Distortion of the Mercury $^1S_0$-$^3P_0$ Clock Line in Two-species Atomic Clock

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I. Introduction

Determining the accuracy of an atomic clock is non-trivial. There are many effects that perturb the clock line transition, the impact of which is difficult to estimate. The use of a two-species atomic clock opens the possibility for a better determination of the clock line frequency due to the ability to use the second atomic species as a tool to determine the magnitude of the perturbation effect. On the other hand, the very nature of the composite system itself provides new systematic effects whose impact must be estimated. Therefore, before implementing a two-species atomic clock, it is desirable to perform diagnostics to determine if this is feasible.

Our work focuses on theoretical calculations for the Hg-Rb mixture. Here we show how the frequency and shape of the mercury clock line $^1S_0$-$^3P_0$ are distorted if overlapped with rubidium atoms. When rubidium atoms (S=1/2) interact with mercury in the excited states (S=1), the resulting potential energy curve can be either S=3/2 or 1/2. In the latter case, the symmetry is the same as for the HgRb molecular ground-state. Since the interaction potential that correlates with the $^3P_0$ state of Hg contains admixture of the S=1/2 state, transitions to the molecular states of Hg($^3P_0$)—Rb are no longer forbidden. This might affect the line shape of the mercury clock line.

II. Methods/Results

The model Lennard-Jones potentials for the ground [1] and excited states [2] allowed for determining the scattering wavefunctions for ^{202}Hg-^{87}Rb (Fig. 1). The wavefunctions were calculated using the DVR algorithm [3]. To study the possible effects related to the collisions of Hg and Rb, the depth of the potential of the excited state was scanned. The magnitude of the scan range was defined by scattering length covering at least one entire bin (Fig. 2).

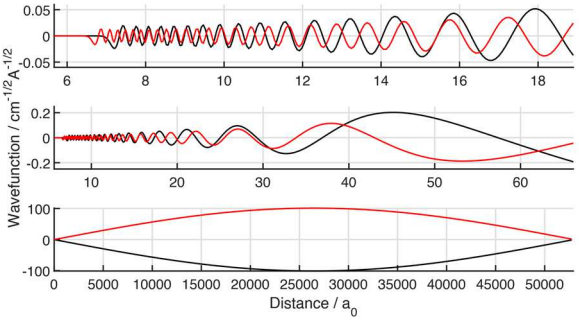

Fig. 1. Calculated lowest scattering wavefunctions describing rubidium collisions with mercury in ground (black line) and excited (red line) states. Three graphs show the wavefunctions in different interaction ranges.

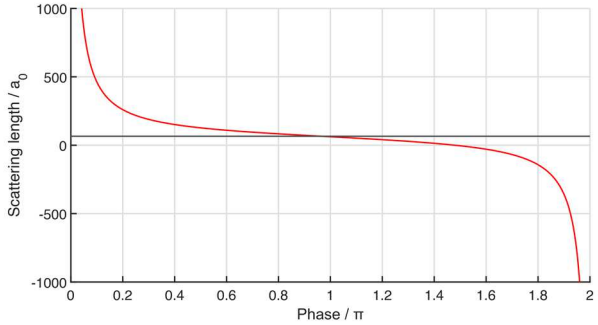

Fig. 2. Dependence of the scattering length calculated for the lowest scattering excited state in the 5 nK limit (red line) on the phase. The phase changes while scanning the depth of the RbHg* potential through the entire bin. The black solid line indicates the mean scattering length $\bar{a} = 65.7\ a_0$.

The wave functions were necessary to get the S-matrices, which determine the pressure broadening cross-sections [4]. We calculated the clock line-shape parameters, the pressure broadening Γ (Fig. 3) and shift Δ (Fig. 4)

$$\Gamma = n_b \mathrm{Re}(v\sigma(j_i, j_f)),$$

$$\Delta = -n_b \mathrm{Im}(v\sigma(j_i, j_f)),$$

$$\sigma(j_i, j_f) = \frac{\pi}{k_j^2}\left((2J_i+1)(2J_f+1)(-1)^{l+l'}\left(\delta_{j_i,j_f} - S_{J_i}S_{J_f}^*\right)\right).$$

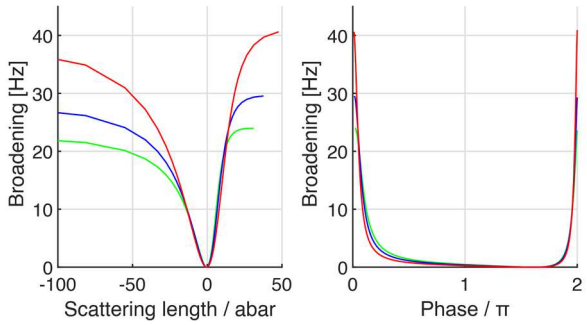

Fig. 3. Dependence of the estimated clock-line broadening for non-averaged collision energy of 1 μK (red line), 2 μK (blue line), and 3 μK (green line) on the scattering length of RbHg* (left panel) and the phase (right panel). The values are obtained for the atomic density of $n_b = 10^{11}\ cm^{-3}$.

The j_i and j_f denote the initial and final states, respectively, n_b is the number density of the perturber, v is the relative emitter-perturber speed, k is the wave vector of the lowest scattering wavefunction. The calculations were performed in the low-temperature limit, where only the lowest partial wave $l = 0$ is taken into account.

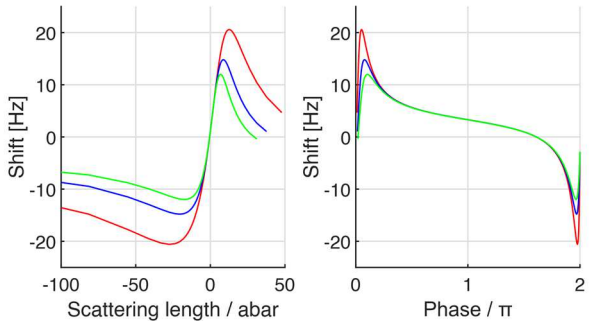

Fig. 4. Dependence of the estimated clock-line shift for non-averaged collision energy of 1 μK (red line), 2 μK (blue line), and 3 μK (green line) on the scattering length of RbHg* (left panel) and the phase (right panel). The values are obtained for the atomic density $n_b = 10^{11}\ cm^{-3}$.

III. CONCLUSIONS

Our *ab initio* calculations allowed us to determine how the spectral line parameters, both its shift and shape, are perturbed by collision with another atomic species. This approach was general, yet it eventually allowed us to apply this to a Hg-Rb mixture, where we investigated how the $^1S_0$-$^3P_0$ mercury clock line is perturbed upon collisions with the rubidium atoms. These results are crucial for diagnosing whether it is possible to construct a two-species Rb-Hg atomic clock.

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REFERENCES

[1] M. Borkowski et al., Phys. Rev. A 96, 063411 (2017).

[2] P. S. Żuchowski et al., Phys. Rev. A 90, 012507 (2014).

[3] E. Tiesinga, C. J. Williams, and P. S. Julienne, Phys. Rev. A 57, 4257–4267 (1998).

[4] T. Orlikowski, Eur. Phys. J. D 28, 187 (2004).