Scattering lengths of calcium and barium isotopes

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We have calculated the \( s \)-wave scattering length of all the even isotopes of calcium (Ca) and barium (Ba) in order to investigate the prospect of Bose-Einstein condensation (BEC). For Ca we have used an accurate molecular potential based on detailed spectroscopic data. Our calculations show that Ca does not provide other isotopes alternative to the recently Bose condensed \( ^{40}\text{Ca} \) that suffers strong losses because of a very large scattering length. For Ba we show by using a model potential that the even isotopes cover a broad range of scattering lengths, opening the possibility of BEC for at least one of the isotopes.

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I. INTRODUCTION

Knowledge of the \( s \)-wave scattering length plays a crucial role in the achievement of Bose-Einstein condensation (BEC) in ultracold atomic gases [1]. A positive sign of the scattering length indicates that a Bose-Einstein condensate is stable, whereas a negative sign indicates an unstable or collapsing condensate. Also, its magnitude is crucial in the formation of BEC, as it determines the elastic and inelastic collision rates. For efficient evaporative cooling, a large scattering length is required; however, for a too-large scattering length, three-body recombination loss limits the formation and collisional stability of a BEC. This gives rise to a range of about 50–440 \( a_0 \) [6], limiting the size and stability of BEC.

In general, isotopes of an element have different scattering lengths. Therefore, the ability of BEC formation depends crucially on the chosen isotope. For instance, the scattering length of \( ^{84}\text{Sr} \) is 123 \( a_0 \) [15], which made it an ideal candidate to achieve BEC despite its low abundance of only 0.6% [16], as compared to the more abundant \( ^{86}\text{Sr} \) (10%, 800 \( a_0 \) [15]) and \( ^{88}\text{Sr} \) (83%, –2 \( a_0 \) [15]), either suffering strong losses [9] or requiring sympathetic cooling with another isotope [10], respectively. The \( ^{86}\text{Sr} \) isotope has a large scattering length of about 440 \( a_0 \) [6], limiting the size and stability of BEC.

Motivated by the success of BEC in Sr and Yb even isotopes and \( ^{40}\text{Ca} \), we carried out calculations to obtain the scattering lengths for all the even (bosonic) isotopes of Ca and Ba, for which mass and abundance are summarized in Table I. Laser cooling and trapping of all stable Ca isotopes have been reported [17,18]. The demonstration of magneto-optical trapping of Ba [19] has opened its use for ultracold collision studies, photoassociation spectroscopy, and Bose-Einstein condensation. Recently, an optical clock based on ultracold Ba has been proposed [20].

II. THEORY

The scattering properties of ground-state atoms are obtained from the underlying two-body ground-state potentials. For alkaline-earth-metal atoms, there is only one molecular ground-state potential, namely the singlet \( ^1\Sigma_\parallel^+ \) potential. Furthermore, the lack of nuclear spin and, therefore, hyperfine structure for the even (bosonic) isotopes highly reduces the number of collision channels compared with the alkali metal systems.

To calculate the \( s \)-wave scattering length, we solve the 1D radial Schrödinger equation with zero angular momentum and vanishing kinetic energy.

\[
\psi''(R) + \frac{2\mu}{\hbar^2} \left[ E - V(R) \right] \psi(R) = 0, \tag{1}
\]

where \( \mu \) is the reduced mass, \( R \) the internuclear distance, \( V(R) \) the Born-Oppenheimer potential (here the \( ^1\Sigma_\parallel^+ \) potential), and \( E \) the kinetic energy (below \( \mu K \)). The asymptotic form of the wavefunction is \( \psi(R) \propto \sin[k(R - a)] \), where \( k = \sqrt{2\mu E/\hbar^2} \), and \( a \) is the scattering length. We fit the asymptotic form to the solution of Eq. (1) for large \( R \) in order to obtain \( a \). Within the Born-Oppenheimer approximation, the potentials are identical for all the isotopes of a particular atomic system. Therefore, for a given potential \( V(R) \), one only needs to adjust \( \mu \) to obtain \( a \) for all the isotopes.

To obtain reliable scattering lengths, accurate potentials are needed. With the exception of systems with only a few electrons, like metastable helium [22], ab initio potentials are in general not accurate enough and constraints from experimental data are required. For \( ^{40}\text{Ca} \), an analytic representation of the \( ^1\Sigma_\parallel^+ \) potential based on an extensive set of experimental data from the Tiemann group is available [23]. For \( ^{138}\text{Ba} \), alternative to the recently Bose condensed \( ^{40}\text{Ca} \) that suffers strong losses because of a very large scattering length.
TABLE I. Mass and abundance of all stable even isotopes of Ca and Ba [21].

