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RESEARCH ARTICLE

Exact wave functions for atomic electron interacting with photon fields

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Many nonlinear quantum optical physics phenomena need more accurate wave functions and corresponding energy or quasienergy levels to account for. An analytic expression of wave functions with corresponding energy levels for an atomic electron interacting with a photon field is presented as an exact solution to the Schrödinger-like equation involved with both atomic Coulomb interaction and electron–photon interaction. The solution is a natural generalization of the quantum-field Volkov states for an otherwise free electron interacting with a photon field. The solution shows that an N-level atom in light form stationary states without extra energy splitting in addition to the Floquet mechanism. The treatment developed here with computing codes can be conveniently transferred to quantum optics in classical-field version as research tools to benefit the whole physics community.

Keywords Volkov–Coulomb problem, driven N-level atom, exact wave functions and energy levels, non-perturbative quantum electrodynamics, strong laser fields

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The main purpose of this paper is to present an exact solution for an atomic electron interacting with both atomic Coulomb field and photon field. An interacting quantum–mechanic system can be described by a Schrödinger equation with interaction terms, but only few of them can be solved exactly. In 1935, Volkov [1] published an exact solution to the Dirac equation for an otherwise free electron interacting with an electromagnetic plane wave. The so-called Volkov–Coulomb (VC) problem is the one for obtaining wave functions and corresponding energy levels of a system which contains an electron interacting with both the atomic Coulomb potential and the potential due to the electron–light interaction. On the theoretical side, this problem is a long-standing unsolved basic problem. On the experimental side, many nonlinear phenomena have been discovered in strong laser physics since late 70s, such as above-threshold ionization (ATI), Freeman resonances, high harmonic generations (HHG), Kapitza–Dirac (KD) effect, tomographic reconstruction of atomic orbits, and so on. In quantum information physics, detailed studies on multi-level atom in laser fields are needed. All theoretical analyses on these physics effects need more accurate wave functions for atoms interacting with light. The recent, exact solution for a driven two-level atom [3] shows that the true resonances are Freeman resonances [4] where an integer number of field-photon energy coincides with the interaction-shifted energy spacing.

The history of exact solutions for otherwise free electron interacting with quantum field of light is also long. Berson found solutions to the Dirac equation for the quantized single-mode linearly polarized em wave in the Bargman representation; Bergou et al. found solutions to the Dirac equation in quantized single-mode circularly polarized em plane wave [5–7]. During the past years, this author and his collaborators obtained exact solutions for a relativistic electron interacting with an arbitrarily polarized single-mode photon field [8, 9] and that interacting with multi-mode photon field in one propagation direction [10]. We also found solutions for a non-relativistic electron interacting with multi-mode photon fields in multiple propagation directions [11–13]. These quantum-field Volkov solutions and the scattering theory [14], as the main part of the nonperturbative quantum electrodynamics (NPQED) theory, have been used in the treatment of multi-photon ionizations in strong laser fields. A notable success of the NPQED theory was the interpretation of the half Kapitza–Dirac effect [2, 15, 16].

To solve the VC problem, two assumptions can be made as the starting points: 1) N-level atom. For a real atom, it contains a finite number of non-excited bound states, an enumerable sequence of excited bound states, and a non-enumerable number of continuum states. With reasonable cutoff on highly excited states and by discretizing the continuum states, one may express a real atom as an N-level atom. ii) Known atom. There is no reason to solve the equation of motion for an atom interacting with light if the wave-functions and the corresponding energy levels of the atom are previously unknown. Atomic physicists have many fruitful results for atomic wave functions from Hartree [17] and Slater's [18] pioneer work till progress in recent years [19, 20]. All many-body atomic wave functions can be expressed in terms of single-body wave functions. Most of these single-body wave functions have analytical expressions on the angular part with numerical expressions on the radial part. These known wave functions can all be used as input parameters in the current solution scheme.

To treat atoms in strong laser field, some numerical techniques have been developed to solve the time-dependent Schrödinger equation for a simple atom, say a hydrogen or helium atom, interacting with classical light. These numerical solutions and applications can be seen in references [21–23]. In the solution processes to the time-dependent Schrödinger equation, the Floquet formulation is frequently used [24, 25].

