Проявления эффекта дефекта масс в атомных часах

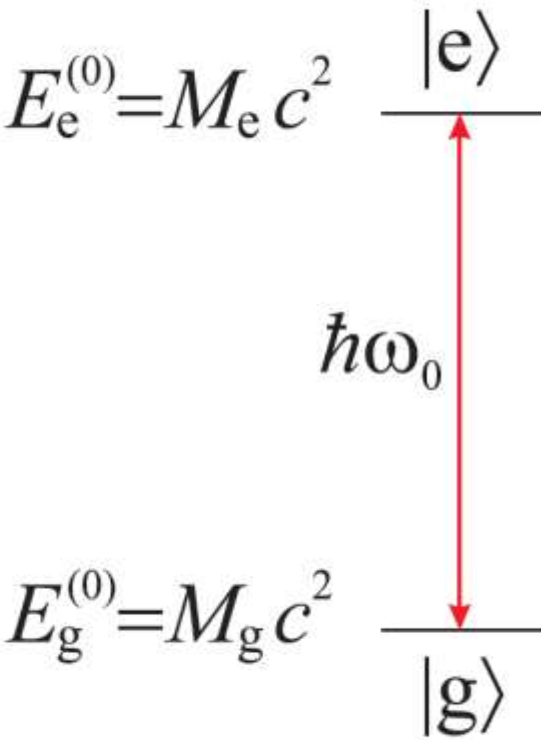
В.И.Юдин, А.В.Тайченачев

Новосибирский государственный университет

Институт лазерной физики СО РАН

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.

Main idea



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), we can find the rest masses of our particle, M_g and M_e, for the states $|g\rangle$ and $|e\rangle$, respectively: $E_g = M_g c^2$ and $E_e = M_e c^2$.

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 is the following:

$$M_e c^2 = M_g c^2 + \hbar\omega_0 \quad \Rightarrow \quad M_e = M_g + \frac{\hbar\omega_0}{c^2}$$

Gravitational shift 1

We show how the mass defect allows us to formulate a very simple explanation of the gravitational redshift, even with a classical description of the gravitational field (as classical Newtonian 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 as:

$$E_g = M_g c^2 + M_g U_G = M_g c^2 (1 + U_G / c^2)$$

$$E_e = M_e c^2 + M_e U_G = M_e c^2 (1 + U_G / c^2)$$

Then we find the frequency of the transition $|g\rangle \leftrightarrow |e\rangle$ in the gravitational field:

$$\omega = \frac{E_e(U_G) - E_g(U_G)}{\hbar} = \omega_0 \left(1 + \frac{U_G}{c^2}\right)$$

Gravitational shift 2

This expression coincides (to leading order) with a well known result based on general relativity theory:

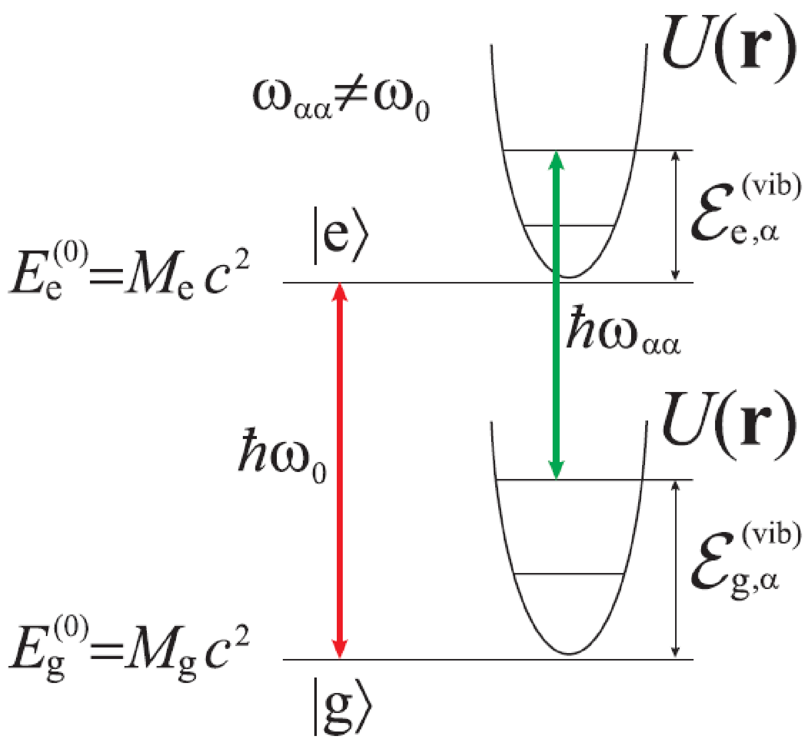
$$\omega = \omega_0 \sqrt{1 + \frac{2U_G}{c^2}} \approx \omega_0 \left(1 + \frac{U_G}{c^2}\right)$$

