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A Simplified Wave Function for Dressed Atoms*

LI Shu-min, CHEN Ji, ZHOU Zi-fang, ZHANG Sheng-tao

(*Open Laboratory of Bond Selective Chemistry, Department of Modern Physics, University of Science and Technology of China, Hefei 230027, China*)

Abstract: A wave function for laser dressed atom is derived as a perturbative solution of the time-dependent Schrödinger equation in the velocity gauge. With the use of the average excitation energy approximation and the closure approximation, the solution is reduced to a time-dependent operator acting on the "bare" atomic state. In soft-photon approximation, the average excitation energy only appears in the first and second order terms of field frequency. Such a simplified dressed wave function is useful in the calculation of laser-assisted scattering, especially in the laser-assisted rearrangement collisions.

Key words: laser field; atom; dressed wave function; velocity gauge

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With the development of laser technology, laser-assisted electron-atom and ion-atom collisions received considerable attentions from both theoretical and experimental aspects[1−4]. In the theoretical treatment of these processes, the laser field may be considered as a classical electromagnetic field when the number of photons in a laser mode is high enough [1]. The state of incident or scattered electron is usually described by the Volkov state [1,5] or the Coulomb-Volkov state[6,7]. The former is an exact solution of the time-dependent Schrödinger equation for a "free" electron moving in a monochromatic electromagnetic field, while the latter is a Coulomb function modulated by the laser in the same way as in the Volkov state. In both wave functions, the laser-electron interaction are considered up to infinite orders. As to the state of an atom in the radiation field (the dressed state), no exact solution seems available except the solutions in the two-state (or three-state) model for the resonant case. In the investigation of the laser-assisted electron-atom collisions, the atomic target is initially treated as a static potential with neglecting the laser dressing, before Joachain and co-workers found that the dressing effect of target plays an important role in the intense-laser-assisted collisions[8−11]. Joachain et al employed a first order perturbative solution of the time-dependent Schrödinger equation in the length gauge to describe the dressing of target atom. They suppose that the laser field is monochromatic and spatially homogeneous, described by a classical vector potential

$$\boldsymbol{A}(t) = \boldsymbol{A}_0 \cos(\omega t) , \quad (1)$$

or electric field strength

$$\boldsymbol{\varepsilon}(t) = \boldsymbol{\varepsilon}_0 \sin(\omega t) , \quad (2)$$

where $\boldsymbol{\varepsilon}_0 = (\omega/c)\boldsymbol{A}_0$ (c is the velocity of light in vacuum), then the dressed wave function of the

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atomic state characterized by quantum number k reads [11,12],

$$\psi_k(\boldsymbol{r}_1,\cdots,\boldsymbol{r}_Z,t) = \Big[\Phi_k(\boldsymbol{r}_1,\cdots,\boldsymbol{r}_Z) - \sin(\omega t)\sum_n \frac{\omega_{nk}}{\hbar(\omega_{nk}^2-\omega^2)}\cdot \boldsymbol{\varepsilon}_0\cdot\langle n\mid\sum_{j=1}^{Z}\boldsymbol{r}_j\mid k\rangle\,\Phi_n(\boldsymbol{r}_1,\cdots,\boldsymbol{r}_Z) - \mathrm{i}\cos(\omega t)\sum_n\frac{\omega}{\hbar(\omega_{nk}^2-\omega^2)}\boldsymbol{\varepsilon}_0\cdot\langle n\mid\sum_{j=1}^{Z}\boldsymbol{r}_j\mid k\rangle\,\Phi_n(\boldsymbol{r}_1,\cdots,\boldsymbol{r}_Z)\Big]\cdot e^{-\frac{i}{\hbar}W_k t-\frac{ie}{\hbar c}\boldsymbol{A}\cdot\sum_{j=1}^{Z}\boldsymbol{r}_j} \tag{3}$$

