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Probing Non-Newtonian gravity by photoassociation spectroscopy

M Borkowski¹, A A Buchachenko², R Ciuryło¹, P S Julienne³, H Yamada¹, K Yuu¹, K Takahashi⁴, Y Takasu⁴, and Y Takahashi⁴,⁵

¹ Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Grudziadzka 5, 87-100 Torun, Poland
² Skolkovo Institute of Science and Technology, 100 Novaya Street, Skolkovo, Moscow Region, 143025, Russia and Institute of Problems of Chemical Physics RAS, Chernogolovka, Moscow Region 142432, Russia
³ Joint Quantum Institute, National Institute of Standards and Technology and the University of Maryland, 100 Bureau Drive, Stop 8423, Gaithersburg, Maryland 20899-8423, USA
⁴ Department of Physics, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan
⁵ CREST, Japan Science and Technology Agency, Chiyoda-ku, Tokyo 102-0075, Japan

E-mail: mateusz@fizyka.umk.pl

Abstract. State of the art photoassociative measurements of bound state energies in the ground state Yb₂ molecule are used to establish limits on non-Newtonian gravity at Yukawa ranges of nanometers.

1. Introduction

Several cosmological theories [1–3] predict deviations from the usual 1/R behavior of the gravitational interaction. Those supposed corrections to the gravitational interaction between masses \( m_1 \) and \( m_2 \) at a distance \( R \) are usually expressed in terms of a Yukawa-type potential \( V_{\text{corr}}(R) \):

\[
V_{\text{Newton}}(R) + V_{\text{corr}} = -G \frac{m_1 m_2}{R} \left( 1 + \alpha \exp(-R/\lambda) \right).
\]  (1)

Since so far no experimental evidence of such deviations has been found, experimental efforts have concentrated on giving limits on the magnitude \( \alpha \) of this ‘correction’ as a function of the Yukawa range \( \lambda \). In this work we place similar limits in the range of \( \lambda = 0.1 \text{ nm} \) to \( \lambda = 1000 \text{ nm} \) by measuring bound state energies of Yb₂ and modelling the interactions between Yb atoms using mass-independent Born-Oppenheimer potentials. This way we can place limits on the mass-dependent part of the interaction and, by proxy, an upper bound on non-Newtonian gravity.

2. Measurements

Several bound state energies of the ground state Yb₂ have been measured using two-color photoassociation spectroscopy [4–6] in the Raman configuration, with \( ^1S_0 \rightarrow ^3P_1 \rightarrow ^0\Sigma_u^+ \) intermediate states. To avoid thermal broadening [7], the measurements were performed in Bose-Einstein condensates of ytterbium atoms. Techniques for forming such samples have already been
described elsewhere [8–10]. The photoassociation lines had a Lorentzian FWHM of about 1 kHz, as seen in Figure 1(a). The following systematic shifts were taken into account: shift due to the photoassociation lasers, the trapping laser and the density of atoms. The systematic shifts were eliminated by linear extrapolation, as seen in figs. 1(b)-(d). A total of 13 bound rovibrational state energies with rotational quantum numbers \( J = 0 \) or 2 has been measured with error bars \( \approx 500 \text{ Hz} \): two for \(^{168}\text{Yb} \), six for \(^{170}\text{Yb} \) and five for \(^{174}\text{Yb} \) and will be published elsewhere [11].

3. Interactions
Thanks to the single spinless \(^1\text{S}_0 \) ground state of the Yb atom, the interactions in the ytterbium dimer are described by a single Born-Oppenheimer potential. We have developed four such potential curves. The short range part of the potential could either be a Lennard-Jones type model potential [5], or an \textit{ab initio} based curve [14]. Our short range curves are shown in the upper panel of Figure 2. The long range part could be the standard \( R^{-6} \) van der Waals interaction or one that accounted for the Casimir-Polder effect, as tabulated for Yb\(_2\) in [15].