Thus, the combination of special relativity ($E = Mc^2$) and quantum mechanics (definition of the frequency of atomic transitions) leads to a formally noncontradictory explanation of the gravitational shift, which describes different experiments with atomic clocks in a spatially nonuniform gravitational field $U_G(\mathbf{r})$. We emphasize that the gravitational shift was derived without including time dilation, which is taken as a basis of Einstein's theory of relativity. Therefore, the developed mass defect approach can be considered as "quasi-classical" explanation of gravitational shift.

Shifts for atoms (ions) trapped in confinement potential 1

For simplicity, we will consider a stationary confinement potential $U(\mathbf{r})$, which we take to be the same for both states $|g\rangle$ and $|e\rangle$. Such a situation can occur both for clocks based on neutral atoms in optical lattice and those based on trapped ions. In this case, we use the standard formalism that quantizes the energy levels with translational degrees of freedom:

$$\widehat{H}_j|\Psi_j(\mathbf{r})\rangle = \mathcal{E}_j^{(\mathrm{vib})}|\Psi_j(\mathbf{r})\rangle\,, \quad \widehat{H}_j = \frac{\hat{\mathbf{p}}^2}{2M_j} + U(\mathbf{r})$$



where Hamiltonian H_j and state $|\Psi_j(\mathbf{r})\rangle$ describe the translational motion of the particle in the j-th internal state $|j\rangle$ (j = g;e), and $\mathbf{r}$ is coordinate of atomic center-of-mass.

Because of the mass defect ($M_e \neq M_g$), the energy levels for the lower and upper states differ: $\mathcal{E}_g^{(\mathrm{vib})} \neq \mathcal{E}_e^{(\mathrm{vib})}$

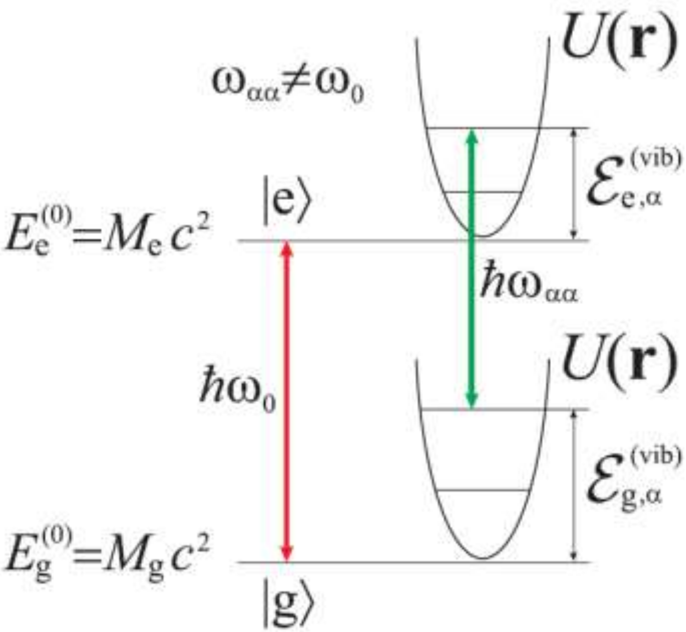
Shifts for atoms (ions) trapped in confinement potential 2