provides that the field strength is weak enough in comparison with the internal Coulomb field of atom (for atomic hydrogen, $\varepsilon_0 \ll 5.14\times 10^9$ V/cm) although strong enough by laboratory standards. Here $\Phi_n(\boldsymbol{r}_1,\cdots,\boldsymbol{r}_Z)\equiv |n\rangle$ and W_n are respectively the eigen state and eigen value of the undressed atom, and $\omega_{nk}=(W_n-W_k)/\hbar$ the Bohr frequency. This dressed wave function was also used by other authors to investigate laser-assisted collisions[13-17]. In Eq. (3), a space-time dependent gauge factor $\exp\{-\frac{ie}{\hbar c}\boldsymbol{A}(t)\cdot\sum_{j=1}^{Z}\boldsymbol{r}_j\}$ has been introduced to ensure gauge consistency. For the laser-assisted direct scattering, such gauge factors are exactly the same in both initial and final states, thus it is cancelled out in the scattering matrix. However in the rearrangement channel, the gauge factors in initial and final states are different, and not cancelled each other. This may result in difficulties in reducing of the scattering amplitude into lower fold numerical integrals. In addition, such a dressed state involves the coupling to an infinite number of "bare" atomic states, which causes the calculation rather cumbersome and computer-time consuming, even makes the calculation practically forbidden[3]. To simplify the dressed wave fuction for complex atoms, Jochain et al introduced an average excitation energy approximation (AEEA) by which all the Bohr frequencies in the infinite series were replaced by an averaged value[8,9]. However, when the energy levels of atom were far-between, this approximation may result in considerable error.

In this article, we improve the dressed wave function by working straight forwardly in the velocity gauge [18] in order to avoid the appearance of the above mentioned space-time-dependent gauge factor. The laser-atom interaction is considered as a first order time-dependent perturbation. In the low frequency and high frequency limits, the dressed state is reduced further.

Consider an atom of atomic number Z which is initially at an eigen state Φ_k, and then adiabatically embedded in a background laser field of Eq. (1). The time-dependent Schrödinger equation for such a dressed atom is

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi(\boldsymbol{r}_1,\cdots,\boldsymbol{r}_Z,t) = \left\{\frac{1}{2m}\sum_{j=1}^{Z}\left[\hat{\boldsymbol{p}}_j+\frac{e}{c}\boldsymbol{A}(t)\right]^2+V(\boldsymbol{r}_1,\cdots,\boldsymbol{r}_Z)\right\}\psi(\boldsymbol{r}_1,\cdots,\boldsymbol{r}_Z,t)\,. \tag{4}$$

The term of A^2 in this equation can be removed by a standard gauge transformation

$$\psi(\boldsymbol{r}_1,\cdots,\boldsymbol{r}_Z,t) = e^{-\mathrm{i}\frac{Ze^2}{2mc^2\hbar}\int_{-\infty}^{t}A^2(t')dt'}\varphi(\boldsymbol{r}_1,\cdots,\boldsymbol{r}_Z,t)\,. \tag{5}$$

Then the new wave function satisfies

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\varphi(\boldsymbol{r}_1,\cdots,\boldsymbol{r}_Z,t) = [H_A+H_I(t)]\,\varphi(\boldsymbol{r}_1,\cdots,\boldsymbol{r}_Z,t)\,, \tag{6}$$

where H_A is the Hamiltonian for the "bare" atom,

$$H_A = \sum_{j=1}^{Z}\frac{\hat{\boldsymbol{p}}_j^{\,2}}{2m}+V(\boldsymbol{r}_1,\cdots,\boldsymbol{r}_Z) \tag{7}$$

and its Schrödinger equation is assumed exactly solvable. Whereas

$$H_1(t) = \frac{e}{mc} \boldsymbol{A}(t) \cdot \sum_{j=1}^{Z} \hat{\boldsymbol{p}}_j \tag{8}$$

is the field-atom interaction in the velocity gauge. It can be treated as a time-dependent perturbation for it is much more weak than the Coulomb field of the atom. Based on these hypotheses, Eq. (6) is then readily solved by using the first order time-dependent perturbation theory [19] to yield,

$$\varphi_k(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_Z, t) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} W_k t} \Big\{ \Phi_k(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_Z) - \frac{1}{2\hbar} \sum_{n \neq k} \Big[\frac{\mathrm{e}^{\mathrm{i}\omega t}}{\omega_{nk} + \omega} + \frac{\mathrm{e}^{-\mathrm{i}\omega t}}{\omega_{nk} - \omega} \Big] \cdot \\ \langle n \mid \frac{e}{mc} \boldsymbol{A}_0 \cdot \sum_{j=1}^{Z} \hat{\boldsymbol{p}}_j \mid k \rangle \Phi_n(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_Z) \Big\} . \tag{9}$$