<table>
<thead>
<tr>
<th>Isotope</th>
<th>40</th>
<th>42</th>
<th>44</th>
<th>46</th>
<th>48</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass (amu)</td>
<td>39.963</td>
<td>41.959</td>
<td>43.955</td>
<td>45.954</td>
<td>47.953</td>
</tr>
<tr>
<td>Abundance (%)</td>
<td>96.941</td>
<td>0.647</td>
<td>2.086</td>
<td>0.004</td>
<td>0.187</td>
</tr>
</tbody>
</table>

such an accurate potential is not available. Here we rely on the analytical representation according to the Tang-Toennies potential model [24], which has been shown to be able to reproduce accurately the $X^1\Sigma^+_g$ potentials of Ca$_2$ [25] and Sr$_2$ [24]. The used Ca$_2$ and Ba$_2$ potentials are shown in Fig. 1.

III. RESULTS

A. Calcium

Information on the Ca$_2$ $X^1\Sigma^+_g$ potential has been gathered by several spectroscopic methods, including photoassociation spectroscopy [26–28], Fourier-transform spectroscopy [29], and filtered laser excitation technique [23]. Based on these detailed spectroscopic data, an interval of the scattering length for $^{40}$Ca is determined to be 340–700 $a_0$ [28]. In the $^{40}$Ca BEC experiment, a scattering length of $a \approx 440 a_0$ was estimated from a measurement of the chemical potential [6], without quoting an uncertainty. Therefore, we take the scattering length range of 340–700 $a_0$ as the starting point of our calculations.

We have taken the analytical representation and parameter values of the Ca$_2$ $X^1\Sigma^+_g$ potential from Ref. [23] (see Fig. 1). We allow the $C_6$ long-range coefficient to vary within a factor 0.991 to 1.003 from its reported value [23], in order to reproduce the scattering length interval for $^{40}$Ca. We then take the mass as a variable parameter and calculate the scattering length for the full mass interval spanned by the stable even isotopes. In this way we transfer the knowledge on $^{40}$Ca to the other isotopes.

The results for Ca are shown in Fig. 2. The plotted mass is twice the reduced mass, which for homonuclear collisions simply is the atomic mass. The dashed vertical lines indicate the masses of the even isotopes, from which the scattering lengths for homonuclear collisions are directly read off. Two calculations are shown, obtained from potentials with $C_6$ coefficients that give rise to 340 $a_0$ (red closed circles) and 700 $a_0$ (blue closed squares) for $^{40}$Ca. The scattering length shows the expected behavior as a function of mass, with a regular pattern of scattering resonances. They can be understood from the mass dependence of the vibrational splitting and, therefore, the number of bound states. A scattering resonance appears at those mass values at which a new vibrational state becomes bound, i.e., where the least bound vibrational state has zero binding energy. We find that accidentally all even isotopes are located close to such a scattering resonance, giving rise to large positive or negative scattering lengths.

The scattering length intervals for the different isotopes are given in Table II. It is clear that Ca does not provide an isolate with a favorable scattering length. At most one can state that $^{42}$Ca has a slightly smaller scattering length than $^{40}$Ca. In addition, the interisotope scattering lengths are given for collisions between $^{40}$Ca and the other isotopes.

TABLE II. Scattering lengths of even Ca isotopes (left), as well as interisotopic scattering lengths for all combinations with $^{40}$Ca and $^{42}$Ca+$^{40}$Ca (right).

<table>
<thead>
<tr>
<th>$a$ (units of $a_0$)</th>
<th>$a$ (units of $a_0$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>40 + 40</td>
<td>+340±700 [28]</td>
</tr>
<tr>
<td>42 + 42</td>
<td>+320±640</td>
</tr>
<tr>
<td>44 + 44</td>
<td>+460±1800</td>
</tr>
<tr>
<td>46 + 46</td>
<td>±∞</td>
</tr>
<tr>
<td>48 + 48</td>
<td>−230±120</td>
</tr>
</tbody>
</table>
and $^{42}\text{Ca} + ^{44}\text{Ca}$. Here we find favorable scattering lengths for $^{40}\text{Ca} + ^{42}\text{Ca}$, $^{40}\text{Ca} + ^{46}\text{Ca}$, and $^{42}\text{Ca} + ^{44}\text{Ca}$. Taking into consideration the large scattering length of $^{44}\text{Ca}$ and $^{46}\text{Ca}$, the only interesting mixture in view of sympathetic cooling is $^{40}\text{Ca} + ^{42}\text{Ca}$.