The frequency shift: $\Delta\omega = \omega - \omega_0 = \left(\mathcal{E}_{\rm e}^{(\rm vib)} - \mathcal{E}_{\rm g}^{(\rm vib)}\right)/\hbar$

We write the Hamiltonian for upper state H_e in the following form:

$$\widehat{H}_{\rm e} = \widehat{H}_{\rm g} + \Delta\widehat{H}, \quad \Delta\widehat{H} = \frac{\hat{\mathbf{p}}^2}{2M_{\rm e}} - \frac{\hat{\mathbf{p}}^2}{2M_{\rm g}} = \frac{M_{\rm g} - M_{\rm e}}{2M_{\rm g}M_{\rm e}}\hat{\mathbf{p}}^2 = -\frac{\hbar\omega_0}{2c^2}\frac{\hat{\mathbf{p}}^2}{M_{\rm g}M_{\rm e}}$$

where the operator ΔH can be considered as small perturbation.



In this case, we obtain the following estimation of the relative value of shift:

$$\frac{\Delta\omega}{\omega_0} \approx -\frac{1}{2c^2}\frac{\langle\Psi_{\rm g}|\hat{\mathbf{p}}^2|\Psi_{\rm g}\rangle}{M_{\rm g}M_{\rm e}} \approx -\frac{1}{2c^2}\frac{\langle\Psi_{\rm g}|\hat{\mathbf{p}}^2|\Psi_{\rm g}\rangle}{M_{\rm g}^2}$$

Shifts for atoms (ions) trapped in confinement potential 3

$$\frac{\Delta\omega}{\omega_0} \approx -\frac{1}{2c^2}\frac{\langle\Psi_g|\hat{\mathbf{p}}^2|\Psi_g\rangle}{M_g M_e} \approx -\frac{1}{2c^2}\frac{\langle\Psi_g|\hat{\mathbf{p}}^2|\Psi_g\rangle}{M_g^2}$$

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:

$$\omega \approx \omega_0[1 - \mathbf{v}^2/(2c^2)] = \omega_0[1 - (\mathbf{p}/M)^2/(2c^2)]$$

We believe that the mass-defect approach corresponds to the canonical quantum-mechanical scheme, while the time dilation approach can be considered as a phenomenological quasi-explanation. Both these approaches are not equivalent each to other - they coincide only in the second order Doppler.

Micromotion shift 1

In the case of dynamic confinement of the particle in time-dependent potential $U(t;\mathbf{r})$ (for example, in rf Paul trap for ions), the mass defect concept is also applicable and can explain, in particular, the frequency shift, which is usually interpreted as the micromotion shift. Indeed, in the case of relatively high rf frequency in Paul trap

$$\phi(t,\mathbf{r}) = V_{\rm dc}\, a(\mathbf{r}) + V_{\rm rf}\, b(\mathbf{r}) \cos(ft)$$

there is well-working approximation of so-called pseudopotential, which can be expressed (in context of mass defect) as following:

$$U^{(j)}_{\rm pseudo}(\mathbf{r}) = eZ_iV_{\rm dc}\, a(\mathbf{r}) + \frac{W_{\rm rf}(\mathbf{r})}{M_j}, \quad W_{\rm rf}(\mathbf{r}) = \frac{e^2Z_i^2V_{\rm rf}^2}{4f^2}(\vec{\nabla} b(\mathbf{r}))^2$$

$$\mathcal{E}^{(\rm vib)}_{j,\alpha} \ll \hbar f$$

Micromotion shift 2

$$U^{(j)}_{\rm pseudo}(\mathbf{r}) = eZ_i V_{\rm dc}\, a(\mathbf{r}) + \frac{W_{\rm rf}(\mathbf{r})}{M_j}, \quad W_{\rm rf}(\mathbf{r}) = \frac{e^2 Z_i^2 V_{\rm rf}^2}{4f^2}(\vec{\nabla} b(\mathbf{r}))^2$$

where the first term is connected with the static electric potential, and the second term is related to the micromotion and it is produced by the rf oscillating potential.

