Calculation of the elastic scattering parameters in an ultra-cold Fermi-Bose and Bose-Bose Fr vapor

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The calculations of the elastic scattering properties of ultracold-francium isotopes are reported in the detail. A parametric model potential for the triplet molecular states of the Fr₂ is represented, and the scattering lengths at and the effective range $r_e$ are calculated using WKB and Numerov methods for Fr-Fr in the triplet state. The convergence of these scattering properties as the depending on a $K_0$ parameter and core radius is also investigated using two method as Quantum Defect Theory and analytical formula of symkovisky.

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I. INTRODUCTION

In the Bose-Einstein condensation of alkali metal atoms, about francium atom has been known very little knowledge except trapping and cooling until now [1]. Because it has too much energy coming from nuclear reaction and no stable long-lived isotopes. Ultracold atomic collisions gained renew an important have came out a necessity of research as result of the atomic trapping and cooling when energy levels, hyperfine structure intervals and isotopes shifts for Fr isotopes is intensely studied in detailed [2, 3]. Calculations of ultracold elastic scattering properties for this atom haven’t been seen in literature until now. Reason of this is that experimental work on Fr has been lacking mostly due to no stable long-lived isotope [4, 5]. Collisions of alkali metal atoms except Fr atom at a few mill degrees Kelvin temperatures have been studied recently in many experiments [6, 7, 8, 9, 10, 11]. Theoretical work about scattering on Fr has been scant and only a few published papers exist [12].

The character of the interaction between atoms in low-temperatures is determined by signs ($\pm$) and magnitude of the scattering length $a$: for bosonic and fermionic atoms with $a > 0$ Bose condensate is stable, for $a < 0$ it is unstable [13]. The Pauli Exclusion Principle (which was determined experimentally) states that no two fermion particles can occupy the same state at the same time. They must have some way of being distinguished, whether by location, spin state, or some other property. That means that if one fermion is in a local ground or minimum energy state, the next fermion in the area must be in a higher energy state. For bosons, however, the Pauli Exclusion Principle is irrelevant by definition – so all of the bosons can be in the same state at the same time. They don’t have to be distinguishable from each other. When this happens, a Bose-Einstein Condensate is stable. Accurate calculations of $s$-wave scattering length and effective range for diatomic potentials are important due to the elastic collisions in these temperatures dominated by $s$-wave or low wave scattering. The accurate determination of scattering length depends on choosing the interaction potentials. Collision processes at near-zero temperatures ($\sim \mu K$) are sensitive to the details of the interaction potentials between the colliding systems.

In this paper, we have calculated scattering lengths $a$, effective ranges $r_e$ and cross section for collisions of Fr-Fr isotopes at ultracold temperatures with the semiclassical method (WKB) [14] and also solved the Schrödinger equation using Numerov method numerically [15]. The interaction of francium isotopes in triplet ($3^1\Sigma_u^+$) is described by short and long range potentials. This interaction potential $V(r)$ for Fr atom was parametered by using coefficients found in the literature. These calculated scattering properties using this potential are compared for two methods. We investigated the convergence of some scattering properties obtained with help of these methods as the dependence of the core radius and a $K^0$ parameter using Quantum Defect Theory [16] and the analytic calculations of the scattering lengths obtained by Szmytkowski [17].

II. PROCESSES

The scattering length is defined from the asymptotic behavior of the solution of the radial Schrödinger equation at zero energy:

$$\left[ \frac{d^2}{dr^2} - 2\mu V(r) + k^2 + \frac{l(l+1)}{r^2} \right] y_l(r) = 0$$

in atomic unit. Asymptotic behavior of the wave function is

$$y(r) = s \, r + s_0,$$
as \( r \to \infty \), where \( s \) and \( s_0 \) are constants. The sc length is given by

\[
a = -\frac{s}{s_0},
\]

here coefficients are obtained by using WKB from semiclassical behavior and with help of the solution at zero-energy. eq. 3 is transformed to the form 18:

\[
a = \tilde{a}\{1 - \tan\{\varphi - \pi/8\}\}
\]

in atomic unit, where \( \tilde{a} \) is the “mean” or “typical” scattering length determined by the asymptotic behavior potential through the parameter \( \gamma = \sqrt{2\mu k} \) deduced mass, and \( \kappa = c_6 \) is Van der Waals constant atom-atom interactions:

\[
\tilde{a} = \sqrt{2\gamma}(3/4)/\Gamma(1/4)
\]