**B. Barium**

Knowledge of the $\text{Ba}_2$ $X^1\Sigma^+_g$ potential is sparse because of a limited amount of experimental data [30,31], which cover only a small part of the vibrational spectrum. Similarly, theoretical data is scarce. The binding energies of $\text{Ba}_2$ were calculated by Jones [32]. First wave function based quantum chemical calculation was reported by Ref. [33] and most recently by Ref. [34]. The most accurate calculations of the long-range coefficients $C_6$, $C_8$, and $C_{10}$ are reported by Porsev and Derevianko [35,36].

We have used the Tang-Toennies potential [37] of Ref. [24] to model the $\text{Ba}_2$ $X^1\Sigma^+_g$ potential as

$$V(R) = A e^{-bR} - \sum_{n=3}^{5} \left[ 1 - e^{-bR} \sum_{k=0}^{2n} \frac{(bR)^k}{k!} \right] \frac{C_{2n}}{R^{2n}},$$

where the short-range parameters (in a.u.) $A = 105.4$ and $b = 0.9657$ are obtained from rescaling an accurate $\text{Sr}_2$ $X^1\Sigma^+_g$ potential [38], using the measured fundamental vibration frequency [31], and taking the long-range coefficients from Refs. [35,36] (see Fig. 3).

Although we do not expect the potential to be accurate enough to predict the scattering length, we can use it to investigate its mass dependence. The result is shown in Fig. 3 (black closed circles). We observe that the spacing between the resonances is larger than that between the even isotopes, giving rise to a variety of scattering lengths among the different isotopes. Therefore, it is very probable that at least one of the isotopes has a favorable scattering length for BEC formation.

In addition, we have investigated the effect of the theoretical uncertainty in the reported $C_6$ coefficient, $5160 \pm 74$ a.u. [35,36]. We have repeated the above calculation with the upper (red closed squares) and lower (blue closed triangles) limits (see Fig. 3). Note that these adjustments in $C_6$ also require small changes in $A$ and $b$ [24]. The uncertainty in $C_6$ gives rise to a large spread in the scattering length, which can also be seen as a large shift along the mass axis, as indicated by the arrow. This means that even if an accurate short-range potential would be available, still no precise prediction of the scattering length is possible. On the other hand, whereas the scattering length itself is extremely sensitive to details of the potential, the spacing between the scattering resonances is not. Therefore, once scattering length information of one of the isotopes becomes available, the simple Tang-Toennies potential is sufficient to predict the scattering lengths of all the other isotopes,$^1$ at least at an accuracy that allows one to choose the best isotope to achieve BEC.

**IV. CONCLUSION AND OUTLOOK**

In summary, we have investigated the s-wave scattering lengths of the Ca and Ba even (bosonic) isotopes. An experimentally accurate ground-state potential of $\text{Ca}_2$ enabled us to calculate the scattering lengths for all the isotopes, taking knowledge of $^{40}\text{Ca}$ scattering length as a reference. We have observed that accidentally scattering resonances appear near all even isotopes, leading to large positive and negative scattering lengths for all isotopes. Only $^{42}\text{Ca}$ shows a small improvement in terms of scattering length compared to $^{40}\text{Ca}$. Therefore, alternative methods to that of evaporative cooling are interesting for $\text{Ca}$, such as direct laser cooling into quantum degeneracy using a narrow transition [39].

In addition, scattering lengths for all the even Ba isotopes have been investigated using a Tang-Toennies model potential. In contrast to the Ca case, here the scattering lengths vary strongly over the isotopes, resulting in a high probability that at least one isotope has a favorable scattering length to produce a BEC. More accurate knowledge of the ground-state $\text{Ba}_2$ potential, including the long-range coefficients, based on experimental data that covers the full vibrational spectrum is needed for an improved determination of the scattering lengths. However, once experimental knowledge on the scattering length of one isotope becomes available, the scattering lengths of all the other isotopes can be predicted with the present model potential.

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$^1$We have applied the Tang-Toennies potential model for $\text{Ca}_2$ [25] and $\text{Sr}_2$ [24], from which we have obtained similar results as in Sec. III A and Ref. [15], respectively, when fine-tuning the $C_6$ coefficient to reproduce the scattering length of one particular isotope.
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