It has been proved that the Schrödinger eigenvalue equation for a non-relativistic electron interacting with a photon field cannot preserve the light-like property of the photon field. This problem was removed by introducing the Schrödinger-like equation [26], which describes a non-relativistic (NR) atomic electron in a single-mode photon field as

$$\left\{\frac{1}{2m_e}[-\mathrm{i}\nabla - e\boldsymbol{A}(-\boldsymbol{k}\cdot\boldsymbol{r})]^2 + \omega\hat{N} + U(\boldsymbol{r})\right\}\Psi(\boldsymbol{r}) = \mathcal{E}(\hat{N})\Psi(\boldsymbol{r}) \tag{1}$$

where

$$\mathcal{E}(\hat{N}) \equiv \frac{1}{2m_e}[(p_0 - \omega\hat{N})^2 - m_e^2] + \omega\hat{N} \tag{2}$$

and $\hat{N} \equiv (aa^\dagger + a^\dagger a)/2$ is the number operator of the photon field. In the current approach, the atomic Coulomb potential $U(\boldsymbol{r})$ can be assumed to be of a quite general type, such as an arbitrarily central, local or nonlocal potential. One will find that the word "central" can even be removed or weakened after the main result is derived. The single-mode photon field is described by

$$\boldsymbol{A}(-\boldsymbol{k}\cdot\boldsymbol{r}) = g(\epsilon\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}a + \epsilon^*\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}a^\dagger)$$

and $g = (2V_\gamma\omega)^{-1/2}$, V_γ being the normalization volume of the photon field. The polarization vectors ϵ and ϵ^* are defined by the relations

$$\epsilon\cdot\epsilon^* = 1, \quad \epsilon\cdot\epsilon = \cos\xi\mathrm{e}^{\mathrm{i}\Theta}, \quad \epsilon^*\cdot\epsilon^* = \cos\xi\mathrm{e}^{-\mathrm{i}\Theta}$$

The angle ξ is the degree of polarization. For example

$$\epsilon = [\epsilon_x\cos(\xi/2) + \mathrm{i}\epsilon_y\sin(\xi/2)]\mathrm{e}^{\mathrm{i}\Theta/2}$$

The final version of the exact expression of the wave-function for an atomic electron interacting with a photon field is

$$\Psi(\boldsymbol{r}) = V_e^{-1/2}\int\frac{\mathrm{d}^3\boldsymbol{P}}{(2\pi)^3}\sum_{\gamma\alpha js}\mathrm{e}^{\mathrm{i}[\boldsymbol{P}+(u_p-j)\boldsymbol{k}]\cdot\boldsymbol{r}} \times C_{\gamma s}\mid n_0+j+s\rangle\mathcal{X}_{-j}(z_1^{(\gamma)}, z_2)K_\alpha^{(\gamma)}\Phi_\alpha(\boldsymbol{P}) \tag{3}$$

where $\Phi_\alpha(\boldsymbol{P})$ stands for the atomic momentum wave function of the αth orbit. Here the Greek indices α and γ denote the order of atomic states and the English indices j and s denote the transferred photon numbers with n_0 being the surrounding photon numbers. For this wave function, the corresponding energy eigenvalue or the total energy of the two-potential system, is

$$p_0 = m_e + E + \left(n_0 + \frac{1}{2} + u_p\right)\omega \tag{4}$$

In the expression of the wave function, $\{\boldsymbol{K}^{(\gamma)}\}$ is a set of N-dimensional column vectors with a unit length. We choose the vector $\boldsymbol{K}^{(\gamma)}$ as the γth eigenvector of the matrix Z given by Eq. (10) and Eq. (11) in the later context.

