Mapping out atom-wall interaction with atomic clocks

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We explore a feasibility of measuring atom-wall interaction using atomic clocks based on atoms trapped in engineered optical lattices. Optical lattice is normal to the wall. By monitoring the wall-induced clock shift at individual wells of the lattice, one would measure a dependence of the atom-wall interaction on the atom-wall separation. We rigorously evaluate the relevant clock shifts and show that the proposed scheme may uniquely probe the long-range atom-wall interaction in all three qualitatively-distinct regimes of the interaction: van der Waals (image-charge interaction), Casimir-Polder (QED vacuum fluctuations) and Lifshitz (thermal bath fluctuations). The analysis is carried out for atoms Mg, Ca, Sr, Cd, Zn, and Hg, with a particular emphasis on Sr clock.

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Atomic clocks define the unit of time, the second. Usually the environmental effects (e.g., stray fields) degrade the performance of the clocks. One may turn this around and by measuring shifts of the clock frequency, characterize an interaction with the environment. The most fundamental experiments of this kind search for a potential variation of fundamental constants \cite{1}, where the “environmental agent” is the fabric of the Universe itself, affecting the rate of ticking of atomic clocks. In this paper, we evaluate a feasibility of using atomic clocks to measure basic laws of atom-wall interactions. We find that a certain class of atomic clocks, the optical lattice clocks, are capable of accurately characterizing the atom-wall interaction. Moreover, this is a unique system where the atom-wall interaction may be probed in all three qualitatively-distinct regimes of the interaction: van der Waals (image-charge interaction), Casimir-Polder (QED vacuum fluctuations) and Lifshitz (thermal bath fluctuations).

An advantage of working with optical lattices lies with a tight spatial confinement at the lattice sites. Commonly, the accuracy of determination of the atom-wall interaction is limited by the spatial extent of an atomic ensemble \cite{2}. In optical lattices, the size of ultracold atom wave-function can be reduced to a small fraction of the lattice laser wavelength. An idealized setup for measuring atom-wall interaction is shown in Fig. 1. The conducting surface of interest acts as a mirror for the laser beam normally incident on the surface. The resulting interference of the beams forms an optical lattice. Laser operates at a “magic” wavelength $\lambda_m$ specific to the atom (see Table I). For all tabulated magic wavelengths, atoms are attracted to maxima of the laser intensity and one could work with 1D optical lattices. The first pancake-shaped atomic cloud would form at $\lambda_m/\sqrt{2}$ distance from the mirror. The subsequent adjacent clouds are separated by a distance $\lambda_m/\sqrt{3}$. Ref. \cite{10} discusses an experimental procedure for loading atoms into sites close to a mirror.

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In optical lattice clocks, ultracold atoms are trapped in minima (or maxima) of intensity of a standing wave of a laser light (optical lattices) operated at a certain “magic” wavelength \cite{1,6}. The laser wavelength is tuned so that the differential light perturbations of the two clock levels vanishes exactly. Such ideas were experimentally realized \cite{2,8,9} for optical frequency clock transitions in divalent atoms, such as Sr, yielding fractional accuracies at a $10^{-16}$ level \cite{9}. The clock transition is between the ground $^1S_0$ and the lowest-energy excited $^3P_0$ state. $J = 0$ spherical symmetry of the clock states makes the clock insensitive to stray magnetic fields and environmentally-induced decoherences.

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FIG. 1: (Color online) Idealized setup for measuring atom-wall interaction with optical lattice clocks. Clouds of ultracold atoms are trapped in an optical lattice operating at a “magic” wavelength. By monitoring the wall-induced clock shift at individual trapping sites, one measures a dependence of the atom-wall interaction on the atom-wall separation.

Two earlier proposals, by Florence \cite{10} and Paris \cite{13} groups, considered trapping divalent atoms in optical lat-
TABLE I: Fractional shifts of the $^1S_0 - ^3P_0$ clock transitions in divalent atoms due to presence of an ideal conducting surface. The second column lists clock frequencies. Values of magic wavelengths, $\lambda_m$, in Sr and Yb are experimental [11, 12] and are our theoretical results for other atoms. The differences of the static polarizabilities $\alpha(0)$ and the van der Waals coefficients $C_3$ for the two clock levels are tabulated in the fourth and fifth columns. Finally, we list the fractional-shift parameters $\beta_{CP}$, $\beta_{vdW}$ and $\beta_L$, Eq. (5). Notation $a[b]$ stands for $a \times 10^b$.