With employing the communication relation

$$[H_A, \boldsymbol{r}_j] = -\frac{\mathrm{i}\hbar}{m} \hat{\boldsymbol{p}}_j , \tag{10}$$

Eq. (9) becomes

$$\varphi_k(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_Z, t) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} W_k t} \Big\{ \Phi_k(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_Z) - \frac{e}{\hbar c} \sum_n \Big[\frac{\mathrm{i}\omega_{nk}^2}{\omega_{nk}^2 - \omega^2} \cos(\omega t) + \frac{\omega\, \omega_{nk}}{\omega_{nk}^2 - \omega^2} \sin(\omega t) \Big] \cdot \\ \langle n \mid \boldsymbol{A}_0 \cdot \sum_{j=1}^{Z} \boldsymbol{r}_j \mid k \rangle \Phi_n(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_Z) \Big\} , \tag{11}$$

here we have taken the fact $\langle k | \boldsymbol{p}_j | k \rangle = 0$ into account, and removed the restriction $n \neq k$ in the sum. Substitute Eq. (11) into Eq. (5), we finally obtain the dressed wave function of the atom

$$\psi_k(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_Z, t) = \Big\{ \Phi_k(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_Z) - \frac{e}{\hbar c} \sum_n \Big[\frac{\mathrm{i}\omega_{nk}^2}{\omega_{nk}^2 - \omega^2} \cos(\omega t) + \frac{\omega\, \omega_{nk}}{\omega_{nk}^2 - \omega^2} \sin(\omega t) \Big] \cdot \\ \langle n \mid \boldsymbol{A}_0 \cdot \sum_{j=1}^{Z} \boldsymbol{r}_j \mid k \rangle \Phi_n(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_Z) \Big\} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} W_k t - \mathrm{i}\frac{Ze^2}{2mc^2\hbar} \int_{-\infty}^{t} A^2(t') \mathrm{d}t'} \\ = \Big\{ \Phi_k(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_Z) - \frac{e}{\hbar \omega} \sum_n \Big[\frac{\mathrm{i}\omega_{nk}^2}{\omega_{nk}^2 - \omega^2} \cos(\omega t) + \frac{\omega\, \omega_{nk}}{\omega_{nk}^2 - \omega^2} \sin(\omega t) \Big] \cdot \\ \langle n \mid \boldsymbol{\varepsilon}_0 \cdot \sum_{j=1}^{Z} \boldsymbol{r}_j \mid k \rangle \Phi_n(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_Z) \Big\} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} W_k t - \mathrm{i}\frac{Ze^2}{2mc^2\hbar} \int_{-\infty}^{t} A^2(t') \mathrm{d}t'} . \tag{12}$$

Here the gauge factor $\exp\{-\frac{\mathrm{i}Ze^2}{2mc^2\hbar} \int_{-\infty}^{t} A^2(t') \mathrm{d}t'\}$ is time-dependent only. In calculating the laser-assisted collisions, such a gauge factor is usually cancelled out in the scattering matrices for it is exactly the same in both initial and final channels. Eq. (12) is especially suitable to treat the laser-assisted rearrangement collisions.

Further more, under the AEEA, the wave function of Eq. (12) can be further simplified. Suppose that all the Bohr frequencies may be replace by an average value $\bar{\omega}_k$, then Eq. (12) becomes

$$\psi_k(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_Z, t) = \Big\{ 1 - \Big[\mathrm{i} \Big(1 + \frac{\omega^2}{\bar{\omega}_k^2 - \omega^2} \Big) \cos(\omega t) + \frac{\omega\, \bar{\omega}_k}{\bar{\omega}_k^2 - \omega^2} \sin(\omega t) \Big] \frac{e}{\hbar \omega} \boldsymbol{\varepsilon}_0 \cdot \sum_{j=1}^{Z} \boldsymbol{r}_j \Big\} \cdot \\ \Phi_k(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_Z)\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar} W_k t - \mathrm{i}\frac{Ze^2}{2mc^2\hbar} \int_{-\infty}^{t} A^2(t') \mathrm{d}t'} , \tag{13}$$

here we have used the closure relation $\sum_n | n \rangle \langle n | = 1$. In this expression, the infinite series of coupled states in Eq. (12) is reduced into a time-dependent operator acting on a "bare" atomic state.