The generalized phased Bessel (GPB) functions of complex variables are defined as [27]

$$\mathcal{X}_j(z_1, z_2) \equiv \sum_{r=0}^{\pm\infty}\mathrm{X}_{j-2r}(z_1)\mathrm{X}_r(z_2) \tag{5}$$

in terms of single phased Bessel functions of one complex variable,

$$\mathrm{X}_j(z) = \mathrm{J}_j(\mid z\mid)\mathrm{e}^{\mathrm{i}j\arg(z)} \tag{6}$$

The detailed evaluation of z_1 and z_2, in the large-photon-number (LPN) limit, are

$$z_1 = 2\left(\sqrt{\frac{u_p}{m_e\omega}}\right)\boldsymbol{p}\cdot\epsilon$$

$$z_2 = \frac{1}{2}u_p\cos\xi\mathrm{e}^{\mathrm{i}\Theta} \tag{7}$$

where u_p is the ponderomotive energy per laser-field photon energy given below:

$$u_p = \frac{2\pi e^2 I}{m_e \omega^3} \tag{8}$$

where I is the intensity of the light beam. The fine structure constant is defined as $\alpha \equiv e^2$. (If $\alpha \equiv e^2/(4\pi)$, the 2π factor in the last expression should be replaced by 1/2.) The second variables of different GPB functions are the same since u_p does not depend on $\boldsymbol{p}$ in the NR electron case. The variable z_1 can be directly used as the first argument in the GPB function for the otherwise-free electron case. While in the two-potential case it is calculated with the eigenvectors $\boldsymbol{K}^{(\gamma)}$ of matrix Z,

$$Z\boldsymbol{K}^{(\gamma)} = \lambda^{(\gamma)}\boldsymbol{K}^{(\gamma)} \tag{9}$$

which has elements

$$z_{\alpha\beta} \equiv \int \frac{\mathrm{d}^3\boldsymbol{P}}{(2\pi)^3} \varPhi_\alpha(\boldsymbol{P})^* \varPhi_\beta(\boldsymbol{P}) \mid z_1 \mid \tag{10}$$

and eigenvectors $\{\boldsymbol{K}^{(\gamma)}\}$ forming a set of N-dimensional column vectors with a unit length. We choose the vector $\boldsymbol{K}^{(\gamma)}$ as the γth eigenvector of the matrix Z. With the definition

$$z_1^{(\gamma)} = \lambda^{(\gamma)} \mathrm{e}^{\mathrm{i}\varphi_1} \tag{11}$$

The coefficients $C_{\gamma s}$ are the Fourier coefficients of a set of complex function $C_1(\tau), \cdots, C_N(\tau)$ of a real variable τ which is a phase angle related to the photon states. These complex function satisfy the following ordinary differential equations:

$$\begin{aligned} \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}\tau}C_\beta(\tau) &+ \sum_{\gamma=0}^{N} E^{[0]}_{\beta\gamma}(\tau) C_\gamma(\tau) \\ &= EC_\beta(\tau), \quad \beta = 1, \cdots, N \end{aligned} \tag{12}$$

where

$$E^{[0]}_{\beta\gamma}(\tau) = \left[\sum_j X_j(z_1^{(\gamma)} - z_1^{(\beta)}) \mathrm{e}^{\mathrm{i}j\tau}\right] K^{[0]}_{\beta\gamma} \tag{13}$$

with

$$K^{[0]}_{\beta\gamma} \equiv \boldsymbol{K}^{(\beta)\dagger} E^{[0]} \boldsymbol{K}^{(\gamma)} \tag{14}$$

In the single-mode case, when the eigenvalues of the dipole matrix Eq. (10) are real, the Eq. (13) can be simplified by dropping the phase angle φ_1 which makes only a constant phase shift on τ,

$$E^{[0]}_{\beta\gamma}(\tau) = \mathrm{e}^{\mathrm{i}(\lambda_\gamma - \lambda_\beta)\sin\tau} K^{[0]}_{\beta\gamma} \tag{15}$$

One can see that the new solution is a natural generalization of the non-relativistic quantum-field Volkov solution shown as follows [11, 27]:

$$\begin{aligned} \Psi_{\boldsymbol{P}n} = V_e^{-1/2} \sum_l & \exp\{\mathrm{i}[\boldsymbol{P} + (u_p - l)\boldsymbol{k}] \cdot \boldsymbol{r}\} \\ & \cdot \mathcal{X}_{-l}(z_c, z_s) |n + l\rangle \end{aligned} \tag{16}$$

This differential eigenvalue equation set, Eq. (12), can be solved precisely by numerical methods. Before solving for a driven atom with levels of a large number N, it is necessary to programme the driven atoms in few-level cases first.

