RELATIVISTIC QUANTUM THEORY OF MICROWAVE AND OPTICAL ATOMIC CLOCKS

CHRISTIAN J. BORDÉ

Laboratoire de Physique des Lasers, Université Paris-Nord, Villetaneuse, and Bureau National de Métrologie, Paris, France

Tel +33-608221484, Fax +33-608018459, E-mail: chbo@ccr.jussieu.fr

The accuracy of atomic clocks, in the microwave or in the optical domain, is now such that a new theoretical framework [1] is required, which includes: 1 - A fully quantum mechanical treatment of the atomic motion in free space and in the presence of a gravitational field (most cold atom interferometric devices use atoms in "free fall" in a fountain geometry), 2 - An account of simultaneous actions of gravitational and electromagnetic fields in the interaction zones, 3 - A second quantization of the matter fields to take into account their fermionic or bosonic character in order to discuss the role of coherent sources and their noise properties, 4 - A covariant treatment including spin to evaluate general relativistic effects. A theoretical description of atomic clocks revisited along these lines, is presented, using both an exact propagator of atom waves in gravito-inertial fields [2] and a covariant Dirac equation in the presence of weak gravitational fields [3]. Using this framework, recoil effects, spin-related effects, beam curvature effects, the sensitivity to gravito-inertial fields and the influence of the coherence of the atom source can be discussed in the context of present and future microwave and optical clocks.

The goal of this paper is to introduce a unified picture of microwave and optical clocks using the language of atom interferometry. The wave character of atoms is getting more and more manifest in these devices: the recoil energy $\hbar\delta = \hbar^2 k^2/2M$ is not negligible any more in Cesium clocks ($\delta/\omega \simeq 1.5\ 10^{-16}$). Atom sources may now be coherent sources of matter-waves (atom lasers or atomasers[4]). We have to deal with a very different picture from that of small clocks carried by classical point particles. The atomic frame of reference may not be well-defined. Atomic clocks are thus now fully quantum devices in which both the internal and external degrees of freedom must be quantized. Finally gravitation and inertia play a key role in slow atom clocks. The Einstein red shift and the second-order Doppler shift may become important and thus atomic clocks have to be treated also as relativistic devices.

The wave properties of atoms are fully described by a dispersion law relating the de Broglie frequency to the de Broglie wave vector, which is obtained by the introduction of Planck constant in the law connecting the energy $E(\overrightarrow{p})$ to the momentum $\overrightarrow{p}$. In free space (Figure1):

$$E(\overrightarrow{p}) = \sqrt{M^2c^4 + p^2c^2}$$

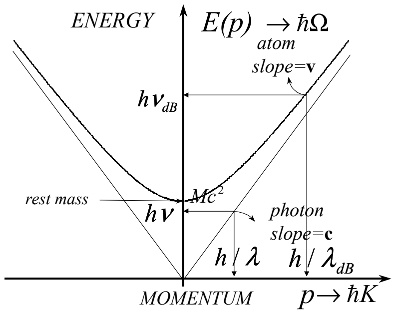

Figure 1

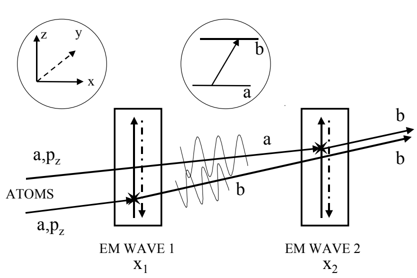

Figure 2

We shall make a systematic use of these energy-momentum diagrams to discuss the problem of interaction of two-level atoms with two separate field zones in a Ramsey excitation scheme (Figure 2). Figures 3 and 4 illustrate the energy and momentum conservation between this two-level atom and effective photons from each travelling wave in the transverse and longitudinal directions and display the recoil energy, the first and second-order Doppler shifts and the transit broadening. It is clear from Fig. 4 that, out of resonance, an additional longitudinal momentum is transferred to the atoms in the excited state.