The potentials were fitted to experimental data using the least-squares method which minimized the difference between experimentally obtained bound state energies and theoretical energies calculated through solving the usual radial Schrödinger equation. Details of the procedure of finding a mass scaled model can be found elsewhere [5, 12, 13]. We find that we are able to reproduce the bound state energies to within a few tens of kHz on average (at \( \chi^2 = 307242 \) for the best model – \textit{ab initio} short range with a van der Waals long range). While the fact that the \textit{ab initio} short range gives better results than a simple model potential is hardly surprising, it is interesting to note that the Casimir-Polder long range always yielded worse fit evidenced by a larger \( \chi^2 \).

4. Limits
The final stage of the data analysis was to augment the interaction potentials with the gravitational interaction as shown in the lower panel of Figure 2. The potentials were fitted repeatedly as \( \alpha \) was ramped to make it possible for other potential parameters to compensate for the obvious shift in the quantum defect caused by the added interaction. This is important, because we are interested in the change in the mass scaling behavior rather than a simple shift.

**Figure 1.** Compensation of systematic errors present in the experiment as shown for the \(^{170}\text{Yb} \) \( \nu = 2, J = 2 \) line position. (a) an example photoassociation spectrum fitted with a Lorentzian lineshape of an FWHM of about 1 kHz, (b) shift due to both photoassociation lasers (molecular optical shift), (c) optical shift due to the far-off-resonant trap (FORT), and (d) the density shift due to the presence of other atoms in the BEC sample.
Figure 2. Upper panel: a comparison between the Lennard-Jones (black line) and ab initio (red) short range potentials. Despite the different shapes and depths both potentials support the same number of bound states, have similar long range \( C_6 \) coefficients and can be used as a basis for a mass-scaled potential model [12, 13]. Lower panel: the impact of the Yukawa potential on the shape of the interaction potential, with the Lennard-Jones potential as an example. For a short \( \lambda = 0.1 \text{ nm} \) only the short range part is affected, but for larger \( \lambda \), the long range part is also changed. For even larger \( \lambda \) no further change at internuclear distances is seen.

Otherwise \( \alpha_{\text{max}} \) would be underestimated, because uncompensated shift from the additional interaction would cause \( \chi^2 \) to grow too quickly. As shown in Figure 3 the behavior was for \( \chi^2 \) to experience a minimum first, and then quickly grow to infinity. This counter-intuitive phenomenon can be explained by the fact that our models take no account of any (real) mass-dependent effects in the molecule, like the beyond-Born-Oppenheimer effects [16] and the \( R \)-dependent isotopic shift [17]. For small \( \alpha \) the non-Newtonian interaction may artificially improve the mass scaling of theoretical bound state energies and therefore decrease \( \chi^2 \). With this in mind, in order to avoid accidental underestimation of the limits on non-Newtonian gravity we pick the

Figure 3. Evolution of the quality of the fit \( \chi^2 \) as the Yukawa coupling \( \alpha \) is ramped. At first the fit is ‘improved’, due to the compensation of mass-dependent effects not included in the theoretical models, but after a certain point \( \chi^2 \) quickly rises to infinity. We choose the limit \( \alpha_{\text{max}} \) so that \( \chi^2(\alpha_{\text{max}}) = \chi^2(\alpha = 0) \), as at this point the non-Newtonian contribution clearly starts to make the fit worse.
Figure 4. Limits on non-Newtonian Yukawa interaction derived from our interaction models (black and red lines depending on the short range, and dashed or solid for the long range part). The ab initio + van der Waals combination provides the most stringent limits. Limits obtained using other methods – neutron scattering (Kamiya et al. [18]), Casimir forces between plates (Klimchitskaya et al. [20]) and classical spectroscopy of HD+ (Salumbides et al. [21]).

point $\alpha_{\text{max}}$ where $\chi^2(\alpha_{\text{max}})$ becomes larger than $\chi^2(\alpha = 0)$, that is, where the theoretical description of the atomic interactions clearly becomes worse.