In the two-level case, the analytically exact solution has been obtained [3]. The numerical results from the current scheme are compared with the step-forward calculation from that solution [28–30]. In the two-photon preresonance case, when $D = 0.6$, one of the energy levels is $-0.107\,131\,400\,930\,337\cdots$. The agreement is up to all figures in both fortran and matlab double precision computing [28].

In the following, we apply the formulas for driven N-level atoms to treat the case of three-level atoms. For a three-level atom, two of the levels belong to the same parity and have no dipole matrix elements between them. In a special case, we may assume that the dipole matrix is in the following form:

$$(z_{\alpha\beta}) = \begin{pmatrix} 0 & 0 & D_{13} \\ 0 & 0 & D_{23} \\ D_{13}^* & D_{23}^* & 0 \end{pmatrix} \tag{17}$$

This matrix can describe a system containing two ground states and one excited state, e.g., $Xe5P1/2$ and $Xe5P3/2$ can be the two ground states in addition to any Rydberg state with an even parity. A system containing one ground state and two excited states can also be expressed in a similar way.

The characteristic equation for this dipole matrix is

$$\begin{aligned} \begin{vmatrix} -\lambda & 0 & D_{13} \\ 0 & -\lambda & D_{23} \\ D_{13}^* & D_{23}^* & -\lambda \end{vmatrix} &= -\lambda^3 + \lambda \mid D_{13} \mid^2 + \lambda \mid D_{23} \mid^2 \\ &= 0 \end{aligned} \tag{18}$$

The three roots are

$$\begin{aligned} &\lambda^{(1)} = -D \\ &\lambda^{(2)} = 0 \\ &\lambda^{(3)} = D \equiv \sqrt{\mid D_{13} \mid^2 + \mid D_{23} \mid^2} \end{aligned} \tag{19}$$

The three column eigenvectors can be expressed as

$$\begin{aligned} \boldsymbol{a}_1 &= \frac{1}{\sqrt{2}}(\cos\varGamma \mathrm{e}^{\mathrm{i}\alpha_1}, \sin\varGamma \mathrm{e}^{\mathrm{i}\alpha_2}, -1)^t \\ \boldsymbol{a}_2 &= (\sin\varGamma \mathrm{e}^{-\mathrm{i}\alpha_2}, -\cos\varGamma \mathrm{e}^{-\mathrm{i}\alpha_1}, 0)^t \\ \boldsymbol{a}_3 &= \frac{1}{\sqrt{2}}(\cos\varGamma \mathrm{e}^{\mathrm{i}\alpha_1}, \sin\varGamma \mathrm{e}^{\mathrm{i}\alpha_2}, 1)^t \end{aligned} \tag{20}$$

where

$$\cos\Gamma e^{i\alpha_1} \equiv \frac{D_{13}}{D}, \quad \sin\Gamma e^{i\alpha_2} \equiv \frac{D_{23}}{D} \tag{21}$$

With these eigenvectors, according to Eq. (14), we construct the following matrix $K^{[0]}$:

$$\frac{1}{2}\begin{pmatrix} E_1^{[0]}\cos^2\Gamma + E_2^{[0]}\sin^2\Gamma + E_3^{[0]} & \frac{1}{\sqrt{2}}\sin(2\Gamma)(E_1^{[0]}-E_2^{[0]})e^{-i\alpha} & E_1^{[0]}\cos^2\Gamma + E_2^{[0]}\sin^2\Gamma - E_3^{[0]} \\ \frac{1}{\sqrt{2}}\sin(2\Gamma)(E_1^{[0]}-E_2^{[0]})e^{i\alpha} & 2E_1^{[0]}\sin^2\Gamma + 2E_2^{[0]}\cos^2\Gamma & \frac{1}{\sqrt{2}}\sin(2\Gamma)(E_1^{[0]}-E_2^{[0]})e^{i\alpha} \\ E_1^{[0]}\cos^2\Gamma + E_2^{[0]}\sin^2\Gamma - E_3^{[0]} & \frac{1}{\sqrt{2}}\sin(2\Gamma)(E_1^{[0]}-E_2^{[0]})e^{-i\alpha} & E_1^{[0]}\cos^2\Gamma + E_2^{[0]}\sin^2\Gamma + E_3^{[0]} \end{pmatrix} \tag{22}$$

