UDC 530.1

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TO THE PROBLEM OF THE HAMILTONIAN FORM FOR A SYSTEM OF TWO-LEVEL ATOMS INTERACTING WITH ELECTROMAGNETIC FIELD

On the basis of the Lagrangian formulation of dynamics of a system of charges and electromagnetic field, the Hamilton operator for a system of one-electron two-level atoms is constructed with taking into account the smallness of an electron mass in comparison with that of a core. In addition, it is taken into consideration that electrons in atoms move basically in a small vicinity of cores. The equivalence of Hamilton operators of the system in the Coulomb gauge and dipole approximation ($\mathbf{x}\cdot\mathbf{E}$-approximation) is established for investigating the system of atoms and electromagnetic field by dint of a unitary gauge transformation. It is ascertained that using the dipole approximation is simpler because calculations in the Coulomb gauge require an additional transformation of physical value operators. It is noted that applying the $\mathbf{p}\cdot\mathbf{A}$-approximation reduces the calculation accuracy compared with the dipole approximation. The investigation is performed in the framework of many-particle theory on the basis of the quantum Liouville equation for the statistical operator of a system.

Keywords: interaction between atoms and electromagnetic field, dipole approximation, Coulomb gauge, two-level atoms, $\mathbf{x}\cdot\mathbf{E}$-approximation, $\mathbf{p}\cdot\mathbf{A}$-approximation.

На базі лагранжового формулювання динаміки системи зарядів і електромагнітного поля будується оператор Гамільтона системи одноелектронних дворівневих атомів із урахуванням малості мас електронів порівняно з масою ядра. Додатково враховано, що електрони в атомах в основному рухаються в малому околі ядра. Встановлено еквівалентність операторів Гамільтона системи в кулонівському калібруванні й у дипольному наближенні ($\mathbf{x}\cdot\mathbf{E}$-наближенні) у дослідженні системи з атомів і електромагнітного поля. Це робиться за допомогою унітарного калібрувального перетворення. Встановлено, що використання дипольного наближення виявляється простішим, оскільки при розрахунках у калібруванні Кулона необхідне додаткове перетворення операторів фізичних величин. Зазначено, що застосування $\mathbf{p}\cdot\mathbf{A}$-наближення зменшує точність обчислень порівняно з дипольним наближенням. Дослідження виконано в рамках багаточастинкової теорії на основі квантового рівняння Ліувілля для статистичного оператора системи.

Ключові слова: взаємодія атомів з електромагнітним полем, дипольне наближення, калібрування Кулона, дворівневі атоми, $\mathbf{x}\cdot\mathbf{E}$-наближення, $\mathbf{p}\cdot\mathbf{A}$-наближення.

На основе лагранжевой формулировки динамики системы зарядов и электромагнитного поля строится оператор Гамильтона системы одноэлектронных двухуровневых атомов с учетом малости масс электронов по сравнению с массой ядра. Дополнительно учтено, что электроны в атомах в основном движутся в малой окрестности ядра. Установлена эквивалентность операторов Гамильтона системы в калибровке Кулона и в дипольном приближении ($\mathbf{x}\cdot\mathbf{E}$-приближении) в исследовании системы из атомов и электромагнитного поля. Это сделано с помощью унитарного калибровочного преобразования. Установлено что использование дипольного приближения оказывается более простым, поскольку при вычислениях в калибровке Кулона необходимо дополнительное преобразование операторов физических величин. Указано, что применение $\mathbf{p}\cdot\mathbf{A}$-приближения понижает точность вычислений по сравнению с дипольным приближением. Рассмотрение выполнено в рамках многочастичной теории на основе квантового уравнения Лиувилля для статистического оператора системы.

Ключевые слова: взаимодействие атомов с электромагнитным полем, дипольное приближение, калибровка Кулона, двухуровневые атомы, $\mathbf{x}\cdot\mathbf{E}$-приближение, $\mathbf{p}\cdot\mathbf{A}$-приближение.

1. Introduction

The problem of interaction between atoms and electromagnetic field is a well-known one, but the literature contains contradictory assertions about the limits of dipole approximation ($\mathbf{x}\cdot\mathbf{E}$-approximation) applicability in comparison with the interaction description in the Coulomb gauge. Besides it, in a number of papers [1] so called $\mathbf{p}\cdot\mathbf{A}$-approximation is used; it is obtained from the theory in the Coulomb gauge via neglecting the vector potential square. It is noted that the dipole approximation Hamiltonian is obtained through the gauge transformation of the Hamilton operator of atoms and electromagnetic field in the Coulomb gauge, but at the same time it is affirmed that their application to solving some physical problems lead to differing results [2]. The present paper task is the discussion of the mentioned problems on the basis of fundamental Lagrangian electrodynamics formulation and the quantization procedure for the proposed classical theory.