In the following, we consider two special cases of the field frequency:

(1) $\omega \ll \bar{\omega}_k$ (soft photon approximation). For this situation, the terms of ω in Eq. (13) may be considered up to the second order to yield,

$$\psi_k(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_Z, t) = \Big\{ 1 - \Big[\mathrm{i} \Big(1 + \frac{\omega^2}{\bar{\omega}_k^2} \Big) \cos(\omega t) + \frac{\omega}{\bar{\omega}_k} \sin(\omega t) \Big] \frac{e}{\hbar \omega} \boldsymbol{\varepsilon}_0 \cdot \sum_{j=1}^{Z} \boldsymbol{r}_j \Big\} \cdot$$

$$\Phi_k(\boldsymbol{r}_1,\cdots,\boldsymbol{r}_Z)\ e^{-\frac{i}{\hbar}W_k t-i\frac{Ze^2}{2mc^2\hbar}\int_{-\infty}^{t}A^2(t')dt'}. \tag{14}$$

This is the very situation occurs in most laser-assisted scattering processes. If we only reserve the zeroth-order term of ω, the dressed state is reduced into the result of Ref. [20]. For instance, in treating the rearrangement collision of positron with a ground state hydrogen ($\hbar\bar{\omega}_0=\frac{4}{9}$ ato. units= 12.09 eV)[18] or helium ($\hbar\bar{\omega}_0=$ 1.15 ato. units= 31.29 eV)[21] in the presence of a Nd: YAG yttrium aluminum garnet laser ($\hbar\omega=$1.17 eV), it is precise enough to reserve ω up to the zeroth or first order in the dressed states.

(2) $\omega\gg\bar{\omega}_k$. In this case, Eq. (13) becomes

$$\psi_k(\boldsymbol{r}_1,\cdots,\boldsymbol{r}_Z,t)=\left\{1+\left[\sin(\omega t)+i\frac{\bar{\omega}_k}{\omega}\cos(\omega t)\right]\frac{e\bar{\omega}_k}{\hbar\omega^2}\boldsymbol{\varepsilon}_0\cdot\sum_{j=1}^{Z}\boldsymbol{r}_j\right\}\cdot$$

$$\Phi_k(\boldsymbol{r}_1,\cdots,\boldsymbol{r}_Z)\ e^{-\frac{i}{\hbar}W_k t-i\frac{Ze^2}{2mc^2\hbar}\int_{-\infty}^{t}A^2(t')dt'}. \tag{15}$$

We note that the perturbative correction is of order ε_0/ω^2.

Generally speaking, the dressed wave functions in different gauges are all equally meaningful and give identical physical results when any problem is solved exactly. It is only when approximations are made that the results given by different gauges can differ, and the different gauges may be useful in different cases[1]. In fact, according to the least coupling principle, the velocity gauge is more "elementary" than the length gauge, since the vector potential of the electromagnetic field is more "elementary" in quantum theory. For instance, in the Aharonov-Bohm effect[22-24], the vector potential has observable effect even though the field strength vanishes. In the velocity gauge, the accuracy of the dressed wave function depends on the ratio of field strength to frequency, the condition

$$\frac{e}{\hbar\omega}\boldsymbol{\varepsilon}_0\cdot\sum_{j=1}^{Z}\boldsymbol{r}_j\ll 1 \tag{16}$$

should be satisfied to ensure the validity of the perturbative solution of Eq. (12). Similar conditions are required in the perturbative solution of length gauge and the Coulomb-Volkov function[25]. When the condition of Eq. (16) is satisfied, the dressed states of Eqs. (3) and (12) may differ by a higher order correction term. The perturbative solutions of both gauges are equally efficient in describing the laser-assisted scattering in all directions. But the former has the advantage for lacking a space-time dependent factor and thus improves the numerical computation by sliding over the difficulty occurred in the reduction of the scattering amplitude.

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缀饰原子的简化波函数*

李书民，陈　激，周子舫，张声涛

(中国科学技术大学近代物理系选键化学开放实验室，安徽 合肥 230027)

摘　要：作为含时薛定谔方程的微扰近似解，在速度规范下给出了激光场中缀饰原子的一个波函数. 利用平均激发能近似和完备关系，可将此波函数简化为一个含时的相乘算符作用于无场时的“裸原子”态上. 在软光子近似下，平均激发能仅出现在光场频率的一阶和二阶项上. 此波函数适用于计算激光辅助的散射过程，特别是重排过程.

关键词：激光场；原子；缀饰波函数；速度规范

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