| atom | $\nu_{clock}$, Hz | $\lambda_m$, nm | $\Delta\alpha(0)$, a.u. | $\Delta C_3$, a.u. | $\beta_{vdW}$ | $\beta_{CP}$ | $\beta_L$ |
|------|-------------------|-----------------|------------------------|-------------------|---------------|-----------|--------|
| Mg   | 6.55[14]          | 466             | 29                     | 0.21              | -3.1[-12]     | -7.9[-13]  | -1.0[-13] |
| Ca   | 4.54[14]          | 739             | 138                    | 0.17              | -8.8[-13]     | -8.6[-13]  | -1.8[-13] |
| Sr   | 4.29[14]          | 813             | 261                    | 0.25              | -1.1[-12]     | -1.2[-12]  | -2.6[-13] |
| Yb   | 5.18[14]          | 759             | 155                    | 0.35              | -1.5[-12]     | -7.6[-13]  | -1.6[-13] |
| Zn   | 9.69[14]          | 416             | 28                     | 0.30              | -4.2[-12]     | -8.2[-13]  | -9.4[-14] |
| Cd   | 9.03[14]          | 419             | 28                     | 0.31              | -4.6[-12]     | -8.7[-13]  | -1.0[-13] |
| Hg   | 1.13[15]          | 362             | 22                     | 0.30              | -5.5[-12]     | -9.8[-13]  | -9.8[-14] |
tices for studying atom-wall interaction. In both proposals the lattices are oriented vertically and ultracold atoms experience a combination of periodic optical potential and linear gravitational potential. In the Florence proposal [10], the atom-wall interaction modifies Bloch oscillation frequencies of atomic wavepackets in this potential. In the Paris proposal [13], laser pulses at different frequencies are used to create an interferometer with a coherent superposition of atomic wavepackets at different sites. Here we consider an alternative: by monitoring the clock shift at individual trapping sites, one measures a distance dependence of the atom-wall interaction.

Qualitative estimates — As the separation \( z \) between an atom and a wall increases, the atom-wall interaction evolves through several distinct regimes: (i) chemical-bond region that extends a few nm from the surface, (ii) van der Walls region, (iii) retardation (Casimir-Polder) region, and (iv) the thermal (Lifshitz) zone. The chemical-bond region is beyond the scope of our paper and we focus on the three longer-range regimes of the interaction between a perfectly conducting wall and a spherically-symmetric atom.

Qualitatively, the van der Waals interaction arises due to an interaction of atomic electrons and nucleus with their image charges

\[
U_{vdW} (z) = -C_3 z^{-3},
\]  

where the coefficient \( C_3 \) depends on an atomic state. It may be expressed in terms of the electric-dipole dynamic polarizability of the atom as

\[
C_3 = \frac{1}{4\pi} \int_0^\infty \alpha (i\omega) d\omega.
\]  

Eq. (1) assumes instantaneous exchange of virtual photons. More rigorous consideration in the framework of QED leads to the Casimir-Polder limit [11]

\[
U_{CP} (z) = -\frac{3}{(8\pi)} \hbar c \alpha (0) z^{-4}.
\]  

Notice the appearance of the speed of light \( c \) in this formula. A transition between the van der Walls and the retardation regions occurs at the length-scale \( \hbar c/\Delta E_\alpha \), where \( \Delta E_\alpha \) is a characteristic value of the atomic resonance excitation energy. Compared to the van der Waals interaction, the retardation potential has a steeper, \( z^{-4} \), dependence on the atom-wall separation.

The Casimir-Polder interaction, Eq. (3), is mediated by vacuum fluctuations of electromagnetic field. At finite temperatures \( T \), populations of the vacuum modes are modified and a new length-scale, \( \hbar c/(k_B T) \), appears. As shown by Lifshitz [13], the distance dependence of the interaction switches back to the inverse cubic dependence of the van der Waals interaction, Eq. (1),

\[
U_L (z) = -\frac{1}{4} k_B T \alpha (0) z^{-3}.
\]  

Due to the interaction with the wall, both clock levels would shift. We may parameterize the resulting fractional clock shifts as

\[
\frac{\delta \nu}{\nu_{\text{clock}}} (z, T) = \begin{cases} \beta_{vdW} \left(\frac{x_m}{z}\right)^3, \\ \beta_{CP} \left(\frac{x_z}{z}\right)^4, \\ \beta_L \left(\frac{x}{(400 A)}\right) \left(\frac{x_m}{z}\right)^3. \end{cases}
\]  

We evaluated coefficients \( \beta \) for the clock transitions in Mg, Ca, Sr, Yb, Zn, Cd, and Hg (see discussion of the method later on). The results are presented in Table I. The estimates of Table I immediately show that the atom-wall interaction is a large effect, corresponding to \( 10^{-10} \) fractional clock shifts at the first wall. This is roughly a million time larger than the demonstrated accuracy of the Sr clock [9].