2. Classical theory of atom interaction with electromagnetic field

The Lagrange function of atom system with one electron in an external electromagnetic field has the form

$$L(t)=\sum_a\left(\frac{M\mathbf{u}_a^2}{2}+\frac{m(\mathbf{u}_a+\mathbf{u}_{ae})^2}{2}+\frac{e^2}{|\mathbf{x}_{ae}|}\right)- \\ -\sum_a e\varphi(\mathbf{x}_a,t)+\sum_a e\varphi(\mathbf{x}_a+\mathbf{x}_{ae},t)+\sum_a\frac{e}{c}\mathbf{u}_a\cdot\mathbf{A}(\mathbf{x}_a,t)-\sum_a\frac{e}{c}(\mathbf{u}_a+\mathbf{u}_{ae})\cdot\mathbf{A}(\mathbf{x}_a+\mathbf{x}_{ae},t) \tag{1}$$

where $\mathbf{x}_a$ is a radius-vector of an a-th atom, $\mathbf{x}_{ae}$ is a radius-vector of the electron in the a-th atom (its origin is at the end of the vector $\mathbf{x}_a$), $\mathbf{u}_a$ and $\mathbf{u}_{ae}$ are corresponding velocities. The interaction between atoms is not taken into account in the expression (1).

In our problem it is convenient to pass to the coordinates of the centers of mass of atoms. Bearing in mind that the core mass is much more than the electron mass $m<<M$, we can confine ourselves with the following approximate expression for the system Lagrange function

$$L(t)=\sum_a\left(\frac{M\mathbf{u}_a^2}{2}+\frac{m\mathbf{u}_{ae}^2}{2}+\frac{e^2}{|\mathbf{x}_{ae}|}\right)-\sum_a e\varphi(\mathbf{x}_a,t)+\sum_a e\varphi(\mathbf{x}_a+\mathbf{x}_{ae},t)+ \\ +\sum_a\frac{e}{c}\mathbf{u}_a\cdot\mathbf{A}(\mathbf{x}_a,t)-\sum_a\frac{e}{c}(\mathbf{u}_a+\mathbf{u}_{ae})\cdot\mathbf{A}(\mathbf{x}_a+\mathbf{x}_{ae},t). \tag{2}$$

Further on, it should be taken into account that the electron is relatively close to the core and the expression (2) can be expanded in a series in $\mathbf{x}_{ae}$. In the result we come to the Lagrange function of the system of atoms in an external electromagnetic field

$$L(t)=\sum_a\left(\frac{M\mathbf{u}_a^2}{2}+\frac{m\mathbf{u}_{ae}^2}{2}+\frac{e^2}{|\mathbf{x}_{ae}|}\right)+\sum_a e\mathbf{x}_{ae}\cdot\frac{\partial\varphi(\mathbf{x}_a,t)}{\partial\mathbf{x}_a}- \\ -\frac{e}{c}\sum_a\left(\mathbf{u}_{ae}\cdot\mathbf{A}(\mathbf{x}_a,t)+\mathbf{u}_{an}\mathbf{x}_{ael}\frac{\partial\mathbf{A}_n(\mathbf{x}_a,t)}{\partial\mathbf{x}_{al}}\right) \tag{3}$$

where in the last term vector indices n and l are used. In this case the Hamilton function of the atom system has the form

$$H(t)=\sum_a\left(\frac{1}{2m}(\mathbf{p}_{ae}+\frac{e}{c}\mathbf{A}(\mathbf{x}_a,t))^2-\frac{e^2}{|\mathbf{x}_{ae}|}\right)+\sum_a\frac{1}{2M}\left(\mathbf{p}_a-\frac{1}{c}\mathbf{d}_{al}\frac{\partial\mathbf{A}(\mathbf{x}_a,t)}{\partial\mathbf{x}_{al}}\right)^2+ \\ +\sum_a\mathbf{d}_a\cdot\frac{\partial\varphi(\mathbf{x}_a,t)}{\partial\mathbf{x}_a} \tag{4}$$

where the corresponding momenta

$$\mathbf{p}_a=M\mathbf{u}_a-\frac{e}{c}\mathbf{x}_{ael}\frac{\partial\mathbf{A}_n(\mathbf{x}_a)}{\partial\mathbf{x}_{al}},\qquad \mathbf{p}_{ae}=m\mathbf{u}_{ae}-\frac{e}{c}\mathbf{A}(\mathbf{x}_a,t) \tag{5}$$

and the electric dipole moment of the atom

$$\mathbf{d}_a=e\mathbf{x}_a+(-e)(\mathbf{x}_a+\mathbf{x}_{ae})=-e\mathbf{x}_{ae} \tag{6}$$

are introduced. Note, that the transition from the Lagrange function (2) to ones similar to (3) is discussed in details in [3].

