{D}{7} & 1 & \frac{D}{5} & \cdots \\ \cdots & \cdots & \cdots & \frac{D}{8} & 1 & \frac{D}{6} \\ \cdots & \cdots & \cdots & \cdots & \frac{D}{9} & 1 \end{vmatrix}. \tag{7}$$

The quasienergies are now given by

$$E_2 = \pm \frac{1}{\pi}\sin^{-1}\left(\frac{\pi}{3}D^2 r_2'\right). \tag{8}$$

We have developed techniques to calculate exactly the coefficients of the expansion of r_2' in D^2,

$$r_2' = 1 - K_1 D^2 + K_2 D^4 - K_3 D^6 + K_4 D^8 + \cdots, \tag{9}$$

in terms of the partial sums

$$\psi(n) = \sum_{k=1}^{n} \frac{1}{k+1}, \quad \phi(n) = \sum_{k=1}^{n} \frac{1}{k^2}. \tag{10}$$

Define $\chi(n)=1/n(n+3)$; then,

$$K_1 \equiv \sum_{n\geq 2} \chi(n) = \frac{13}{36}, \tag{11}$$

$$K_2 \equiv \sum_{n,j\geq 2} \chi(n)\chi(n+j) = \frac{1}{9}\left(\frac{373}{180} - \frac{\pi^2}{6}\right), \tag{12}$$

$$\begin{aligned} K_3 &\equiv \sum_{n,j,l\geq 2} \chi(n)\chi(n+j)\chi(n+j+i) \\ &= \frac{1}{27}\left\{\sum_{m=2}^{4}\frac{1}{m}\sum_{n=2}^{m}\frac{1}{n}\psi(n) - \sum_{n=4}^{5}\frac{1}{n}\psi(n) + \sum_{n=1}^{2}\frac{1}{n}[\psi(n+3)-\psi(3)] + \sum_{n=2}^{4}\frac{1}{n^2}[\psi(n+3)-\psi(3)]\right\} \\ &\quad - \frac{1}{27}\left\{\left[\frac{1}{4}+\frac{\pi^2}{6}-\phi(4)\right]\psi(3) + \sum_{m=1}^{2}\frac{1}{m+2}\sum_{n=1}^{m}\frac{1}{n}[\psi(n+3)-\psi(3)]\right\} - \frac{2}{27}\left[\frac{\pi^2}{6}\psi(3) - \sum_{n=2}^{4}\frac{1}{n}\phi(n+4)\right] \\ &= 3.278683997349973\ldots \times 10^{-3}, \end{aligned} \tag{13}$$

$$K_4 = \sum_{n,j,l,k\geq 2} \chi(n)\chi(n+j)\chi(n+j+l)\chi(n+j+l+k) = 1.402452866666796\ldots \times 10^{-4}. \tag{14}$$

The above exact expression of K_3 gives the reader a flavor of what is going on. For K_4, to save space we did not present its exact expression, but its numerical value to high precision. Similarly the higher-order coefficients are calculated to be [9]

$$K_5 = 4.089694836636745\ldots \times 10^{-6}, \tag{15}$$

$$K_6 = 8.661234370774032\ldots \times 10^{-8}, \tag{16}$$

$$K_7 = 1.393524486588925\ldots \times 10^{-9}, \tag{17}$$

and

$$K_8 = 1.761826370939839\ldots \times 10^{-11}. \tag{18}$$

With these coefficients, the quasienergies can be calculated up to order D^{18}. Our method is applicable to any desired higher order.

We have carried out a numerical evaluation using the above coefficients. We set $D=0.6$ in a sample calculation. (For a hydrogen atom in a laser field of wavelength 243.2 nm, the transition between a $2p$ state and the $1s$ state is at two-photon preresonance; when the intensity is 2×10^{14} W/cm^2, the corresponding dipole coupling has approximately the value $D=0.6$.)

A quasienergy calculated by using above coefficients up to K_7 is $-0.107\ 131\ 400\ 930\ 337\ldots$. The precision of this evaluation is estimated to be better than 15 figures: From Eq. (8) the error due to neglecting K_8 and higher-order terms satisfies

$$|\delta E_2| \leq \frac{1}{3}\frac{1}{\cos(\pi E_2)} K_8 D^{18} \leq 1\times 10^{-15}, \tag{19}$$

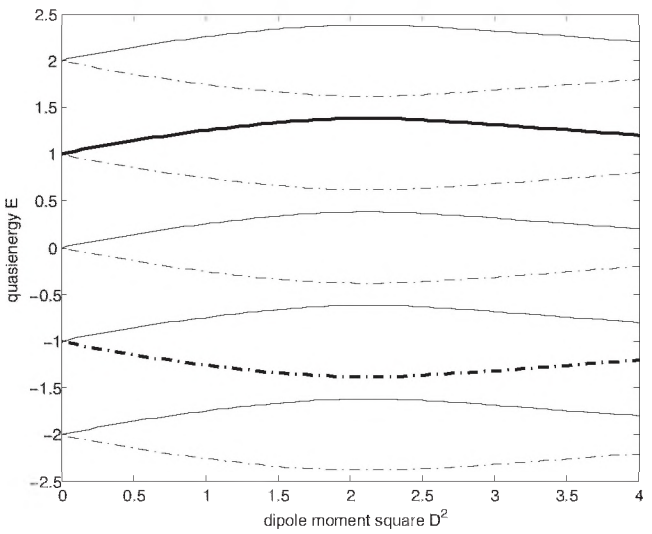

FIG. 1. The two thick lines are the main quasienergy levels, the upper one (solid line) and the lower one (dot-dashed line), which reduce to the original two levels, respectively, when the dipole moment vanishes. The thin lines, in each respective group, are quasienergy levels derived by the Floquet periodicity.

which means the 15 figures for this quasienergy are all accurate.