Figure 4 shows limits on non-Newtonian gravity derived from the four models. The general behavior of $\alpha_{\text{max}}$ is to decrease up to about $\lambda = 2$ nm, where the limits become constant. This is easily understandable, as the non-Newtonian part becomes $V_{\text{corr}} = -\alpha G m_1 m_2 / R$ as $\lambda$ becomes much larger than the internuclear distances $R$ in the molecule. The differences between models are slight. For small $\lambda$ the different long range parts have no impact on the limits while for larger $\lambda$ both the short range and long range parts of the potential matter, as expected.

Our limits can be compared to examples of recent works that derive similar limits using other experimental methods. This is shown as green lines in Figure 4. Both limits from neutron scattering by Kamiya et al. [18] and measurements of Casimir forces between plates by Klimchitskaya et al. are currently more stringent than ours in their respective ranges of $\lambda$. On the other hand, our work is on par with the results of classical molecular spectroscopy of HD+ by Salumbides et al. It is worth noting, that the probable weakest link in our approach is the quality of the interaction potentials: while the experimental error bars are on the order of 500 Hz, the theory matches experiment to about 50 kHz at best. On the other hand all four models are pure Born-Oppenheimer potentials, with no account taken for known mass-dependent effects, namely the $R$-dependent isotopic shift [17] and higher orders of the Born-Oppenheimer approximation [16]. Calculation of these effects for heavy systems like Yb is prohibitively difficult and was only recently undertaken [19]. The inclusion of these effects may pay off handsomely, as the limits are rapidly becoming more stringent with decreasing model $\chi^2$. For instance, at $\lambda = 10$ nm, the Lennard-Jones + van der Waals model yields $\log \alpha_{\text{max}} = 23.2$, as opposed to $\log \alpha_{\text{max}} = 22.7$ for the ab initio + van der Waals model. The $\chi^2$ of the former is twice as large as the latter. By extrapolation: if $\chi^2$ could be reduced by a factor of about 100 (which would require the models to be ten times more accurate than now), $\log \alpha_{\text{max}}$ could be reduced by about 3, putting photoassociation on par with the best current methods.

5. Conclusion
We have used state of the art photoassociation spectroscopy in a Bose-Einstein condensate of ytterbium atoms to measure the binding energies of several isotopomers of the Yb$_2$ molecule to an accuracy of $\approx 500$ Hz. Four interaction models were fitted to the experimental data in an
attempt to reproduce them theoretically. Both ab initio and model short range potentials were implemented, either with a standard van der Waals or the quantum-electrodynamic Casimir-Polder long range interaction. The impact of non-Newtonian gravitylike interactions on the mass scaling behavior of bound state energies was assessed to obtain the limits on the Yukawa coupling constant $\alpha$ at distances $\lambda \sim 1$ nm. Our best limits are only three orders of magnitude worse than the current best from long standing experimental approaches: neutron scattering and measurements of Casimir-Polder interactions. The presented methodology shows great promise for future research as small improvements in the theoretical description of the atomic interactions result in the rapid tightening of the limits on non-Newtonian gravity.

Acknowledgments

We acknowledge K. Enomoto, M. Ando, J. Hutson, and E. Tiemann for their useful comments. This work has been partially supported by the Grant-in-Aid for Scientific Research of JSPS (25220711, 26247064) and Impulsing Paradigm Changing Through Disruptive Technologies (ImPACT) program. It has also been partially supported by the TEAM Programme of the Foundation for Polish Science, co-financed by the EU European Regional Development Fund and by the COST Action CM1405 MOLIM and also partially supported by the National Science Centre grant no. UMO-2014/13/N/ST2/02591. It is part of an ongoing research program of the National Laboratory FAMO in Toruń, Poland. Calculations took place in Wroclaw Centre for Networking and Supercomputing grant no. 353.

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