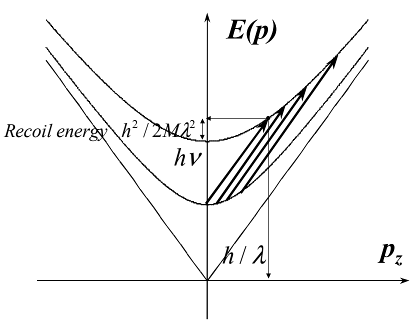

Figure 3

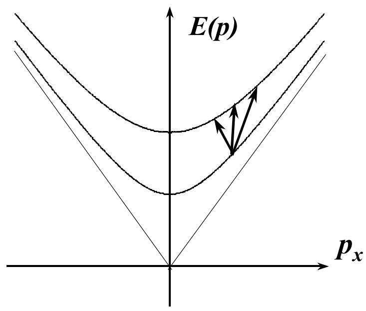

Figure 4

For each field zone, we can calculate the first-order excited state transition amplitude[3,2] for a Gaussian field envelope (as an example):

$$b_{\pm}^{(1)}(\overrightarrow{r},t) = i\sqrt{\pi}e^{i(\pm kz-\omega t+\varphi)}\int \frac{d^3p}{(2\pi\hbar)^{3/2}}\frac{w\Omega_{ba}}{v_x}e^{-w^2(\omega-\omega_{ba}\mp kv_z-\delta)^2/4v_x^2} \quad (1)$$
$$e^{i(\omega-\omega_{ba}\mp kv_z-\delta)(x-x_1)/v_x}e^{i[\overrightarrow{p}\cdot(\overrightarrow{r}-\overrightarrow{r}_0)-E_a(\overrightarrow{p})(t-t_0)]/\hbar}a^{(0)}(\overrightarrow{p},t)$$

as the product of the e.m. carrier times a Rabi frequency and a Rabi envelope, times an additional momentum phase factor for each initial wave packet Fourier component. This additional longitudinal momentum (Fig.4) is proportional to the detuning and is responsible for the Ramsey fringes, since de Broglie waves associated with each path have a different wavelength in the dark zone[11,7] (Fig.2):

$$\int dz b_{1\pm}^{(1)}(\overrightarrow{r},t) b_{2\pm}^{(1)*}(\overrightarrow{r},t) \propto \int dp_z e^{-w^2(\omega-\omega_{ba}\mp kv_z-\delta)^2/2v_x^2} \\ e^{i(\omega-\omega_{ba}\mp kv_z-\delta)(x_2-x_1)/v_x} a^{(0)}(p_z) a^{(0)*}(p_z) \qquad (2)$$

This Ramsey interference pattern has a blue recoil shift δ and is the superposition of fringe sub-systems corresponding to each velocity class, shifted by the first-order Doppler effect. If the transverse velocity distribution is too broad (absence of diaphragm) or in the optical domain, this will blur out the fringes. To make the connection with atom optics, this superposition can be rewritten as a correlation function involving the degree of coherence of the atom source[a]:

$$\int dz a^{(0)}(z \mp \frac{\hbar k}{M}\left(x_2-x_1\right)/v_x, t) a^{(0)*}(z,t) \qquad (3)$$

Fringes will be obtained as long as $\hbar k\left(x_2-x_1\right)/Mv_x$ is smaller than the coherence width of the atom source. A second mechanism, which was considered only recently, is the interaction with oppositely travelling waves in each zone as in Figures 5 and 6:

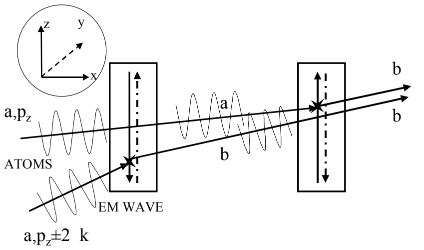

Figure 5

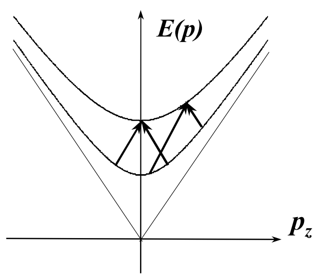

Figure 6

[a]The degree of transverse coherence of a thermal atom source is given by the density matrix element: $\langle z,t|\,\rho\,|z',t'\rangle$ which is simply the free propagator for a "complex time" argument: $t-t'-i\hbar/(k_BT)$. Its width is the thermal de Broglie wavelength h/Mu and it gives rise to the Doppler width k_Bu. Incidentally, an accurate value for the Boltzman constant could be obtained through the accurate frequency measurement of a Doppler width.