To compare, the quasienergy from the usual rotating-wave approximation (RWA) calculation is −1.083 095 189 4 (or −0.083 095 189 4 by the Floquet theorem). Its error is about 22%. The quasienergy from an improved RWA result [1] is −1.120 483 682 2 (or −0.120 483 682 2 by the Floquet theorem), still with an error of 12%. High precision of the predicted quasienergy is clearly guaranteed by the analytically exact expression.

In Fig. 1, we present the quasienergy spectrum, calculated at the two-photon preresonance, versus the dimensionless dipole coupling squared, D^2. Recall that the energy-level spacing is 2 (twice the photon energy) at $D^2=0$ and we have chosen the zero energy to be at the midpoint of the two levels in the absence of a radiation field (i.e., at $D=0$), so the quasienergy spectrum is symmetric with energy zero. The quasienergy shift, corresponding to the well-known Bloch-Siegert (BS) shift [7], increasing with D^2, is shown by the two thick lines. The thin lines are the quasienergies due to the Floquet periodicity: There are two sets of quasienergies [10], corresponding to the quasistationary states derived from the original two levels. For any two quasienergies, if their difference (or sum) is always an integral multiple of photon energy, then they belong to the same (or the distinct) quasistationary states. A weak probe laser beam with appropriate frequency (allowing small detuning) can induce a transition between two quasienergies belonging to distinct quasistationary states. This may be used to test the predicted quasienergies with high precision. To test the nonperturbative nature of our results, we note that a transition induced by a probe beam may happen even between quasienergies with spacing smaller than the original spacing.

In the driven two-level atom model, various atomic effects that affect the atomic levels and wave functions show up only through two parameters: the level spacing 2Δ and the coupling strength D. As shown in Eq. (8), the quasienergy at the preresonance depends only on the coupling D. With this advantage, the measurements of the quasienergy at the two-photon preresonance may provide a new possibility to test quantum *mechanics* to high precision.

Moreover, since the coupling strength D^2 is proportional to the driving laser intensity, measurements of quasienergy at the two-photon preresonance can also be used for calibration of laser intensities with high precision. For example, for the $2p$-$1s$ transition of a hydrogen atom in two-photon preresonance, we have

$$D^2 = |D_{12}|^2 = 2^{11} \times 3^{-8} \alpha \frac{\lambda}{2\pi a_0} u_p. \tag{20}$$

Here $\lambda = 2\pi/\omega$ is the photon wavelength, $\alpha = 1/m_e a_0$ the fine-structure constant, and $u_p = 2\pi e^2 I/m_e \omega^3$ is the ponderomotive parameter—i.e., the ponderomotive energy per field-photon energy, with I being the light field intensity. We see that D^2 is proportional to u_p or to I, numerically, when the field intensity $I = 2.00 \times 10^{14}$ W/cm^2 (or 1.00×10^{15} W/cm^2), $u_p = 0.216$ (or $u_p = 1.08$), and $D^2 = 0.360$ (or $D^2 = 1.80$). The corresponding quasienergies can be easily read from Fig. 1.

The demonstration here for evaluating the infinite determinant r_2 for two-photon preresonance up to high precision gives us confidence that the other preresonance cases can be dealt with in a similar way. According to the theorem proved in this paper, quasienergies for a generic driven two-level atom could be calculated with high precision after the calculation of r_1, r_3, r_4, etc.

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[1] D.-S. Guo, Y.-S. Wu, and L. Van Woerkom, Phys. Rev. A **73**, 023419 (2006).
[2] A. Einstein, Phys. Z. **18**, 121 (1917).
[3] J. H. Eberly and P. W. Milonni, in *Encyclopedia of Physical Science and Technology*, edited by R. Myers (Academic Press, New York, 1987), Vol. II, pp. 471–502.
[4] C. Cohen-Tannoudji, J. Dupont-Roc, and C. Fabre, J. Phys. B **6**, L214 (1973).
[5] R. Loudon, *The Quantum Theory of Light*, 2nd ed. (Oxford University Press, New York, 1983).
[6] M. Sargent III, M. O. Scully, and W. E. Lamb, Jr., *Laser Physics* (Addison-Wesley, London, 1973).
[7] F. Bloch and A. Siegert, Phys. Rev. **57**, 522 (1940).
[8] R. R. Freeman, P. H. Bucksbaum, H. Milchberg, S. Darack, D. Schumacher, and M. E. Geusic, Phys. Rev. Lett. **59**, 1092 (1987).
[9] Y. Wang (private communication).
[10] Ya. B. Zel'dovich, Sov. Phys. JETP **24**, 1006 (1967).