Scattering length also depends a semiclassical calculation at zero energy from classical turning points, where \( y(r_0) = 0 \), to infinity,

\[
\varphi = \int_{r_0}^{\infty} \sqrt{-2\mu V(r)} dr.
\]

It also determines the total number of vibrational levels with zero orbital angular momentum, \( N_{ld} = 5/8 + 1 \), where \( \{ \} \) is the integer part. When a is just below an integer value, eq. 4 is anomalously large negative (see fig 1) \(|a| > \tilde{a}\), which correspond to presence of a virtual bound state. Unlike \( \gamma \) and \( \tilde{a} \), the phase \( \varphi \) depends strongly on the actual shape of the potential. When the phase is large, \( \varphi/\pi \) the scattering length is very sensitive to the slightest change of 1% in phase. For \(-c_6/r^6\) potential type, this expression is adjusted by Flambaum et al. 18 using WKB method, and the exact solution of the radial equation at zero-energy to form

\[
r_e = 2\int_{0}^{\infty} \left\{ u_0^2(r) - u^2(r) \right\} dr. \tag{8}
\]

This integral converges provided \( u(r) \) approaches \( u_0(r) \) rapidly enough as \( r \to \infty \). This requires \( V(r) \) to decrease faster than \( r^{-5} \). For \(-c_6/r^6\) potential type, this expression is adjusted by Flambaum et al. 18 using WKB method and the exact solution of the radial equation at zero-energy to form

\[
r_e = \frac{\sqrt{2\gamma}}{3} \left[ \Gamma(1/4) \frac{\Gamma(3/4)}{\Gamma(1/4)} - \frac{2\sqrt{2\gamma}}{a} + \frac{\Gamma(3/4)}{\Gamma(1/4)} \frac{4\sqrt{2\gamma}}{a^2} \right]. \tag{9}
\]

Then, the mean effective range may be rewritten by replacing \( a \sim \tilde{a} \) into eq. 8 as

\[
r_e = \frac{\sqrt{2\gamma}}{3} \left[ \frac{\sqrt{2\Gamma(1/4) \Gamma(3/4)}}{\Gamma(1/4) \Gamma(3/4)} - \frac{4\sqrt{2\gamma}}{\pi} + \frac{\Gamma(3/4) \frac{4\sqrt{2\gamma}}{\pi}}{\Gamma(1/4) \Gamma(3/4)} \right]. \tag{10}
\]

The low-energy scattering is dominated by the contribution \( l = 0 \). At values of \( k \) close to zero, the \( l = 0 \) phase shifts \( \delta_0 \) can be represented by a power series expansion in \( k \) 20

\[
k \cot \delta_0 = -\frac{1}{a} + \frac{1}{2} r_e k^2 + o(k^3). \tag{11}
\]

\[
FIG. 1: \text{Changes of scattering length as a function of the phase.} \text{The solid point in the left shows triplet Fr isotope interaction. So, the accurate determination of potential type, this expression is adjusted by Flambaum et al. 18 using WKB method, and the exact solution of the radial equation at zero-energy to form}
\]
III. RESULTS AND DISCUSSIONS

A. Potential

The interaction between Fr atoms like the other alkali metal atoms has two features: First, the potential at large distances behave as an inverse power of the interatomic distance, \( v = -\kappa/r^n \) with \( n = 6 \) for spherically symmetric two atoms in their ground state. The asymptotic parameter \( \kappa \equiv C_6 \) is known quite well for most atomic pairs of interest. Second, for alkali metal atoms other than hydrogen and helium the potential curve is generally quite deep and also the electron-exchange part of the atomic interaction is repulsive at smaller distance for the singlet and triplet terms of alkali-metal atoms. “Deep” here means that the wave functions of the atomic pair oscillate many times within the potential well, even at very low collision energies. The interatomic potential supports a large number of vibration levels. This latter feature enables one to use the semiclassical approximation to describe the motion of Fr atoms within potential well.[21]