This is possible only if the initial wave packet has Fourier components which differ by $\pm 2\hbar k$ (size of atomic cloud $< \lambda_{em}$) since:

$$\int dz b_{1\pm}^{(1)}(\overrightarrow{r},t) b_{2\mp}^{(1)*}(\overrightarrow{r},t) \propto \int dz e^{\pm 2ikz} \int dp_z dp_z' \exp\left[i\left(p_z - p_z'\right) z/\hbar\right] ...$$
$$...a^{(0)}(p_z) a^{(0)*}(p_z') \Rightarrow \delta\left(p_z - p_z' \pm 2\hbar k\right) \qquad (4)$$

The resulting signal exhibit fringes with an opposite recoil shift $-\delta$. Unlike the previous one, this signal depends upon the propagation characteristics of the incident atom wave:

$$\int dz b_{1\pm}^{(1)}(\overrightarrow{r},t) b_{2\mp}^{(1)*}(\overrightarrow{r},t) \propto e^{i(\omega-\omega_{ba}+\delta)(x_2-x_1)/v_x}$$
$$.\int dp_z e^{-i(\pm k v_z + 2\delta)(2x_0 - x_2 - x_1)/v_x} \quad a^{(0)}(p_z) a^{(0)*}(p_z \pm 2\hbar k) \qquad (5)$$

This integral is easily calculated for Gaussian wave packets and statistical mixtures (a more realistic strong-field numerical approach to this recoil problem is also presented in this book[22]). If the waist position x_0 of the atom wave is not well-defined (e.g. in a thermal beam), energy conservation requires $kv_z = \mp 2\delta$ and will not be satisfied for most velocities (Fig. 6) and this signal will tend to average out. For a coherent atom wave, if the waist is located at x_1, this second contribution will have the same magnitude as the first one and the overall recoil shift will cancel[22]. If it is focussed at the midpoint $x_0 = (x_1 + x_2)/2$ (perfect time reversal), this signal will be free of Doppler effect and will tend to dominate and impose its opposite recoil shift. This would be the case, for example, of a coherent atom wave with a waist at the top of a fountain clock.

To treat fountain clocks and take gravito-inertial fields into account, we consider quite generally the non-relativistic Schroedinger equation obtained as the non-relativistic limit of a general relativistic equation:

$$i\hbar \frac{\partial |\Psi(t)\rangle}{\partial t} = \left[H_0 + \frac{1}{2M} \overrightarrow{p}_{op}^{\,2} - \overrightarrow{\Omega}(t) \cdot (\overrightarrow{L}_{op} + \overrightarrow{S}_{op}) \right.$$
$$\left. - M\vec{g}(t) \cdot \vec{r}_{op} - \frac{M}{2} \vec{r}_{op} \cdot \overrightarrow{\overrightarrow{\gamma}}(t) \cdot \vec{r}_{op} \right] |\Psi(t)\rangle \qquad (6)$$

where H_0 is an internal atomic Hamiltonian. Gravito-inertial fields are represented by the tensor $\overrightarrow{\overrightarrow{\gamma}}(t)$ and by the vectors $\overrightarrow{\Omega}(t)$ and $\vec{g}(t)$. The same terms can also be used to represent the effect of various external electromagnetic fields. The operators $\overrightarrow{L}_{op} = \vec{r}_{op} \times \overrightarrow{p}_{op}$ and $\overrightarrow{S}_{op}$ are respectively the orbital and spin angular momentum operators. The rotation terms are easily removed with a unitary transformation, which rotates all quantities[2,18]. The exact propagator of this equation has been derived by introducing a vector $\vec{\xi}$ such that

$$\ddot{\vec{\xi}} - \vec{\vec{\gamma}}\,(t) \cdot \vec{\xi} - \vec{g} = 0 \tag{7}$$

and the ABCD matrices of Gaussian optics[2,18]. As an example, for one space dimension z, the following result (corrected from reference [2]) is obtained for the wave packet at (z, t) :

