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Effects of mass defect in atomic clocks

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Abstract. We consider some implications of the mass defect on the frequency of atomic transitions. We have found that some well-known frequency shifts (such as gravitational and quadratic Doppler shifts) can be interpreted as consequences of the mass defect, i.e., without the need for the concept of time dilation used in special and general relativity theories. Moreover, we show that the inclusion of the mass defect leads to previously unknown shifts for clocks based on trapped ions.

1. Introduction

At the present time, atomic clocks are most precise scientific devices. The principle of operation of these quantum instruments is based on modern methods of laser physics and high-precision spectroscopy. In this way, the unprecedented value of fractional instability and uncertainty at the level of 10⁻¹⁸ has already been achieved with the goal of 10⁻¹⁹ on the horizon [1]. Frequency measurements at such a level could have a huge influence on further developments in fundamental and applied physics. In particular, we can foresee tests of quantum electrodynamics and cosmological models, searches for drifts of the fundamental constants, new types of chronometric geodesy, and so on (see, for example, review [2]). However, this level of experimental accuracy requires a comparable level of theoretical support, which would account for systematic frequency shifts of atomic transitions due to different physical effects. Thus, modern atomic clocks are also at the point of interweaving different areas of theoretical physics.

In this paper we develop the mass defect concept with respect to atomic clocks. Historically, considerations of the mass defect have been connected with nuclear physics, where the mass defect explains the huge energy emitted due to different nuclear reactions. However, a quite unexpected result is that this effect has a direct relation to frequency standards, where it leads to shifts in the frequencies of atomic transitions.

The main idea of our approach is as follows. Let us consider an arbitrary atomic transition between the ground (g) and excited (e) states with unperturbed frequency \( \omega_0 = (E_e^{(0)} - E_g^{(0)})/\hbar \), where \( E_e^{(0)} \) and \( E_g^{(0)} \) are the unperturbed energies of the corresponding states (see in Fig.1). Using Einstein's famous formula, \( E=Mc^2 \), which links the mass \( M \) and energy \( E \) of a particle (\( c \) is the speed of light in vacuum), we can find the rest masses of our particle, \( M_g \) and \( M_e \), for the states (g) and (e), respectively:
The fact that $M_g \neq M_e$ is the essence of the so-called mass defect. In our case, the connection between $M_g$ and $M_e$ reads:

$$M_e c^2 = M_g c^2 + \hbar \omega_0 \Rightarrow M_e = M_g + \hbar \omega_0 / c^2$$

We show that the relationship (1) allows us to reinterpret some well-known systematic frequency shifts (e.g. those connected with the time dilation effects) [3,4]. Moreover, our approach predicts some new shifts previously unconsidered, to our best knowledge, in the scientific literature.

2. Gravitational shift
As the first example, let us show how the mass defect allows us to formulate a very simple explanation of the gravitational redshift even under a classical description of the gravitational field (as classical potential $U_G$). Indeed, because the potential energy of a particle in a classical gravitational field is equal to the product $MU_G$ (where $U_G < 0$), we can write the energy of $j$-th state $E_j(U_G)$ as:

$$E_j(U_G) = M_j c^2 + M_j U_G = M_j c^2 (1 + U_G / c^2), \ (j = g,e)$$

(2)

Using eqs.(1) and (2), we find the frequency of the transition $(g) \rightarrow (e)$ in the gravitational field:

$$\omega = \omega_0 (1 + U_G / c^2).$$

(3)

This expression coincides to the leading order with the well-known formula from the general relativity theory:

$$\omega = \omega_0 \sqrt{1 + 2U_G / c^2} \approx \omega_0 (1 + U_G / c^2)$$

(4)

in the limit of weak gravitational field $|U_G|c^2 << 1$.

3. Motion-induced shifts for atoms (ions) trapped in a confining potential
The second example concerns frequency shifts in the presence of a confining potential $U(r)$, which we take to be the same for both states $(g)$ and $(e)$. Such a situation occurs both for clocks based on neutral...
atoms in optical lattice at magic wavelength and those based on trapped ions. In this case, we have the standard task of quantizing the energy levels with translational degrees of freedom:

\[ \hat{H} \left| \psi_{j,a}(r) \right\rangle = E_{j,a}^{\text{vib}} \left| \psi_{j,a}(r) \right\rangle, \quad \hat{H} = \hat{p}^2 / 2M_j + U(r), \]

