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Effect of trapped-ion heating on generalised Ramsey methods for suppressing frequency shifts caused by a probe field in atomic clocks

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Abstract. **Based on a simple one-dimensional model, we consider the effect of trapped-ion heating on the efficiency of generalised Ramsey methods for the probe-induced frequency shift suppression in optical frequency standards based on single ultracold ions. It is shown that ion heating reduces the efficiency of all previously proposed one-loop generalised Ramsey methods, leading in all cases to the appearance of a linear dependence of the reference frequency shift on the residual field frequency shift. Two versions of the most heating stable generalised Ramsey schemes, for which the proportionality coefficient in this dependence is minimal, are demonstrated.**

Keywords: *quantum frequency standard, laser cooling, Ramsey method, Paul trap.*

1. Introduction

The problem of the light shift of the reference transition frequency due to the action of the probe field is a key one for many types of existing and future optical frequency standards on ultracold atoms and ions. Here are some examples, including electric octupole (E3) transition in a single ytterbium ion [1], magnetically induced $^1S_0 \to {}^3P_0$ transitions in even isotopes of atoms of alkaline-earth metals and similar elements [2], optical transitions in multiply charged ions [3], two-photon E1–M1 transitions in Hg, Sr, Yb, and Mg atoms [4], etc.

To date, a number of generalised Ramsey methods (see original work [5–11] and review [12]) have been developed and investigated, allowing one to suppress frequency shifts of this type down to a negligible level ($\delta\omega/\omega < 10^{-18}$). Some of these methods have been implemented in experiments [1, 6, 9, 13], while some have not been yet. Theoretical models do not take into account some real factors, in particular, the heating of the ion in a radio-frequency trap due to electric field fluctuations. The allowance for this heating and the analysis of its impact on the efficiency of methods for the field shift suppression are important scientific problems which are solved in the present work within the framework of simple theoretical models of ion motion (one-dimensional harmonic potential) and heating process (harmonic oscillator in thermal equilibrium with the environment).

Based on the numerical solution of a system of kinetic equations for the elements of the ion density matrix, we have shown that ion heating reduces the efficiency of the previously proposed one-loop generalised Ramsey methods, leading in all cases to the appearance of a linear dependence of the reference frequency shift on the residual field frequency shift. Two most heating stable versions of the generalised Ramsey schemes, i.e. original [5] and hybrid generalised [8] hyper-Ramsey schemes, are revealed, for which the proportionality coefficient in this dependence is minimal.

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2. Generalised Ramsey schemes

The considered generalised Ramsey schemes for frequency shift suppression by the nonresonant action of a strong probe field are based on the resonant interaction of a two-level atom (ion) with a sequence of laser pulses separated by a dark Ramsey interval of duration T (see Fig. 1). Pulse amplitudes, durations, frequencies, and phases are selected to reach the desired effect of the reference frequency shift suppression by the nonresonant shift of working levels during the pulse action. In the cases studied in this work, the ion is in the ground electronic state at the initial time moment. The detectable value (signal) is the probability of finding the ion in the excited electronic state. This probability depends on all parameters of the problem. Pulse amplitudes are the same [$\Omega_1 = \Omega_3 = \Omega_4 = \Omega = \pi/(2\tau)$], and their durations satisfy the relation $\tau_1 = \tau_3/2 = \tau_4 = \tau$. Here Ω_i are the Rabi frequencies for laser pulses (i = 1, 3, 4), the areas of which are $\theta_1 = \pi/2$, $\theta_3 = \pi$ and $\theta_4 = \pi/2$. The frequencies ω_i are the same for all pulses. Consequently, the detunings δ_i of radiation frequencies from the frequency ω_0 of the unperturbed transition are also the same. The frequency ω_i is chosen so as to partially compensate for the nonresonant light shift Δ_{shift}: $\delta_1 = \delta_3 = \delta_4 = \omega - \omega_0 + \Delta_{\text{step}}$, where ω is the laser field frequency during the dark interval, and Δ_{step} is a controlled additive to the probe field frequency during the pulse action. The residual field shift Δ satisfies the condition $|\Delta| = |\Delta_{\text{shift}} - \Delta_{\text{step}}| < \Omega$.