In the weak relativistic theory of atoms interacting with an external electromagnetic field the approximation that corresponds formally to the zero value of the vector potential in (4) is widespread. Then the Hamiltonian (4) takes the form

$$H_1(t)=\sum_a H_{ae}+\sum_a\frac{\mathbf{p}_a^2}{2M}-\sum_a\mathbf{d}_a\cdot\mathbf{E}(\mathbf{x}_a,t)\quad\left(H_{ae}\equiv\frac{\mathbf{p}_{ae}^2}{2m}-\frac{e^2}{|\mathbf{x}_{ae}|}\right), \tag{7}$$

tally with the dipole approximation [5]. This approximation substantiation on the basis of the electromagnetic field gauge choice with $\mathbf{A}(\mathbf{x},t)=0$ and $\varphi(\mathbf{x},t)\neq 0$ seems to be impossible. At the same time the Coulomb gauge is possible

$$\varphi(\mathbf{x},t)=0,\qquad \mathrm{div}\mathbf{A}(\mathbf{x},t)=0, \tag{8}$$

in which we come to the Hamiltonian

$$H_2(t)=\sum_a\left(\frac{1}{2m}(\mathbf{p}_{ae}+\frac{e}{c}\mathbf{A}(\mathbf{x}_a,t))^2-\frac{e^2}{|\mathbf{x}_{ae}|}\right)+\sum_a\frac{1}{2M}\left(\mathbf{p}_a-\frac{1}{c}\mathbf{d}_{al}\frac{\partial\mathbf{A}(\mathbf{x}_a,t)}{\partial\mathbf{x}_{al}}\right)^2 \tag{9}$$

The obtained expression (9) is absent in literature on quantum optics [1, 2, 5] (however, similar problems are discussed in [3, 4]). The distinction is in a new member containing vector potential derivatives. In the next section we show that it is essential for considering the problem of a gauge transformation of the quantum Liouville equation.

3. Quantum theory of atom interaction with a classical electromagnetic field

Let us discuss now the problem of quantization of the theory developed in the previous section. Actually the quantization consists in constructing the operators of physical values. In the quantum theory the following Hamilton operators correspond to the Hamilton functions (7) and (9):

$$\hat{H}_1(t)=\sum_a\hat{H}_{ae}+\sum_a\frac{\hat{\mathbf{p}}_a^2}{2M}-\sum_a\hat{\mathbf{d}}_a\cdot\mathbf{E}(\hat{\mathbf{x}}_a,t)\quad\left(\hat{H}_{ae}\equiv\frac{\hat{\mathbf{p}}_{ae}^2}{2m}-\frac{e^2}{|\hat{\mathbf{x}}_{ae}|},\quad\hat{\mathbf{d}}_a=-e\hat{\mathbf{x}}_{ae}\right) \tag{10}$$

and

$$\hat{H}_2(t)=\sum_a\left(\frac{1}{2m}(\hat{\mathbf{p}}_{ae}+\frac{e}{c}\mathbf{A}(\hat{\mathbf{x}}_a,t))^2-\frac{e^2}{|\hat{\mathbf{x}}_{ae}|}\right)+\sum_a\frac{1}{2M}\left(\hat{\mathbf{p}}_a+\frac{e}{c}\hat{\mathbf{x}}_{ael}\frac{\partial\mathbf{A}(\mathbf{x}_a,t)}{\partial\mathbf{x}_{al}}\bigg|_{\mathbf{x}_a\to\hat{\mathbf{x}}_a}\right)^2. \quad (11)$$

We shall show that the Hamilton operator (10) can be laid in the basis of investigating the electrodynamics of atoms, though its derivation is not substantiated. With this end in view we consider the quantum Liouville equations corresponding to these Hamiltonians

$$\frac{\partial\rho_1(t)}{\partial t}=-\frac{i}{\hbar}[\hat{H}_1(t),\rho_1(t)],\qquad \frac{\partial\rho_2(t)}{\partial t}=-\frac{i}{\hbar}[\hat{H}_2(t),\rho_2(t)]. \quad (12)$$