$$\exp\left[\frac{iM}{\hbar}\dot{\xi}(z-\xi)\right] \exp\left[\frac{iM}{\hbar}\int_{t'}^{t}(\dot{\xi}^2/2 + \gamma\xi^2/2 - g\xi)dt_1\right]$$
$$\int_{-\infty}^{+\infty} dz'\,(M/2\pi i\hbar B)^{1/2} \exp\left[(iM/2\hbar B)(D\,(z-\xi)^2 - 2\,(z-\xi)\,z' + Az'^2)\right]$$
$$\exp\left[iMv_0(z'-z_0)/\hbar\right] F\,(z'-z_0, X_0, Y_0)$$
$$= \exp\left[\frac{iS(t,t_0)}{\hbar}\right] \exp\left[\frac{iM}{\hbar}v(t)\,(z - z(t))\right] F(z - z(t), X(t), Y(t)) \tag{8}$$

$$\begin{aligned} \text{where } S(t,t_0) &= M\dot{\xi}(Az_0 + Bv_0) - \frac{M}{2}\int_{t_0}^{t}(\dot{\xi}^2 + \gamma\xi^2)dt_1 + M\dot{\xi}\xi \\ &+ \frac{M}{2}(ACz_0^2 + DBv_0^2 + 2BCz_0v_0) \\ &= \frac{M}{\gamma^{3/2}}\left[g^2\left(-\frac{x}{2} + \frac{1}{4}\sinh 2x\right) + \frac{\gamma}{4}\left(v_0^2 - 2gz_0 + \gamma z_0^2\right)\sinh 2x \right. \\ &\left. + \sqrt{\gamma}v_0\,(-g + \gamma z_0)\sinh^2 x\right] \end{aligned} \tag{9}$$

is the classical action, with $x = \sqrt{\gamma}(t - t_0)$ and where

$$F\,(z - z_0, X_0, Y_0) = \frac{1}{\sqrt{X_0}} \exp\left[\frac{iM}{2\hbar}\frac{Y_0}{X_0}(z - z_0)^2\right] \tag{10}$$

is a Gaussian (more generally Hermite-Gaussian) wave packet at the initial time t_0 in which the central position z_0, the initial velocity v_0 and the initial complex width parameters X_0, Y_0 in phase space, have to be replaced by their values at time t given by the $ABCD\xi$ transformation law:

$$\begin{aligned} z(t) &= Az_0 + Bv_0 + \xi \quad ; \quad X(t) = AX_0 + BY_0 \\ v(t) &= Cz_0 + Dv_0 + \dot{\xi} \quad ; \quad Y(t) = CX_0 + DY_0 \end{aligned} \tag{11}$$

In the limit where $\gamma \to 0$, $A = D \to 1$, $B \to t - t_0$, $C \to 0$, $\xi \to -(1/2)g(t-t_0)^2$ and $S \to M(t - t_0)\left(v_0^2 - 2gz_0 - 2gv_0(t - t_0) + 2g^2(t - t_0)^2/3\right)/2$.

Let us apply this result to fountain clocks (Fig.7).

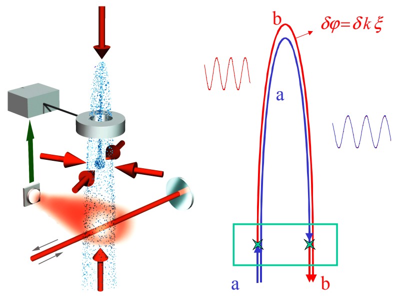

Figure 7

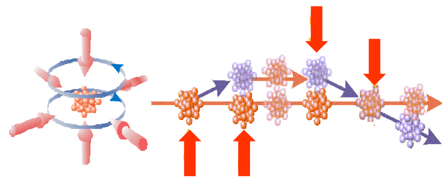

Figure 8

We have seen that the total phase factor acquired by the atomic wave packet is: $\exp\left[\frac{iS(t,t_0)}{\hbar}\right] \exp\left[ip(t)\left(z - z(t)\right)/\hbar\right]$ [b]. On one arm the additional momentum communicated after the first interaction: $\hbar\delta k = \hbar\left(\omega - \omega_{ba} - kv_z - \delta\right)/v_x$ combined with $\xi = -(1/2)gT^2$, in the second phase factor, gives the phase shift responsible for the Ramsey fringes $\delta k \xi$. Note that this phase shift is indeed the same as in the atom gravimeter (see below) and an atom fountain clock is essentially a gravimeter with a recoil momentum communicated longitudinally proportional to the detuning. The phase factor which comes from the action, gives the proper combination of gravitational phase shift and second-order Doppler effect (analogy with the Langevin twin paradox):