For further presentation, it is convenient to consider in explicit form the dependence of excitation probability on laser pulse phases: $P(\varphi_1, \varphi_3, \varphi_4)$. In the case of the original hyper-Ramsey (HR) scheme, the error signal (discriminator) is formed as follows:

$$\Delta E_{\text{HR}} = P(\pi/2, \pi, 0) - P(-\pi/2, \pi, 0).$$

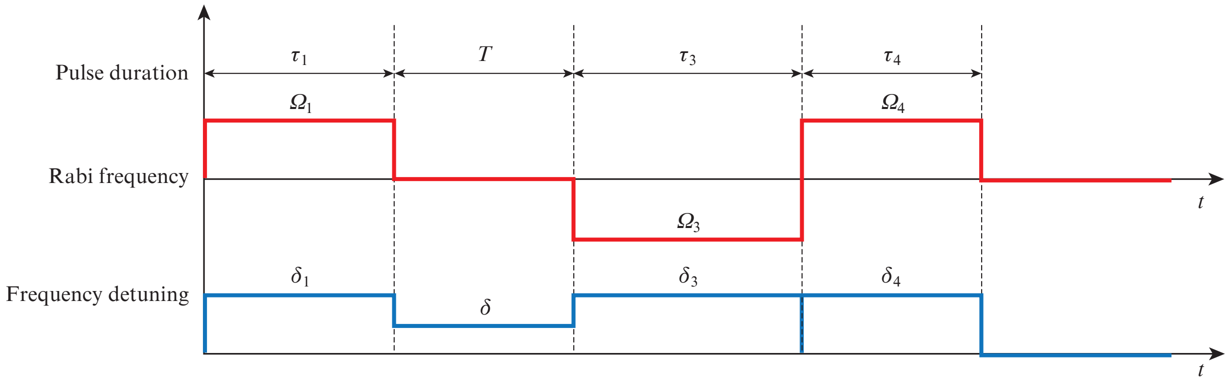

Figure 1. General Ramsey sequence of three laser pulses acting on a two-level atom (see the text).

The reference frequency, to which the probe laser radiation frequency is locked, zeros the error signal. Consequently, as was shown in our paper [5], within the framework of an idealised interaction model based on solving the dynamic Schrödinger equation for a stationary two-level atom in the external field of laser pulses, the reference frequency shift $\delta\omega$ relative to the unperturbed transition frequency, in contrast to the case of the standard Ramsey scheme, has a cubic dependence on the residual field shift: $\delta\omega = (C/T)(\Delta/\Omega)^3$ (C is a numerical factor of the order of unity). This makes it possible to suppress the frequency shift by three to four orders of magnitude to a relative level of less than 10^{-18}. The efficiency of the HR method for suppressing the reference resonance frequency shift by the probe field was confirmed experimentally [1], including the development and design of the optical frequency standard based on a single ytterbium ion, with unprecedented (for ion standards) metrological characteristics [14].

Later in work [6], a modified HR (MHR) scheme was proposed, differing from the original HR scheme by the method of error signal generation:

$$\Delta E_{\rm MHR} = P(\pi/2, \pi, 0) - P(0, \pi, -\pi/2).$$

In this case, as shown in [6] within the framework of same idealised interaction model, the reference frequency shift is zero for any residual field shift values. Several more variants of the so-called generalised HR (GHR) spectroscopy were proposed in [7, 8]. The error signal in these variants is formed by the phase jumps in the second pulse:

$$\Delta E_{\rm GHR}(\varphi) = P(0, \varphi, 0) - P(0, -\varphi, 0),$$

where the value of the phase jump φ may be either $\pi/4$ or $3\pi/4$. In some cases, certain advantages are provided by the formation of a hybrid error signal:

$$\Delta E_{\rm GHR}(\pi/4, 3\pi/4) = (1/2)[\Delta E_{\rm GHR}(\pi/4) - \Delta E_{\rm GHR}(3\pi/4)].$$

For GHR schemes, just as in the case of MHR schemes, the reference frequency shift is zero for any values of the residual field shift if we confine ourselves to the idealised interaction model based on the Schrödinger equation.