Alkali-metal atoms have uncompensated electron spin \( s = \frac{1}{2} \) in the ground state. Therefore, the interaction between two alkali atoms in the ground state results in the formation of a diatomic molecule, which is described by two terms corresponding to the total spin \( s_{ab} = s_a + s_b \) of the system equals to 1 or 0. The state with \( s_{ab} = 0 \) and \( 1 \) corresponds to the singlet state and triplet state, respectively. The probability of the spin exchange is determined by both the dependence of potential curves on the internuclear distance \( r \) and the splitting between singlet and triplet terms. The exchange interaction is analytically calculated using the surface integral method by Smirnov and Chibisov[22], which yields

\[
v_{exc}(r) = \frac{1}{2}(v_u - v_g) = J(A,\alpha,\beta)r^{\frac{3}{2}} + \frac{2}{3} + \frac{1}{\sqrt{\pi}}\Gamma(-\alpha-\beta)r. \tag{12}\]

Where \( \alpha = \beta \) is the ionization energy of francium atom, and \( J \) are constant. In this equation, \( J \) is calculated from the surface integral given in the Ref.[22]. Also we have obtained the value of normalization constant, \( A \) by joining in the range of distances from the nucleus the wave function \( y(r) \), obtained by the Hartree-Fock method, and the asymptotic value of the wave function of Eq. 2 for an electron far from the nucleus but in the Coulomb field of the atomic core. For Fr-Fr, these values of constants are given in Table II.

![Table I: Potential coefficients for Francium-Francium atom in triplet state.](image)

| A       | J     | \( \alpha \) | \( C_3 \) | \( C_6 \) |
|---------|-------|-------------|--------|--------|
| 0.500   | 4.480x10^{-3} | 0.5471     | 4.437  | 5256   |

The long-range part of the interaction potential is given by

\[
v_{long-range} = -\sum \frac{C_m}{r_m^m} f_c(r), \tag{13}\]

which is the sum of Van der Waals terms. The \( C_3 \) and \( C_6 \) Van Der Waals values are given in Table II and had been calculated by Derivianko in literature[23]. The potential of Fr+Fr atom interaction consists of above expressed two terms, the sum of Eqs. 12 and 13 is given as

\[
V^{2s_{AB}}(r) = V(r)_{long-range} + (-1)^{s_{exc}}V(r)_{exc}. \tag{14}\]

Here, for triplet state, \( S_{AB} \) is taken as 1 value. This potential can be useful for other studies.

B. Scattering length and effective range of Fr

The scattering lengths of francium isotopes calculated from Eq. 4 using WKB method for \( V(r) \) are given in the Table II. In order to calculate numerically scattering length, we obtained s-wave phase shift \( \delta_0 \) using the potentials in eq.14 then we do it by solving radial equation using Numerov algorithm at \( e = K^2/2\mu \) in atomic unit and finding \( \delta_0 \) from the asymptotic behavior of the wave function \( y(r) = \sin(kr + \delta_0) \). The phases at small momenta \( k \) are used to extract the scattering length numerically from \( a = \lim(\tan\delta_0/k) \). The scattering lengths obtained via this method are given in the numeric columns of Table III.

![Table II: Scattering lengths of the same species francium isotope interactions in the triplet state. x,y gives isotopes cases.](image)

| Isotopes(\textsuperscript{a}Fr-\textsuperscript{a}Fr) | WKB | Numerov |
|----------------------------------|------|---------|
| 208-208                          | -52.315 | -52.303 |
| 209-209                          | -134.209 | -134.229 |
| 210-210                          | -332.242 | -332.672 |
| 211-211                          | -1779.55 | -1779.490 |
| 212-212                          | 932.576  | 932.598  |
| 213-213                          | 434.477  | 434.481  |
| 214-214                          | 301.464  | 301.461  |
| 215-215                          | 237.152  | 237.151  |
| 216-216                          | 97.235  | 97.226  |
| 223-223                          | 52.0355 | 52.035  |