where $\alpha \equiv \alpha_1 + \alpha_2$. With simplified notations Eq. (22) becomes

$$(K_{\alpha\beta}^{[0]}) = \begin{pmatrix} \bar{E}^{[0]} & -\Delta_1 & -\Delta_2 \\ -\Delta_1^* & E_t^{[0]} - 2\bar{E}^{[0]} & -\Delta_1^* \\ -\Delta_2 & -\Delta_1 & \bar{E}^{[0]} \end{pmatrix} \tag{23}$$

where

$$\begin{aligned} \Delta_1 &\equiv -\frac{1}{2\sqrt{2}}\sin(2\gamma)(E_1^{[0]}-E_2^{[0]})e^{-i\alpha} \\ \Delta_2 &\equiv E_3^{[0]} - \bar{E}^{[0]} \\ E_t^{[0]} &\equiv E_1^{[0]} + E_2^{[0]} + E_3^{[0]} \\ \bar{E}^{[0]} &\equiv \frac{1}{2}(E_1^{[0]}\cos^2\gamma + E_2^{[0]}\sin^2\gamma + E_3^{[0]}) \end{aligned} \tag{24}$$

The differential equation set governing $C_\beta(\tau)$, where $\beta = 1, 2, 3$, is derived as follows. According to the formulas derived for an N-level atom, say Eq. (15), we have

$$(E_{\beta\gamma}^{[0]}(\tau)) = \begin{pmatrix} \bar{E}^{[0]} & -\Delta_1 e^{iD\sin\tau} & -\Delta_2 e^{i2D\sin\tau} \\ -\Delta_1^* e^{-iD\sin\tau} & E_t^{[0]} - 2\bar{E}^{[0]} & -\Delta_1^* e^{iD\sin\tau} \\ -\Delta_2 e^{-i2D\sin\tau} & -\Delta_1 e^{-iD\sin\tau} & \bar{E}^{[0]} \end{pmatrix} \tag{25}$$

Thus, the differential equation set is

$$\begin{aligned} &\left(i\frac{d}{d\tau} + \bar{E}^{[0]}\right)C_1(\tau) - \Delta_1 e^{iD\sin\tau}C_2(\tau) \\ &\qquad -\Delta_2 e^{i2D\sin\tau}C_3(\tau) = EC_1(\tau) \\ &-\Delta_1^* e^{-iD\sin\tau}C_1(\tau) + \left(i\frac{d}{d\tau} + E_t^{[0]} - 2\bar{E}^{[0]}\right)C_2(\tau) \\ &\qquad -\Delta_1^* e^{iD\sin\tau}C_3(\tau) = EC_2(\tau) \\ &-\Delta_2 e^{-i2D\sin\tau}C_1(\tau) - \Delta_1 e^{-iD\sin\tau}C_2(\tau) \\ &\qquad + \left(i\frac{d}{d\tau} + \bar{E}^{[0]}\right)C_3(\tau) = EC_3(\tau) \end{aligned} \tag{26}$$