In this case, the total Hamiltonian for upper state $H_{\rm e}$ can be rewritten in the following form:

$$\hat{H}^{(\rm eff)}_{\rm e} = \hat{H}^{(\rm eff)}_{\rm g} + \Delta\hat{H}^{(\rm eff)},$$

$$\Delta\hat{H}^{(\rm eff)} = \left(\frac{1}{M_{\rm e}} - \frac{1}{M_{\rm g}}\right)\left[\frac{\hat{\mathbf{p}}^2}{2} + W_{\rm rf}(\mathbf{r})\right] = -\frac{\hbar\omega_0}{M_{\rm g} M_{\rm e} c^2}\left[\frac{\hat{\mathbf{p}}^2}{2} + W_{\rm rf}(\mathbf{r})\right]$$

where the operator ΔH can be considered a small perturbation. In the result, we have the frequency shift:

Micromotion shift 3

$$\frac{\Delta\omega_{\alpha\alpha}}{\omega_0} \approx -\frac{1}{M_{\rm g}M_{\rm e}c^2}\left[\frac{\langle\Psi_{{\rm g},\alpha}|\hat{\mathbf{p}}^2|\Psi_{{\rm g},\alpha}\rangle}{2} + \langle\Psi_{{\rm g},\alpha}|W_{\rm rf}(\mathbf{r})|\Psi_{{\rm g},\alpha}\rangle\right]$$

$$\approx -\frac{1}{2c^2}\frac{\langle\Psi_{{\rm g},\alpha}|\hat{\mathbf{p}}^2|\Psi_{{\rm g},\alpha}\rangle}{M_{\rm g}^2} - \frac{\langle\Psi_{{\rm g},\alpha}|W_{\rm rf}(\mathbf{r})|\Psi_{{\rm g},\alpha}\rangle}{M_{\rm g}^2c^2},$$

where the first contribution coincides with 2-nd order Doppler shift, which can be considered also as secular-motion-induced shift. The second contribution can be interpreted as micromotion shift. Note that both these shifts have comparable values, in the general case.

Micromotion shift 4

In the case of purely rf Paul trap with $U_{dc}(\mathbf{r}) = 0$, we have the following relationships for Hamiltonians, vibrational energies and eigenfunctions:

$$\widehat{H}_{\mathrm{e}} = \frac{M_{\mathrm{g}}}{M_{\mathrm{e}}}\widehat{H}_{\mathrm{g}}, \ \mathcal{E}_{\mathrm{e}}^{(\mathrm{vib})} = \frac{M_{\mathrm{g}}}{M_{\mathrm{e}}}\mathcal{E}_{\mathrm{g}}^{(\mathrm{vib})}, \ \Psi_{\mathrm{e}}(\mathbf{r}) = \Psi_{\mathrm{g}}(\mathbf{r})$$

leading to the total fractional frequency shift:

$$\frac{\Delta\omega}{\omega_0} = -\frac{\mathcal{E}_{\mathrm{g}}^{(\mathrm{vib})}}{M_{\mathrm{e}}c^2} \approx -\frac{\mathcal{E}_{\mathrm{g}}^{(\mathrm{vib})}}{M_{\mathrm{g}}c^2}$$

which contains both secular-motion and micromotion contributions.

Previously unconsidered frequency shifts for trapped ions

Besides the reinterpretation of some well-known shifts, the mass defect concept predicts additional contributions for frequency 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.