Some parameters are important in the determination of \( a \) for WKB method. We also obtain these parameters, the mean scattering length \( \bar{a} \) and the zero-energy semiclassical phases \( \varphi \), given in Table III, using values of asymptotic parameter \( \gamma \). Here, the mean scattering length with asymptotic behavior of the potential in Eq. 14 has been calculated from equation 5.
TABLE III: Mean scattering length $\bar{a}$, semiclassical phase shifts $\varphi$ and numbers of the vibration bound states of same-species isotope interactions in the triplet states.

| Isotope Pair | $\bar{a}_{WKB}$ | $\varphi$ | $N_b$ |
|--------------|-----------------|----------|------|
| $^{208}$Fr-$^{208}$Fr | 101.173 | 73.6373 | 22.8145 |
| $^{209}$Fr-$^{209}$Fr | 101.294 | 73.8139 | 22.8709 |
| $^{210}$Fr-$^{210}$Fr | 101.415 | 73.9904 | 23.0387 |
| $^{211}$Fr-$^{211}$Fr | 101.536 | 74.1662 | 23.0945 |
| $^{212}$Fr-$^{212}$Fr | 101.656 | 74.3419 | 23.1503 |
| $^{213}$Fr-$^{213}$Fr | 101.775 | 74.5170 | 23.2058 |
| $^{214}$Fr-$^{214}$Fr | 102.014 | 74.6922 | 23.2613 |
| $^{215}$Fr-$^{215}$Fr | 102.133 | 75.0412 | 23.3167 |
| $^{216}$Fr-$^{216}$Fr | 102.952 | 76.2502 | 23.6462 |

As shown in the Table III, the scattering lengths calculated for the collisions of Francium pairs is in excellently agreement for two method.

Even our results shows that the stability of large condensates requires repulsive interactions (positive $a$), whereas for attractive interactions (negative $a$) it is unstable, only a finite number of atoms can be found in condensate state in a trap. Due to changes in the $V(r)$, scattering length is found as negative value, which lead to a condensate triplet state where the number of atoms is limited to a small critical value determined by the magnitude of $a$. In contrast, we have observed the positive scattering lengths that produce stable condensates. The calculations given in Table III shows that all atoms are found in the same energy levels if interaction atom species are boson, or they display a adopt behavior due to Pauli exclusion principle if interaction atom species are fermion. Also, from scattering lengths given as a function of the semiclassical phase shift in the eq. 1, we say that the minor changes in phase shifts have strongly affected the scattering amplitude. It is also remarked that for $^{212}$Fr-$^{212}$Fr, the analysis in the direct determination of scattering length is weakly dependent on the number $N_b$ of bound states supported by ab-initio potential. In contrast, mass scaling from one isotope to the others depends more strongly on $N_b$.

As shown in Table IV, scattering lengths are unstable against collapse from isotope $^{208}$Fr-$^{208}$Fr to $^{211}$Fr-$^{211}$Fr. Here the both boson-boson and fermion-fermion interactions are unstable. Same case is valid for the other stable isotope interactions.

Also, the effective ranges calculated using Numerov and WKB methods in the function of phase for the $V(r)$ potentials are presented in Table IV. The close agreement between the calculations of $r_x$ from Eqs. 8 and 11 confirms the accuracy of the numerical integration of the partial-wave equation. The size of the scattering lengths and effective ranges is closely related to the position of the last vibration bound states of the energy curves, as can be anticipated by inspection of Eq. 10 and number of vibrational levels $n_x(\varphi/\pi)$ which, consistent with Levinson’s theorem, show that as the binding energy of the highest level tends to zero, the scattering length tends to $\pm$ infinity.