where the Hamiltonian \( \hat{H} \) describes the translational motion of the particle in the \( j \)-th internal state \((j=g,e)\), the wavefunction \( \left| \psi_{j,a}(r) \right\rangle \) corresponds to the \( \alpha \)-th vibrational level \((\alpha=0,1,2,...)\) and \( r \) is coordinate of atomic center-of-mass. Thus, taking into account the translational motion, the atomic wave function is described by the pair products \( \left| j \right\rangle \otimes \left| \psi_{j,a}(r) \right\rangle \). Because of the mass defect \((M_g \neq M_e)\), the energy levels for the lower and upper states differ: \( E_{g,a}^{\text{vib}} \neq E_{e,a}^{\text{vib}} \). Consequently, the frequency \( \omega_{\alpha a} \) between corresponding levels of trapped particle is different from the unperturbed frequency, \( \omega_0 \), with a value \( \Delta \omega \) (see Fig.1): 

\[ \Delta \omega = \omega_{\alpha a} - \omega_0 = \left( E_{e,a}^{\text{vib}} - E_{g,a}^{\text{vib}} \right) / \hbar. \]

For this purpose, we write the Hamiltonian for upper state in the following form:

\[ \hat{H}_g = \hat{H}_e + \Delta \hat{H}; \quad \Delta \hat{H} = \frac{\hat{p}^2}{2M_g} - \frac{\hat{p}^2}{2M_g} = - \frac{\hbar \omega_0}{2M_g M_s} \hat{p}^2. \]

where the operator \( \Delta \hat{H} \) can be considered as a small perturbation. Then using standard perturbation theory, we obtain the following estimate for the relative value of the shift

\[ \frac{\Delta \omega}{\omega_0} \approx \frac{1}{2c^2} \frac{\langle \psi_{j,a} | \hat{p}^2 | \psi_{j,a} \rangle}{M_g^2}. \]

We note that this expression coincides with a well-known relativistic correction, which is the quadratic Doppler shift due to the time dilation effect for moving particle [4]. Indeed, at the present time the following explanation is conventionally used. In accordance with special relativity, the tick rate \( \Delta \tau \) in the moving (with velocity \( \nu \)) coordinate system changes with respect to the tick rate \( \Delta \tau^* \) in motionless (laboratory) coordinate system by the law: 

\[ \Delta \tau = \Delta \tau^* \left(1 - \nu^2 / c^2\right)^{1/2}. \]

As a result, an atomic oscillation with eigenfrequency \( \omega_0 \) is perceived by an external observer to be shifted to 

\[ \omega = \omega_0 \left(1 - \nu^2 / c^2\right)^{1/2}. \]

In the nonrelativistic limit, \( (\nu^2 / c^2)<<1 \), we have: 

\[ \omega = \omega_0 (1 - \nu^2 / 2c^2) = \omega_0 [1 - (p/M)^2 / 2c^2] \]

(where \( p \) is momentum of particle). Then, if we take into account quantum considerations through the replacement \( \hat{p} \rightarrow \hat{p} = -i \hbar \nabla \), we obtain the expression for frequency shift (7).

### 4. Previously unconsidered field-induced shifts for trapped ions

Besides the reinterpretation of some well-known shifts, the mass defect concept predicts additional contributions for field-induced shifts that have not been previously discussed in the scientific literature. We emphasize that these additional shifts are associated with translational degrees of freedom and they vanish if we will not take into account the mass defect.

We will consider a trapped ion (with charge \( eZ_i \)) in the presence of additional weak electric field with potential \( \phi_{\text{add}}(r) \), which describes all controlled and uncontrolled fields except the trapping potential \( U(r) \). Let us show how the additional potential \( \phi_{\text{add}}(r) \) will perturb the vibrational structure formed by \( U(r) \). For this purpose we will use vibrational eigenfunctions \( \left| \psi_{j,a}(r) \right\rangle \), which describe a spatial localization of the ion in the internal states \( \left| j \right\rangle \) \((j=g,e)\) due to the trap potential \( U(r) \), as a basis for perturbation theory on the small additional interaction \( U_{\text{add}}(r) = eZ_i \phi_{\text{add}}(r) \).

The center of the ion localization \( \mathbf{r}_0 \) in the trap is determined by averaging: 

\[ \mathbf{r}_0 = \langle \psi_{j,a} | r \psi_{j,a} \rangle. \]

In this case, we will use the following Taylor series of the operator \( U_{\text{add}}(r) \) at the point of ion localization \( \mathbf{r}_0 \): 

\[ U_{\text{add}}(r) = eZ_i \phi_{\text{add}}(\mathbf{r}_0) - (\mathbf{d} \cdot \mathbf{E}_{\text{add}}(r)) + (\mathbf{Q} \cdot \mathbf{W}_{\text{add}}(r_0)) + ..., \]
where \( \mathbf{E}_{\text{add}}(\mathbf{r}_0) = -\nabla \phi_{\text{add}}(\mathbf{r}) \big|_{\mathbf{r}_0} \) and \( \mathbf{W}_{\text{add}}(\mathbf{r}_0) = \frac{1}{6} \nabla \otimes \nabla \phi_{\text{add}}(\mathbf{r}) \big|_{\mathbf{r}_0} \) are the electric vector and electric tensor, respectively, at the point \( \mathbf{r}_0 \). The operators \( \mathbf{d} \) and \( \mathbf{Q} \) correspond to the mesoscopic dipole and quadrupole moments of ion cloud in a trap:

\[
\mathbf{d} = eZ_i(\mathbf{r} - \mathbf{r}_0) \\
\mathbf{Q}_{ij} = eZ_i \left\{ \frac{1}{2} (\mathbf{r} - \mathbf{r}_0)_i (\mathbf{r} - \mathbf{r}_0)_j - \delta_{ij} |\mathbf{r} - \mathbf{r}_0|^2 \right\}
\]  

(9)

As we see, that apart from the well-known electronic dipole and quadrupole moments the charge spatial distribution connected with motion of ion in a trap leads to mesoscopic multipole moments coupled to the weak additional electric field and its gradients.

Let us consider now the first order shift:

\[
\Delta_{\mathbf{d},\alpha} = \left\{ \frac{\Psi_{j,\alpha}}{\hbar} \left| \mathbf{d}_{\text{add}} \right| \Psi_{j,\alpha} \right\} = \left( \frac{\mathbf{Q}_{j,\alpha} \cdot \mathbf{W}_{\text{add}}(\mathbf{r}_0)}{\hbar} \right),
\]

(10)

where \( \mathbf{Q}_{j,\alpha} = \left\{ \Psi_{j,\alpha} \left| \mathbf{Q} \right| \Psi_{j,\alpha} \right\} \). The shift of the clock transition frequency reads

\[
\delta_{\alpha} = \Delta_{\mathbf{d},\alpha} - \Delta_{\mathbf{e},\alpha} = \left( \frac{\Delta \mathbf{Q}_{\alpha} \cdot \mathbf{W}_{\text{add}}(\mathbf{r}_0)}{\hbar} \right).
\]

(11)

Here the residual quadrupole moment caused by the mass defect

\[
\Delta \mathbf{Q}_{\alpha} = \left\{ \Psi_{e,\alpha} \left| \mathbf{Q} \right| \Psi_{e,\alpha} \right\} - \left\{ \Psi_{g,\alpha} \left| \mathbf{Q} \right| \Psi_{g,\alpha} \right\}
\]

(12)

has nonzero value because the wavefunctions describing the translational motion in the excited and ground states are different in general case. Estimate of order of magnitude gives

\[
|\Delta \mathbf{Q}_{\alpha}| \approx eZ_i R^2 \frac{\hbar \alpha_0}{Mc^2},
\]

where \( R \) is the size of ion cloud and \( M \approx M_{e,g} \). Though the expression (12) contains a very small multiplier, \( \frac{\hbar \alpha_0}{M c^2} \ll 1 \), the size of ion localization \( R \) significantly exceeds the Bohr radius \( \alpha_0 \). Indeed, \( R \approx 10^2 - 10^3 \alpha_0 \) even for the deeply-cooled ion to the lowest vibrational level in the confined potential \( U(\mathbf{r}) \) (i.e., for the quantum limit of cooling), and \( R \approx 10^4 \alpha_0 \) for the upper vibrational states, which are populated if the ion is laser-cooled to the usual Doppler temperature (mK range). As a result, the quadrupole shift of the clock transition, modified by the mass defect, can be metrologically significant for modern and future optical frequency standards. For example, let us consider an atomic clock based on the transition \( ^1S_0 \rightarrow ^3P_0 \) in the ion \( ^{27}\text{Al}^+ \) [5]. Because of the zero electronic angular momentum for the clock transition, \( J_e = J_g = 0 \), the quadrupole moment, associated with internal degrees of freedom, is very small (\( |\mathbf{Q}| \sim 10^{-6} \alpha_0^2 \), see Ref. [6]). However, for the residual quadrupole moment caused by mass defect we have the estimate

\[
|\Delta \mathbf{Q}_{\alpha}| \approx 2 \times (10^{-2} - 10^{-6}) \alpha_0^2
\]

for \( R \approx 10^2 - 10^4 \alpha_0 \). Such values of the quadrupole moment may be important for atomic clocks with fractional uncertainty at the level of \( 10^{-18} - 10^{-19} \).

5. Conclusion
We have considered some manifestations of the mass defect in atomic clocks. As a result, some well-known systematic shifts, previously interpreted as the time dilation effects in the frame of special and general relativity theories, can be considered as a consequence of the mass defect in quantum mechanics. Furthermore, our approach has predicted a series of previously unknown shifts for ion clocks. These results are important for high precision optical atomic clocks and can be interesting for theoretical quantum physics.

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