3. Trapped-ion heating and recoil effect in interrogating the clock transition

Deviations from an idealised model of the atom–field interaction can be physically stipulated by the presence of relaxation processes of various types in the system, including the dephasing of optical oscillations due to the finite width of radiation spectrum of a probe laser [15]. From this viewpoint, trapped-ion heating with allowance for its translational degrees of freedom and the recoil effect in absorption and emission of photons of the probe field leads to a specific relaxation in the atomic subsystem.

As is known [16], heating of a single ion occurs in the presence of noise electric fields at the point of ion location, which leads to the appearance of fluctuating forces acting on the ion. If the fluctuation spectrum overlaps the frequencies of vibrational motion of the ion in the trap, fluctuating forces can significantly increase the energy of vibrational motion. There are a number of possible sources of these noise fields: thermal Johnson noise caused by the resistance of the trap electrodes and external circuits; fluctuating patch-potentials (for example, due to randomly oriented domains on the surface of electrodes); external noise electric fields; fields generated by fluctuating currents; etc. There are quite extensive literature in which experimental data and theoretical developments in this field of research are systematised (see, for example, original work [17–20] and review [21]).

Consider a two-level atom (ion) interacting with a sequence of pulses, taking into account the vibrational degrees of freedom of the ion in a one-dimensional harmonic potential well. With allowance for the heating of the ion, its state becomes mixed, and we have to use an approach based on the ion density matrix ρ and the kinetic equation:

$$\frac{\partial\rho}{\partial t} = \frac{\rm i}{\hbar}[H_0, \rho] - \frac{\rm i}{\hbar}[V, \rho] + \left(\frac{\partial\rho}{\partial t}\right)_{\rm heating}, \qquad (1)$$

where

$$H_0 = -\hbar\delta|{\rm e}\rangle\langle{\rm e}| + \hbar\omega_{\rm v}(a^+a + 1/2),$$

$$V = \hbar\Omega|{\rm e}\rangle\langle{\rm g}|\exp({\rm i}kx) + {\rm h.c.}$$

are the Hamiltonian of the trapped ion and the ion–probe field interaction operator, written in the resonance approximation in a rotating basis; the expressions in square brackets are the commutators of the operators; $\delta = \omega - \omega_0$ is the detuning of the field frequency from the unperturbed transition frequency between the ground, $|{\rm g}\rangle$, and excited, $|{\rm e}\rangle$, electronic states; $\omega_{\rm v}$ is the oscillation frequency of the trapped ion; a^+ and a are the operators of creation and annihilation of a quantum of vibrational motion; x is the operator of the ion coordinate in the trap; and k is the wave number. The last term in the quantum kinetic equation (1) describes a change in the ion density matrix due to heating. In the simplest model of a harmonic oscillator interacting with environment under conditions of thermodynamic equilibrium, this contribution has a form (see, for example, [22])

$$\left(\frac{\partial\rho}{\partial t}\right)_{\text{heating}} = K(\bar{N}+1)\Big(a\rho a^{+} - \frac{1}{2}\{a^{+}a,\rho\}\Big) + K\bar{N}\Big(a^{+}\rho a - \frac{1}{2}\{aa^{+},\rho\}\Big),$$

where K is the phenomenological rate constant; the terms in curly brackets are the anti-commutators of the operators; and $\bar{N} = \{\exp[\hbar\omega_{\text{v}}/(k_{\text{B}}T)] - 1\}^{-1} = k_{\text{B}}T/(\hbar\omega_{\text{v}}) \gg 1$ is the average equilibrium number of excitation quanta. At an oscillation frequency of ~ 1 MHz and room temperature, we obtain $\bar{N} \approx 10^7$. The experimentally measured heating rate $v = K\bar{N}$ usually varies in the range of $1-10^3$ s^{-1} (see review [21] and references therein).