Mass defect quadrupole shift 1

We assume that the ion is localized in an rf Paul trap, and also we assume that the functions $|\Psi_g(\mathbf{r})\rangle$ and $|\Psi_e(\mathbf{r})\rangle$, formed by the controlled trap potential, are known. Then we can calculate the shift, produced by the weak uncontrolled external field $E_{ext}(\mathbf{r})$, as quadrupole shift in the frame of perturbation theory. For this purpose, we consider the ion as a point charge $Z_i|e|$, when the operator of its mesoscopic quadrupole moment is determined as a standard symmetrical tensor of the second order:

$$\hat{Q}_{lm} = Z_i|e|\left(3r_l r_m - \delta_{lm}|\mathbf{r}|^2\right), \quad (l, m = 1, 2, 3)$$

In this case, the residual quadrupole moment, conditioned by mass defect, is determined by the difference tensor:

$$\Delta Q_{lm}^{(\text{m-def})} = \langle\Psi_e|\hat{Q}_{lm}|\Psi_e\rangle - \langle\Psi_g|\hat{Q}_{lm}|\Psi_g\rangle$$

In the general case, we have $|\Psi_g(\mathbf{r})\rangle \neq |\Psi_e(\mathbf{r})\rangle$ due to the mass defect, and an order-of-magnitude estimate is the following:

$$|\Delta Q^{(\text{m-def})}| \sim |\langle\Psi_g|\hat{Q}_{lm}|\Psi_g\rangle|\frac{\hbar\omega_0}{Mc^2} \sim Z_i|e|R^2\frac{\hbar\omega_0}{Mc^2}$$

Mass defect quadrupole shift 2

$$|\Delta Q^{(\text{m-def})}| \sim |\langle\Psi_{\rm g}|\hat{Q}_{lm}|\Psi_{\rm g}\rangle|\frac{\hbar\omega_0}{Mc^2} \sim Z_i|e|R^2\frac{\hbar\omega_0}{Mc^2}$$

where R is the typical size of wavefunction (size of the localization of an ion cloud in the trap), and $M \approx M_{g,e}$. Though this expression contains a very small multiplier, $\hbar\omega_0/Mc^2 \ll 1$, however the size of ion localization R significantly exceeds the Bohr radius a_0. Indeed, $R \sim 10^2$–$10^3\ a_0$ 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 $R \sim 10^4\ a_0$ for the upper vibrational states, which are populated if the ion is laser-cooled to the usual so-called Doppler temperature (mK range).

Mass defect quadrupole shift 3

$$|\Delta Q^{(\text{m-def})}| \sim |\langle \Psi_g | \hat{Q}_{lm} | \Psi_g \rangle| \frac{\hbar\omega_0}{Mc^2} \sim Z_i |e| R^2 \frac{\hbar\omega_0}{Mc^2}$$

Some estimations:

$^{27}Al^+$. Because of the zero electronic angular moment for the clock transition, $J_g=J_e=0$, the quadrupole moment, associated with internal degrees of freedom, is very small ($|\Delta Q| \sim 10^{-6}|e|(a_0)^2$, see in Ref. [K. Beloy, et al., Phys. Rev. A **95**, 043405 (2017)]). However, on the basis of our formula (24), we estimate $|\Delta Q^{(\text{m-def})}| \sim 2\times(10^{-2}–10^{-6})|e|(a_0)^2$ for $R \sim 10^2–10^4 a_0$.

$^{229}Th^{3+}$. In Ref. [C. J. Campbell, et al., Phys. Rev. Lett. **108**, 120802 (2012)], the quadrupole moment (associated with internal degrees of freedom) for the clock transition was estimated to be: $|\Delta Q| \sim 10^{-5}|e|(a_0)^2$. Using our formula, we find $|\Delta Q^{(\text{m-def})}| \sim 10^{-2}–10^{-6}|e|(a_0)^2$ for $R \sim 10^2–10^4 a_0$.