Fortran codes and Matlab codes have been made by this author to solve for wave functions and corresponding energies of generic few-level atoms. In Matlab programming, the coefficients of the ordinary differential equation set for a generic N level atom can be constructed conveniently, even without writing the coefficients explicitly. Test run of the codes has been made for up to 5-level atoms. In programming this quantum mechanic system, it is found that these systems do not allow a continuous boundary condition. One cannot start the integration from an arbitrary value of $C_1(0), \cdots, C_N(0)$. One must select the correct boundary condition, which is unknown previously, to force the trial solution to have the correct period. The author applied the golden cut method, i.e., the 0.618 method, to the selection of the boundary condition (or the initial condition) and the energy eigenvalue to optimize the periodicity of the solution. In the computational selection process, once the correct periodicity is reached, the wave function possesses the correct boundary condition and the correct energy eigenvalue. The energy value allows an additive integer constant which features the periodicity of the driving field by the Floquet theorem. As an example, a three-level atom at $E_1^{[0]} = -1.5$ (per laser photon energy), $E_2^{[0]} = 0.1$, and $E_3^{[0]} = 1$ is calculated at dipole matrix elements $D_{13} = 0.6\cos\Gamma$ and $D_{23} = 0.6\sin\Gamma$ with $\Gamma = \pi/6$. The obtained three independent energy levels are $E_1 = -0.7772$, $E_2 = -1.063$, and $E_3 = 1.440$. Each of the energy levels can add up an arbitrary integer (positive or negative) according to Floquet theorem. Each of the coefficient wave function $C_\alpha(\tau)$ ($\alpha = 1, 2, 3$) describes a curve in the complex plane which is a closed smooth curve. The calculated curves are presented in Fig. 1.

The ordinary differential equation set developed here looks similar to the equation set in classical field quantum optics if one treats the phase variable τ as time. Thus all the theoretical treatments developed here with computing codes can be transferred into a version as in classical-field theory. Thus the main results obtained in this paper can be used as research tools to benefit quantum optics and other related areas.

Conclusions in Physics

i) An N-level atom interacting with quantized light form stationary states.

ii) Light does not cause additional energy splitting

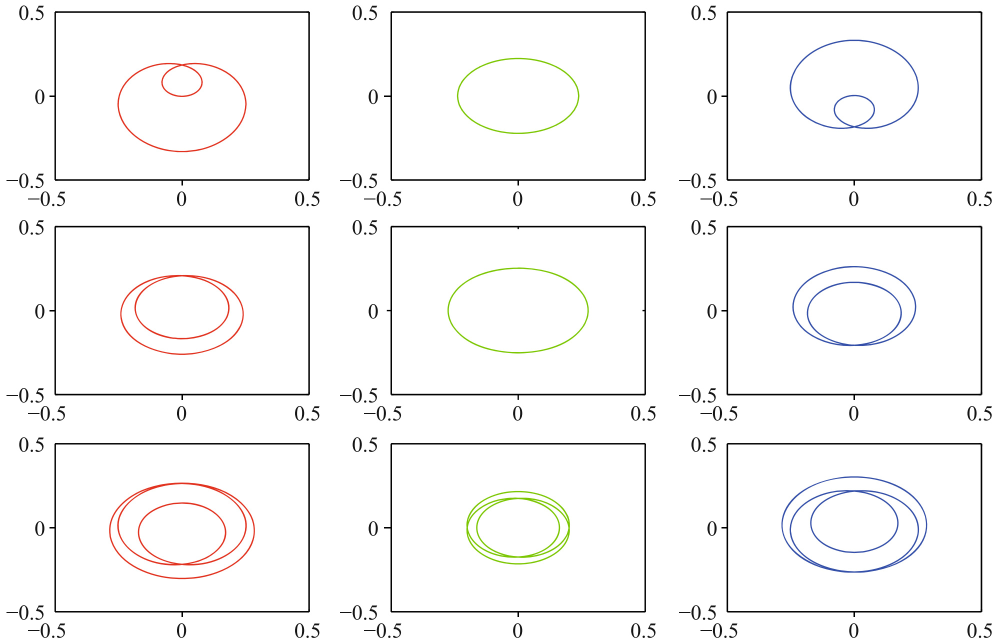

Fig. 1 The each row corresponds a coefficient wave function $C_1(\tau)$, $C_2(\tau)$, and $C_3(\tau)$. The row 1, row 2, and row 3 (from top to bottom) corresponds to energy levels E_1, E_2, and E_3 respectively.

for an N-level atom besides the integer additive energy spacing due to the Floquet mechanism. Floquet mechanism sets up the equivalent groups of the states. The number of different equivalent groups still keeps as N.

iii) When a spacing between a pair of truly different energy levels shifts with light intensity to an integer spacing, Freeman resonances may occur.

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