If the oscillation frequency of the trapped ion is much greater than the detuning and the Rabi frequency ($\omega_{\text{v}} \gg \delta$, Ω), then the so-called secular approximation is valid, within which the off-diagonal elements of the density matrix, related to vibrational quantum numbers n, can be neglected. For the elements being diagonal in n, the kinetic equation is reduced to an infinite chain of coupled equations:

$$\frac{\partial\rho_n^{\text{eg}}}{\partial t} = -\,\mathrm{i}\Omega(n)(\rho_n^{\text{gg}} - \rho_n^{\text{ee}}) + \left(\frac{\partial\rho_n^{\text{eg}}}{\partial t}\right)_{\text{heating}},$$

$$\frac{\partial\rho_n^{\text{ee}}}{\partial t} = -\,\mathrm{i}[\Omega(n)\rho_n^{\text{ge}} - \rho_n^{\text{eg}}\Omega^{*}(n)] + \left(\frac{\partial\rho_n^{\text{ee}}}{\partial t}\right)_{\text{heating}},$$

$$\frac{\partial\rho_n^{\text{gg}}}{\partial t} = -\,\mathrm{i}[\Omega^{*}(n)\rho_n^{\text{eg}} - \rho_n^{\text{ge}}\Omega(n)] + \left(\frac{\partial\rho_n^{\text{gg}}}{\partial t}\right)_{\text{heating}}, \qquad (2)$$

$$\left(\frac{\partial\rho_n^{(ij)}}{\partial t}\right)_{\text{heating}} = -v(2n+1)\rho_n^{(ij)} + v(n+1)\rho_{n+1}^{(ij)} + vn\rho_{n-1}^{(ij)},$$

$$i,j = \text{e, g}.$$

In these equations, the Rabi frequency for a transition between the states with a given vibrational quantum number $|\text{g},n\rangle \to |\text{e},n\rangle$ depends on n due to the recoil effect and the finite size of the localisation region of the wave functions of the harmonic oscillator's eigenstates:

$$\Omega(n) = \langle n|\Omega\exp(\mathrm{i}kx)|n\rangle = \Omega\exp(-\eta^2/2)\,L_n(\eta^2),$$

where the square of the Lamb–Dicke parameter η is determined by the ratio of the recoil frequency to the vibrational frequency: $\eta^2 = \hbar k^2/(2M\omega_{\text{v}}) = \omega_{\text{r}}/\omega_{\text{v}} \ll 1$ (M is the mass of the atom), and the Laguerre polynomials allow the expansion in powers of the small parameter: $L_n(\eta^2) \approx 1 - n\eta^2 + n(n-1)\eta^4/4 + \ldots$. Thus, the ion heating and recoil effect lead to a decrease in the effective Rabi frequency compared to the nominal one at $n = 0$. In addition, in the course of evolution, the dispersion of Rabi frequencies increases with populating of higher vibrational levels.

4. Numerical solution and discussion

In order to quantitatively characterise the impact of trapped-ion heating on the efficiency of various generalised Ramsey methods for the reference frequency shift suppression by the nonresonant action of the probe field, we numerically solve the system of dynamic equations (2) under assumption that, at the initial time moment, the ion is in the ground electronic state with the Boltzmann distribution over vibrational levels:

$$\rho|_{t=0} = \sum_n p_n|\text{g},n\rangle\langle\text{g},n|,$$

$$p_n = \frac{1}{1+n_0}\left(\frac{n_0}{1+n_0}\right)^n,$$

where

$$n_0 = \sum_n np_n \approx \frac{k_{\text{B}}T_0}{\hbar\omega_{\text{v}}}$$

is the average initial number of vibrational excitations; T_0 is the temperature of the laser-cooled ion (as a rule, this temperature is the Doppler cooling limit of the order of several millikelvins). In finding the numerical solution, an infinite chain of equations is cut off at a certain maximum number n_{max}. To determine this maximum number, we use an exact analytical result for the total population probability of vibrational levels:

$$p_n(t) = \frac{1}{1+n(t)}\left[\frac{n(t)}{1+n(t)}\right]^n,$$

$$n(t) = n_0 + vt, \qquad (3)$$

$$1 - \sum_{n=0}^{n_{\max}} p_n(t) \leqslant \varepsilon = 0.01.$$

Here, ε is the number limiting the calculation accuracy. The remaining parameters of the numerical calculation problem were chosen close to those used in experiments on the spectroscopy of octupole transition in a single ytterbium ion [1, 14]: $v = 3\Omega$, $\tau\Omega = \pi/2$, $T\Omega = 2\pi$, $n_0 = 20$, and $\eta = 0.1$. At the nominal Rabi frequency $\Omega = 10$ Hz, the interrogation cycle duration is 0.2 s, and the estimate by formulas (3) of the maximum vibrational quantum number to be taken into account in the calculations gives $n_{\max} = 270$.