$$\left(S_b - S_a\right)/\hbar = -\omega_{ba}\left[1 + \frac{1}{6}\frac{v_0^2}{c^2}\right]\left(\frac{2v_0}{g}\right) \tag{12}$$

In the optical domain, more interaction zones are necessary to close the interferometer[19,9] and cancel the transverse phase shift (see figure 8). These interactions may be separated in space or in time as in recent realizations of optical clocks[7,20,21], which use magneto-optical traps of Ca, Sr or Mg. The theory of optical clocks begins with perturbative and numerical approaches around 1977 [19]. A more sophisticated theory, which is still used to describe experimental results, introduces 2x2 ABCD matrices in the internal spinor space of the two-level system and free propagation between pulses/field zones and was first published in 1982[16,17]. In 1990, the ABCDξ formalism for atom wave propagation in gravito-inertial fields has been presented, for the first time, in

[b]Quite generally, the phase shift along each arm $\left(S\left(t,t_0\right) - \left[\vec{p}\left(t\right).\vec{r}\left(t\right)\right]_{t_0}^{t}\right)/\hbar$ is equal to minus the time integral of the kinetic energy.

Les Houches[18]. The strong field S-matrix treatment of the electromagnetic field zones was then published in 1994[12,8]. In 1995, the problem of Rabi oscillations in a gravitational field has been treated in analogy/complementarity with the frequency chirp in curved wave-fronts[14]. Finally the dispersive properties of the group velocity of atom waves in strong e.m. fields have been described as a generalization of the dynamical scattering theory of neutrons in neutron beam splitters[10,13,15]. To-day we combine all these elements in a new sophisticated and realistic quantum description of optical clocks. This effort is also underway for atomic inertial sensors and is essential to develop strategies to eliminate the inertial field sensitivity of optical clocks[20]. A complete general relativistic derivation of phase shifts was published in 1999[3]. Using the 4-D Stokes theorem the spin-independent part of this phase shift can be written:

$$\begin{aligned} -\hbar\delta\varphi &= \oint \frac{c^2}{2E(\vec{p})} p^\mu h_{\mu\nu} p^\nu dt = \oint \frac{1}{2} p^\mu h_{\mu\nu} dx^\nu \\ &= \frac{1}{2} \iint d\sigma^{\mu\nu} \left(\partial_\mu A_\nu - \partial_\nu A_\mu\right) \text{ with } A_\nu = \frac{1}{2} p^\mu h_{\mu\nu} \end{aligned} \tag{13}$$

in analogy with electromagnetism. This formula gives:

$$\delta\varphi = -\vec{k}.\vec{g}T(T+T') \tag{14}$$

for the gravitational phase shift[9,6] as the flux of a gravitoelectric field $-c^2\vec{\nabla}h_{00}/2 = \vec{g}$ through a space-time area (which is the case above for the fountain clock), whereas the Sagnac phase shift[c] is the flux of a gravitomagnetic field $c^2\vec{\nabla}\times\vec{h} = 2c\vec{\Omega}$ through an area $\vec{A}$ in space[9,6], which clocks usually do not have:

$$\delta\varphi = \frac{2c\vec{\Omega}.\vec{A}}{\hbar c/M} \tag{15}$$

The spin-dependent terms and related effects in atom interferometers can be found in [3]. Their effect on atomic clocks needs to be carefully evaluated, especially for the spin-rotation interaction, since, unlike the magnetic field, the gravitomagnetic field cannot be shielded.

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[c]This Sagnac phase shift (in units of 2π) can be written as the projection of the orbital angular momentum (in units of $\hbar$) of the interfering particles. An example of nuclear Sagnac interferometer is provided by rotating molecules, for which this phase shift is naturally quantized.

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