Rigorous consideration — In general, as the atom-wall separation is varied, there is a smooth transition between the three interaction regimes. To properly describe the crossover regions, we employ an expression by Babb et al. [10], which may be represented as

\[
U (z, T) = -\frac{k_B T}{4z^3} \left[ \alpha (0) + \sum_{\ell=1}^\infty \alpha (i\omega) I \left( \xi_{2\ell} \frac{2z}{c} \frac{c}{2z} \omega_p \right) \right],
\]  

where the atomic dynamic polarizability is convoluted with \( I(\zeta, \chi) = (1 + \zeta^2 \chi^2) \Gamma (3, \zeta) + \zeta^4 \chi^4 \Gamma (0, \zeta) - 3\zeta^2 \chi \Gamma (2, \zeta) + 2\zeta^4 \chi^2 \Gamma (1, \zeta) - \zeta^6 \chi^2 \Gamma (-1, \zeta) \) at Matzubara frequencies

\[
\xi_l = \frac{2\pi}{\hbar k_B T} l, \quad l = 0, 1, 2, \ldots,
\]  

\( \Gamma (n, \zeta) \) being the incomplete gamma function. In addition to recovering various limiting cases, Eq. (6) also accounts for realistic properties of conducting wall (described by plasma frequency \( \omega_p \)).

Atomic properties enter the atom-wall interaction through the dynamic electric-dipole polarizability of imaginary frequency \( \alpha (i\omega) \). For the two clock levels the perturbation of the clock frequency may be expressed in terms of the difference \( \Delta \alpha (i\omega) = \alpha_{2p} (i\omega) - \alpha_{2g} (i\omega) \). We carried out calculations of \( \alpha (i\omega) \) and \( \alpha (i\omega) \) for Mg, Ca, Sr, Yb, Zn, Cd, and Hg atoms. We used the \( ab \) initio relativistic configuration interaction method coupled with many-body perturbation theory. The summation over intermediate states entering the polarizability was carried out using the Dalgarno-Lewis method. Details of the formalism may be found in Refs. [17, 18]. Detailed dynamic polarizabilities \( \alpha (i\omega) \) and \( C_3 \) coefficients for the ground states of alkaline-earth atoms may be found in Ref. [18].

Dynamic polarizabilities of Sr atom are shown in Fig. 2. Notice that the individual polarizabilities \( \alpha_{2p} (i\omega) \) and \( \alpha_{2g} (i\omega) \) slowly decrease as \( \omega \) increases. At large frequencies each polarizability approaches the same asymptotic limit \( \alpha (i\omega) \sim N_e/\omega^2 \), \( N_e \) being the number of
atomic electrons. As a result, compared to the individual
α(ω), the differential polarizability, Δα(ω), is strongly
peaked around ω = 0. Only the Matsubara frequencies
inside this peak are relevant in Eq. [6]. In this regard,
it is worth noting that when evaluating C3 coefficients
for individual levels with Eq. [2], it was found [19] that
neglecting core excitations while computing α(ω) could
substantially underestimate C3 for heavy atoms. Here
we deal with the differential shift and a simpler approach
of summing over few first valence excitations does pro-
vide the dominant part of the effect. Curiously, Δα(ω)
passes through zero at ω = 0.05 a.u. This is reminiscent of
the “magic” frequency for the perturbation of the clock
transition by laser field which is expressed in terms of
differential polarizability of real argument, Δα(ω).

![Graph](image)

**FIG. 2:** (Color online) Dynamic polarizabilities of imaginary
frequency α(ω) of the Sr clock levels, 5s5p3P1 (dotted line)
and 5s21S0 (dashed line) as a function of frequency. Differential
polarizability Δα(ω) = α3P1(ω) − α1S0(ω) is shown
with a solid line. All quantities are in atomic units.