The results of numerical calculations are presented in Fig. 2. It can be seen that the trapped-ion heating reduces the efficiency of all the generalised Ramsey methods considered in this work, leading to the appearance of a linear dependence of the reference frequency shift on the residual field shift. In addition, in the case of the MHR scheme, the graph of this dependence does not intersect the origin of the coordinates, i.e. a shift in the reference frequency even occurs at a zero residual shift, which makes this scheme unsuitable to supress the frequency shift to a relative level less than 10^{-18}. For other schemes, we obtain the following proportionality coefficients in the corresponding linear dependences (the slopes of the straight lines at the origin of the coordinate):

$$\left(\frac{\delta\omega}{\Delta}\right)_{\text{HR}} = -0.040, \quad \left(\frac{\delta\omega}{\Delta}\right)_{\text{GHR}(\pi/4)} = 0.135,$$

$$\left(\frac{\delta\omega}{\Delta}\right)_{\text{GHR}(3\pi/4)} = -0.140, \quad \left(\frac{\delta\omega}{\Delta}\right)_{\text{GHR}(\pi/4,3\pi/4)} = -0.003.$$

If we accept that the residual field shift is controlled at a level of 10 MHz (as in work [14]), then only the two most heating

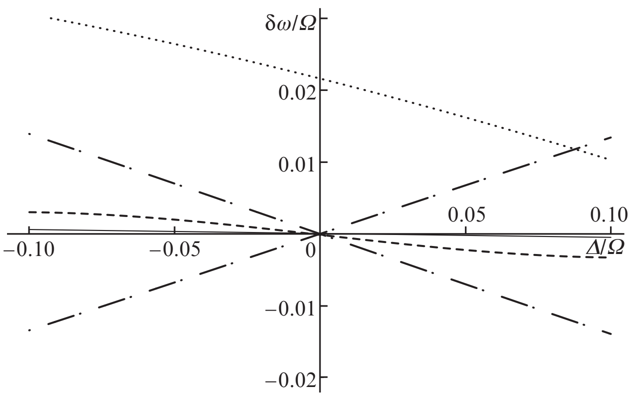

Figure 2. Reference frequency shift $\delta\omega$ vs. the residual field shift Δ for various generalised Ramsey schemes: (dashed line) HR, (dotted line) MHR, (dash-dotted lines) GHR($\pi/4$) and GHR($3\pi/4$), and (thin solid line) hybrid GHR($\pi/4, 3\pi/4$) schemes.

stable schemes would provide the suppression of the reference frequency shift down to a relative level less than 10^{-18}, in particular, 6×10^{-19} in the case of the original HR scheme and 5×10^{-20} in the case of the hybrid GHR scheme.

5. Conclusions

Heating of ions reduces the efficiency of the above-considered generalised Ramsey schemes for the field shift suppression by the ion–probe field interaction. In all cases, we observe a linear dependence of the clock frequency on the residual field shift near zero. In some cases [MHR, GHR ($\pi/4$) and GHR ($3\pi/4$) schemes], this may be an obstacle to attaining a relative clock uncertainty of less than 10^{-18}.

There are three interrelated factors that lead to a decrease in the efficiency of the methods we have investigated. The first factor is a decrease in the effective Rabi frequency in the course of the ion interrogation cycle, caused by the heating and recoil effect. The second factor is an increase in the dispersion of Rabi frequencies in accordance with the distribution of ions in vibrational levels. These two factors are dominant in the limit $\nu\tau \ll 1$, when heating during the pulse action can be neglected, and a change in the distribution in vibrational levels occurs during the dark interval. However, in experiments, as a rule, the inverse relation $\nu\tau > 1$ holds, and the dephasing of optical oscillations caused by ion heating during the pulse action is added to the first two factors. Two of all above-considered generalised Ramsey schemes, namely, the original HR scheme and the hybrid GHR ($\pi/4, 3\pi/4$) scheme, can be classified as the most insensitive to heating.

It should be noted the effect of heating on the two-loop autobalanced Ramsey schemes [9, 10] and the development of special schemes insensitive to heating require a separate study.

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