Statistical operators $\rho_1(t)$ and $\rho_2(t)$ are connected with a unitary transformation

$$\rho_1(t)=U(t)\rho_2(t)U(t)^+,\qquad \hat{U}(t)\equiv\exp\left(-i\frac{e}{\hbar c}\sum_a\hat{\mathbf{x}}_{ae}\cdot\mathbf{A}(\hat{\mathbf{x}}_a,t)\right). \quad (13)$$

In fact, the formulas

$$U(t)\hat{\mathbf{p}}_{ae}U(t)^+=\hat{\mathbf{p}}_{ae}-\frac{e}{c}\mathbf{A}(\hat{\mathbf{x}}_a,t),\qquad U(t)\hat{\mathbf{p}}_aU(t)^+=\hat{\mathbf{p}}_a-\frac{e}{c}\hat{\mathbf{x}}_{ae}\cdot\frac{\partial\mathbf{A}(\mathbf{x}_a,t)}{\partial\mathbf{x}_a}\bigg|_{\mathbf{x}_a\to\hat{\mathbf{x}}_a} \quad (14)$$

are valid, that follows from the canonical commutation relations

$$[\hat{\mathbf{x}}_{an},\hat{\mathbf{p}}_{bl}]=i\hbar\delta_{ab}\delta_{nl},\qquad [\hat{\mathbf{x}}_{aen},\hat{\mathbf{p}}_{bel}]=i\hbar\delta_{ab}\delta_{nl}. \quad (15)$$

The transformation laws (14) lead to the identity

$$U(t)\hat{H}_2(t)U(t)^+=\hat{H}_1(t)+\sum_a\hat{\mathbf{d}}_a\cdot\mathbf{E}(\hat{\mathbf{x}}_a,t), \quad (16)$$

which proves that solutions of equations (12) are connected by the unitary transformation (13) because

$$\mathbf{E}_n(\mathbf{x},t)=-\frac{1}{c}\frac{\partial\mathbf{A}_n(\mathbf{x},t)}{\partial t}. \quad (17)$$

Note, that gauge unitary transformations for problems of the theory of nonequilibrium processes are discussed in the literature (see, for example, [4, 6, 7]).

In papers devoted to the description of atom-field interaction it is noted that using the Hamilton operators $\hat{H}_1(t)$ and $\hat{H}_2(t)$ can lead to non-coordinated results at average value calculations [2]. It follows from our consideration that such a formula is valid for calculating the average values of physical variables

$$\overline{A}=\mathrm{Sp}\,\rho_1(t)\hat{A}=\mathrm{Sp}\,\rho_2(t)U(t)^+\hat{A}U(t). \quad (18)$$

In other words, if the statistical operator $\rho_2(t)$ is used for average value calculation, the operators of physical values should be subjected to the unitary transformation (13). Thus, using the statistical operator $\rho_1(t)$ and Hamiltonian $\hat{H}_1(t)$ is more convenient.

Now we shall discuss the Hamilton operator $\hat{H}_1(t)$ in the approximation of two-level atoms. Electron states in the a-th atom are described with Dirac vectors $|a,\alpha\rangle$

$$\hat{H}_{ae}|a,\alpha\rangle = E_\alpha|a,\alpha\rangle, \quad \langle a,\alpha|a,\alpha'\rangle = \delta_{\alpha\alpha'}, \quad \sum_\alpha |a,\alpha\rangle\langle a,\alpha| = \hat{1}_a \tag{19}$$

where for two-level atoms $\alpha,\alpha',\ldots = 1,2$. Matrix elements for the dipole moment operator of the electron in the a-th atom are given by formulas [5]

$$\langle a,\alpha|\mathbf{d}_a|a,\alpha\rangle = 0, \quad \langle a,1|\mathbf{d}_a|a,2\rangle = \langle a,2|\mathbf{d}_a|a,1\rangle = \mathbf{d}_a; \qquad \mathbf{d}_a = \mathbf{n}_a d, \quad \mathbf{n}_a^2 \equiv 1. \tag{20}$$