With the computed Δα(ω), we evaluate the atom-
wall clock shifts, Eq. [4]. We use plasma frequency ωp =
9 eV (gold wall) and consider several temperatures T =
77 K, 300 K, and 600 K. Results for Sr lattice clock are
shown in Fig. 3. Individual points represent shifts in
individual wells of the optical lattice. First well is placed
at λm/4 and subsequent wells are separated by λm/2.
Roughly the first 20 wells produce a fractional clock shift
above the already demonstrated 10⁻¹⁶ accuracy limit [3].
We observe that over 20 wells the clock shift varies by
six orders of magnitude. As temperature of the surface
is increased, the clock shifts become more pronounced.

It is worth pointing out that Eq. [3] assumes that the
temperatures of the environment and the wall are the
same (otherwise see Refs. [20, 21]). Moreover, the clock
shifts in Fig. 3 do not include the conventional black-
body-radiation shifts ( ~ T³). The corresponding tem-
perature coefficients are tabulated in Ref. [22].

![Graph](image)

**FIG. 3:** (Color online) Fractional clock shifts for Sr as a func-
tion of separation from a gold surface at three temperatures,
T = 77 K (blue dots), T = 300 K (red squares), and T = 600 K
(brown diamonds). Individual points represent shifts in indi-
vidual trapping sites of the optical lattice. First well is placed
at λm/4 and subsequent points are separated by λm/2.

Indeed, in Fig. 4 we draw a ratio

$$\eta(z, T) = U(z, T)/U_{CP}(z).$$  \(7\)

Parameter η is equal to one in the region where the
Casimir-Polder approximation is valid. From Fig. 4 we
observe that the transition between the van der Waals
and the CP regimes occurs around well number four. The
position of the second transition region, from the CP to
the Lifshitz regimes depends on the temperature. For
T = 77 K, this crossover is delayed until well number 25
(not shown on the Fig. 4). T = 600 K represents an-
other extreme, as the van der Waals region immediately
transforms into the Lifshitz region. Atom-wall interac-
tion at room temperature, T = 300 K, represents an
intermediate case, where the Casimir-Polder approxima-
tion is valid over several wells, and all the three domains
decome distinguishable.

We shown that the lattice clocks can be used to
detect all three qualitative-distinct mechanisms of the
atom-wall interaction. In this regard, the lattice
clocks offer a unique opportunity to map out both van
der Walls—Casimir-Polder and Casimir—Polder-Lifshitz
transition regions. This distinguishes the clocks from pre-
vious experiments: the former transition was probed in
Ref. [24], while the latter was detected in Ref. [21]. None
of the experiments so far has been able to map out both
transitions simultaneously.

The accuracy of determination of the atom-wall inter-
action is affected by how well the position of the clouds
with respect to the surface is determined. At each well
of the optical lattice, the atomic center-of-mass wave-
function is spread over some distance Δz. Then the
clock shift acquires a width, leading to an uncertainty
δU(z, T)/U(z, T) ≈ 3δz/2 ≈ 6/N_w η_{LTD} (λ_{clock}/λ_m),
where $\eta_{LD} = \lambda^{-1} \left( \frac{h}{2M \omega_{ho}} \right)^{1/2}$ is the Lamb-Dicke parameter for an atom of mass $M$ and $\omega_{ho}$ is the harmonic oscillator frequency of the trapping potential along the $z$-axis. $N_w$ is the site number counting from the surface. For a typical value of $\eta_{LD} \approx 0.1$, the error in determination of the atom-wall interaction would be in the order of a few per cent.

The accuracy can be potentially improved by increasing the intensity of the lattice laser, $I_L$, as the size of atomic cloud $\Delta z \propto 1/I_L^{1/4}$. At the same time, the factors limiting the maximum of intensity relate to the performance of the clock itself. The major factors here are hyperpolarizability (fourth order AC Stark shift) and photon scattering rate, which scale as $I_L^2$ and $I_L$, respectively. Depending on a specific trapping site, the intensity of the lattice laser could be optimized to attain a better accuracy. Finally, we notice that the present scheme could be extended to recently proposed micro-Magic lattice clocks [24], operating in a more convenient microwave domain.

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FIG. 4: (Color online) Sr clock shift of Fig. 3 normalized to the Casimir-Polder limit, Eq. (7) at $T = 77\,K$ (blue dots), $T = 300\,K$ (red squares), and $T = 600\,K$ (brown diamonds).

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