Higher intensity interactions of light with quantum systems in non-relativistic quantum mechanics

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The Ehrenfest theorem has been applied to a non relativistic two-body quantum system in order to investigate its interaction with an electromagnetic wave with high intensity. The obtained equation of motion for such system was found to be only conditionally equivalent to the classical equations of motion for a charged particle in an electromagnetic field.

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I. INTRODUCTION

The Ehrenfest's theorem [1] shows that the classical and the quantum motions are equivalent when the position and momentum vectors are replaced by their corresponding expectation values [2].

Considering the Schrödinger equation:

$$i\hbar \frac{\partial \psi(\vec{x},t)}{\partial t} = -\frac{\hbar^2}{2m} \vec{\nabla}^2 \psi(\vec{x},t) + V(\vec{x}) \psi(\vec{x},t),$$

$$-i\hbar \frac{\partial \psi(\vec{x},t)^{\dagger}}{\partial t} = -\frac{\hbar^2}{2m} \vec{\nabla}^2 \psi(\vec{x},t)^{\dagger} + V(\vec{x}) \psi(\vec{x},t)^{\dagger}, \qquad (1)$$

Or equivalently:

$$[\vec{x}_i, \mathcal{H}(\vec{P})] = i\hbar \frac{\partial \mathcal{H}(\vec{P})}{\partial \vec{p}_i} \tag{2}$$

$$[\vec{p}_i, \mathcal{H}(\vec{x})] = -i\hbar \frac{\partial \mathcal{H}(\vec{X})}{\partial \vec{x}_i}$$
(3)

The results from the Ehrenfest theorem for the time derivatives of the expectation values of momentum and position are:

$$\frac{d}{dt}\langle x\rangle = -\frac{i\hbar}{m} \int \psi^{\dagger} \frac{\partial}{\partial x} \psi d\tau = \frac{1}{m} \langle p_x \rangle. \tag{4}$$

$$\frac{d}{dt}\langle p_x \rangle = \langle -\frac{\partial V(\vec{x})}{\partial x} \rangle. \tag{5}$$

(4) and (5) yield the *classical* equations of motion when the expectation values are replaced by the original vectors.

The Ehrenfest theorem will be used in the following fashion to obtain the equation of motion for a particle in a non-relativistic quantum system under perturbation of a light source with high intensity. First an interaction hamiltonian will be obtained for the system and then by using the canonical commutation relations in (2) and (3), $\frac{d}{dt} < \vec{P} >$ will be obtained which at the end will yield the equation of motion.

II. MODEL

1. The electromagnetic wave

Consider an electromagnetic plane wave of wave vector \vec{k} and angular frequency $\omega = ck$. With a proper choice of gauge, scalar potential $U(\vec{r},t)=0$,

$$\vec{A}(\vec{r},t) = A_0 \,\vec{e}_z \,e^{i(ky-wt)} + A_0^* \,\vec{e}_z \,e^{-i(ky-wt)} \tag{6}$$

With \vec{E} and \vec{B} in the z and x directions respectively.

We then have:

$$\vec{E}(\vec{r},t) = -\frac{\partial}{\partial t}\vec{A}(\vec{r},t) \tag{7}$$

$$\vec{B}(\vec{r},t) = \vec{\nabla} \times \vec{A}(\vec{r},t) \tag{8}$$

$$\vec{E}(\vec{r},t) = \mathcal{E}(\vec{r}) \ \vec{e}_z \cos(ky - wt) \tag{9}$$

$$\vec{B}(\vec{r},t) = \mathcal{B}(\vec{r}) \vec{e}_x \cos(ky - wt) \tag{10}$$

We set:

$$i\omega A_0 = \frac{\mathscr{E}(\vec{r})}{2} \tag{11}$$

$$ikA_0 = \frac{\mathcal{B}(\vec{r})}{2} \tag{12}$$

Where $\frac{\mathscr{E}(\vec{r})}{\mathscr{B}(\vec{r})} = \frac{w}{k} = c$

2. The Interaction Hamiltonian

The interaction Hamiltonian (ignoring the interaction between the spin magnetic moment of the electron with the magnetic field of the wave) can be written as [3]:

$$H = \frac{1}{2m} [\vec{P} - q\vec{A}(\vec{R}, t)]^2 + V(R) + mc^2$$
 (13)

The atomic Hamiltonian is:

$$H_0 = \frac{\vec{P}^2}{2m} + V(R) + mc^2 \tag{14}$$

H can be written as $H_0 + W(t)$. Subsequently:

$$W(t) = -\frac{q}{m}\vec{P}.\vec{A}(\vec{R},t) + \frac{q^2}{2m}[\vec{A}(\vec{R},t)]^2$$
 (15)

In low limit intensities (i.e ordinary light sources), the second term of the expression (15) can be ignored but for higher intensities one should keep the second term in the interaction hamiltonian before trying to calculate the evolution of $\langle \vec{R} \rangle(t)$ and consequently the force acting on the particle.

3. Evolution of $\langle \vec{R} \rangle$ (t) and the equation of motion

Expression (13) can be re-written based on equations (6) and (11) in the following form:

$$W(t) = \frac{q\mathscr{E}(\vec{r})}{m\omega} P_z \sin \omega t + \frac{q^2 \mathscr{E}^2(\vec{r})}{2m \omega^2} \sin^2 \omega t$$
 (16)

At this point, the evolution of $\langle \vec{R} \rangle(t)$ can be calculated using the Ehrenfest's theorem and canonical commutation relations. Therefore

$$\frac{d}{dt} < \vec{R} > = \frac{1}{i\hbar} < \vec{R}, H >$$

$$= \frac{\langle \vec{P} \rangle}{m} + \frac{q\mathscr{E}(\vec{r})}{m\omega} \vec{e}_z \sin \omega t$$
(17)

$$\frac{d}{dt} < \vec{P} > = \frac{1}{i\hbar} < \vec{P}, H >$$

$$= - < \nabla V(R) >$$

$$- \frac{q}{m\omega} \vec{e}_z P_z \sin \omega t < \nabla \mathcal{E}(\vec{r}) >$$

$$- \frac{q^2}{2m\omega} \vec{e}_z \sin^2 \omega t < \nabla \mathcal{E}^2(\vec{r}) >$$
(18)

From equations (17) and (18) and setting $\vec{r} = \vec{R}$, the formula for the force acting on the particle is obtained:

$$m\frac{d^{2}}{dt^{2}} < \vec{r} > = - < \nabla V(r) >$$

$$-\frac{q}{m\omega} \vec{e}_{z} P_{z} \sin \omega t < \nabla \mathcal{E}(\vec{r}) >$$

$$-\frac{q^{2}}{2m\omega} \vec{e}_{z} \sin^{2} \omega t < \nabla \mathcal{E}^{2}(\vec{r}) >$$

$$+q\mathcal{E}(r) \vec{e}_{z} \cos \omega t$$

$$(19)$$

III. DISCUSSIONS

The equation of motion in (19) is only equivalent to the classical equation of motion when $\mathscr{E}(\vec{r})$ is a constant. The effect of the variation of $\mathscr{E}(\vec{r})$ with r and the higher intensity approximation (the second term in equation (15) introduce the following term in (19):

$$-\frac{q^2}{2m\omega}\vec{e}_z\sin^2\omega t < \nabla\mathscr{E}^2(\vec{r}) >$$

Which acts like an additional *drag* force on the particle. At this point a fully relativistic treatment of this problem is needed to investigate the results. It is fortunate that the Ehrenfest theorem is also valid in quantum field theories (see for example ref. 2).

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