Here we take into account that in the absence of external field the average dipole moment of an atom equals to zero for the reasons of rotational invariance. The dipole moment d of the transition between the states $\alpha = 1,2$ is the same in all the atoms ($d^* = d$), but its orientation described by the unitary vector $\mathbf{n}_a$, is different. The Hamilton operator (10) with taking into account formulas (19) and (20) can be put down as

$$\hat{H}_1(t) = \sum_a \left(\frac{\hat{\mathbf{p}}_a^2}{2M} + E_0\hat{\mathbf{R}}_{az} - 2\hat{\mathbf{R}}_{ax}(\mathbf{d}_a \cdot \mathbf{E}(\hat{\mathbf{x}}_a, t)) \right) \qquad (E_0 \equiv E_1 - E_2) \tag{21}$$

where Dicke operators $\hat{\mathbf{R}}_n$ [8], which are expressed via the Pauli matrixes, are introduced

$$\hat{\mathbf{R}}_{al} \equiv \frac{1}{2}\sum_{\alpha,\alpha'} |a,\alpha\rangle\langle a,\alpha'|\boldsymbol{\sigma}_{l,\alpha\alpha'}; \quad \boldsymbol{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \boldsymbol{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{22}$$

and a constant connected with the beginning of atom energy readings is omitted.

4. Quantum theory of atom interaction with a quantum electromagnetic field

In accordance with the idea of quantization the Hamilton operator of a system consisting of atoms and electromagnetic field is given by the formula

$$\hat{H}_1 = \sum_a \left(\frac{\hat{\mathbf{p}}_a^2}{2M} + E_0\hat{\mathbf{R}}_{az} - 2\hat{\mathbf{R}}_{ax}(\mathbf{d}_a \cdot \hat{\mathbf{E}}^t(\hat{\mathbf{x}}_a)) \right) + \sum_{\mathbf{k},\alpha} \hbar\omega_k c_{\alpha\mathbf{k}}^+ c_{\alpha\mathbf{k}} \qquad (\omega_k \equiv kc, \quad k \equiv |\mathbf{k}|). \tag{23}$$

Here the external field in (21) $\mathbf{E}(\mathbf{x})$ is substituted with the operator of transversal electric field $\hat{\mathbf{E}}^t(\mathbf{x})$. It can be shown that a longitudinal electric field introduces a direct Coulomb interaction between atoms if in the framework of the Coulomb gauge the scalar potential is chosen in a proper way rather than considered to be equal to zero. The transversal electric field operator $\hat{\mathbf{E}}^t(\mathbf{x})$ is taken here in the form [2]

$$\hat{\mathbf{E}}^t(\mathbf{x}) = \sum_{k,\alpha} \left(\frac{2\pi\omega_k\hbar}{V} \right)^{1/2} \left(\mathbf{e}_\alpha(\mathbf{k}) c_{\alpha\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} + \mathbf{e}_\alpha^*(\mathbf{k}) c_{\alpha\mathbf{k}}^+ e^{-i\mathbf{k}\cdot\mathbf{x}} \right) \tag{24}$$

where the complex polarization vectors $\mathbf{e}_\alpha(\mathbf{k})$ corresponding to the circular polarization are used. The last item in (23) is the Hamilton operator of the free electromagnetic field. As a result, we come to the standard Hamilton operator of a system of atoms and electromagnetic field [1, 2, 5, 9, 10].

Note, that one can find in the literature different expression for operator of the transversal electric field

$$\hat{\mathbf{E}}^t(\mathbf{x}) = i\sum_{k,\alpha}\left(\frac{2\pi\omega_k\hbar}{V}\right)^{1/2}\left(\mathbf{e}_\alpha(\mathbf{k})c_{\alpha\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{x}} - \mathbf{e}^*_\alpha(\mathbf{k})c^+_{\alpha\mathbf{k}}e^{-i\mathbf{k}\cdot\mathbf{x}}\right) \quad (25)$$

(see, for example, [6]). Expressions (24) and (25) are connected by the canonical transformation of creation and annihilation operators $c^+_{\alpha\mathbf{k}} \to -ic^+_{\alpha\mathbf{k}}$, $c_{\alpha\mathbf{k}} \to ic_{\alpha\mathbf{k}}$ and both can be used.

5. Conclusions

Proceeding from the fundamental Lagrangian formulation of dynamics for a system of one-electron atoms and electromagnetic field, the equivalence of Hamilton operators in the Coulomb gauge and dipole approximation ($\mathbf{x}\cdot\mathbf{E}$-approximation) is shown. In the framework of the multi-particle theory on the basis of the quantum Liouville equation for the statistical operator of the system, it is ascertained that the both approaches lead to the same average values of physical variables at the proper transformation of their operators. Incidentally the application of the theory based on the dipole approximation is simpler. The inexpedience of using for the Hamilton operator in the Coulomb gauge the $\mathbf{p}\cdot\mathbf{A}$ approximation where the vector potential square is neglected follows from the established equivalence of the discussed approaches.

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Received 15.03.2015