Mass defect quadrupole shift 4

$$\Delta Q_{lm}^{(\text{m-def})} = \langle \Psi_\text{e} | \hat{Q}_{lm} | \Psi_\text{e} \rangle - \langle \Psi_\text{g} | \hat{Q}_{lm} | \Psi_\text{g} \rangle$$

However, this quadrupole shift is absent for spherically-symmetrical states, when $\langle \Psi_g | Q_{lm} | \Psi_g \rangle = 0$ and $\langle \Psi_e | Q_{lm} | \Psi_e \rangle = 0$.

Also the residual quadruple shift vanishes for purely rf Paul trap, because of $|\Psi_e(\mathbf{r})\rangle = |\Psi_g(\mathbf{r})\rangle$:

$$\widehat{H}_\text{e} = \frac{M_\text{g}}{M_\text{e}} \widehat{H}_\text{g}\,, \ \mathcal{E}_\text{e}^{(\text{vib})} = \frac{M_\text{g}}{M_\text{e}} \mathcal{E}_\text{g}^{(\text{vib})}, \ \Psi_\text{e}(\mathbf{r}) = \Psi_\text{g}(\mathbf{r})$$

Mass defect ac-Stark shift 1

To see another manifestation of mass defect, let us consider a previously unknown contribution to the ac-Stark shift in the presence of extraneous weak low-frequency field, $E(t) = (E_s e^{-i\nu t} + c.c.)$

The standard expression for the dynamic shift of the n-th vibrational level in the lower state |g⟩ has the form:

$$\Delta_{\mathrm{g}}^{(n)} = \sum_m \left[\frac{|E_s|^2 |\mathcal{D}_{\mathrm{g}}^{mn}|^2/\hbar}{\hbar\nu - \mathcal{E}_{\mathrm{g}}^{(m)} + \mathcal{E}_{\mathrm{g}}^{(n)}} + \frac{|E_s|^2 |\mathcal{D}_{\mathrm{g}}^{mn}|^2/\hbar}{-\hbar\nu - \mathcal{E}_{\mathrm{g}}^{(m)} + \mathcal{E}_{\mathrm{g}}^{(n)}} \right]$$

$$\mathcal{D}_{\mathrm{g}}^{mn} = \langle \Psi_{\mathrm{g}}^{(m)} | \widehat{\mathcal{D}} | \Psi_{\mathrm{g}}^{(n)} \rangle ,$$

where $D = Z_i |e| \mathbf{r}$ is the operator of the mesoscopic dipole moment of the localized ion cloud.

Similarly we can determine the shift for the n-th vibrational level in the upper state |e⟩.

Mass defect ac-Stark shift 2

Note that the square of the ion-cloud dipole moment has the order-of-magnitude of $|D|^2 \sim (Z_i|e|)^2(R_n)^2$ (where R_n is typical size of localization of wavefunction $|\Psi_{\mathrm{g}}(\mathbf{r})\rangle$), which is many orders greater than the square of the atomic dipole moment $\sim |e|^2(a_0)^2$.

The residual mass defect ac-Stark shift:

$$|\omega - \omega_0| = |\Delta_{\mathrm{e}}^{(n)} - \Delta_{\mathrm{g}}^{(n)}| = |\Delta_{\text{m-deff}}^{(n)}| \sim |\Delta_{\mathrm{g}}^{(n)}| \frac{\hbar\omega_0}{Mc^2}$$

which can exceed the ac-Stark shift connected with low-requency polarizability, which is associated with internal degrees of freedom.

In a similar way, we can find new contributions to the black body radiation (BBR) shift, linear and quadratic Zeeman shifts, and so on.

Summary

1. We have considered some manifestations of the mass defect in atomic clocks. As a result, some well-known systematic shifts (2-nd order Doppler, micromotion, gravitational), 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.

2. Furthermore, mass defect approach has predicted a series of previously unknown shifts for ion clocks.

Thank you very much for your attention!