C. Convergence of scattering length and effective range

Analytical calculations of scattering lengths is important in investigation of convergence of the scattering length and the effective range. In many approaches used to solve collision problems in atomic physics, the tree dimensional configuration space is divided into two regions separated by a spherical shell (a core boundary) of radius $\rho$. In the inner region ($r < \rho$) the short-range interaction between two colliding particles is very complicated and a scattering equation must be solved independently for each combination of particles. In contrast, it $\rho$ is chosen sufficiently large the scattering problems in the outer region ($r > \rho$) may be reduced to potential scattering with the long-range potential accurately approximated by simple analytical expression. A numerical solution in this region is usually easily approachable.

Two of these methods are analytical calculations derived by Radoslaw Szmytkowski for inverse problems and Quantum Defect Theory described by Gao.

Radoslaw Szmytkowski solved the radial schrödinger equation at zero energy for inverse type of long-range interaction analytically with solutions expressed in terms of the Bessel, Whittaker and Legendre functions, respectively. They derive exact analytical converge formulae for the scattering lengths. The expressions depend on the short-range scattering length, core radius and parameters characterizing the long-range part of the interaction. In Table IV we obtained the convergence of the ultra cold scattering length of Francium atom using the formulae of Szmytkowski. These formulae are given in that paper as eqs. (75), (76). As shown in the table, this method confirms convergence of the scattering length for $^{212}$Fr-$^{212}$Fr. Here, only, the convergence of the scattering length calculated from WKB method is given, and the same behavior can also be seen in the numerical calculation.
TABLE V: Convergence of scattering length calculated by WKB with the formulae of Szmytkowski for $^{212}\text{Fr}^{-212}\text{Fr}$.

| ρ  | $a_0$  | $a_0^2$ |
|----|--------|---------|
| 10 | -73.2943 | -1.69E+09 |
| 100 | 53.1953 | -46796 |
| 500 | 929.775 | 929.775 |
| 1000 | 3932.426 | 3932.426 |
| 5000 | 3932.569 | 3932.569 |
| 10000 | 3932.575 | 3932.575 |
| 50000 | 3932.576 | 3932.576 |

Quantum defect theory of atomic collisions is presented by Gao. Based on the exact solutions of the Schrödinger equation for an attractive $1/r^6$ potential, the theory provides a systematic interpretation of molecular bound states and atom-atom scattering properties and establishes the relationship between them. He finds a definition for the scattering length and the effective range and establishes the relationship between them. He finds a definition for the scattering length and the effective range and establishes the relationship between them.

$$a_{l=0} = \frac{2\pi}{\Gamma(1/4)^2} \frac{K^0 - 1}{K^0} \beta_6$$

$$r_{l=0} = \frac{\Gamma(1/4)^2}{3\pi} \frac{|K^0|^2 + 1}{|K^0|^2} \beta_6$$

where $\beta_6 = (2\mu C_6)^4$ and $K^0$ is the analytic function of energy.

Figure 2 shows the scattering length and the effective range curve plotted using the eqs. (15) and ones (dotted points) obtained by the mean WKB formulas. Our graphical representations show that as $K^0$ goes to infinity, the QDT results converge excellently to values obtained by WKB method in Fig. 2. Even, it may be said that the difference calculation of these properties gives similar results for any ultracold atom-atom collision in these two methods.

D. The zero energy cross sections

It is also known in more text book that the low energy scattering is always dominated by the $l = 0$ partial wave, the corresponding phase shift being given by

$$\delta_0 = ka$$

(16)

The triplet elastic cross sections can be defined by

$$\sigma_{el.}^t = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l + 1) \sin^2 \delta_l$$

(17)

where $l = 0$, $\sin \delta_0 \equiv \delta_0$ in limit of zero-energy and Eq. (17) is transformed using eq. (16) to $\sigma_{el.}^t = 4\pi a^2$. This result is valid for fermion-fermion interaction, but it is multiplied with 2 value due to symmetric wave function. If systems are bosonic one. Table VI shows zero energy cross sections adopted for two method. It concludes that zero energy cross sections is expected to be smaller than that of other alkali metal atom, because of it is a heavier atom.

FIG. 2: Convergence of the scattering length and the effective range calculated with QDT as a function of $K^0$ parameter when $K^0$ goes infinity.

TABLE VI: Triplet cross section of different francium isotopes calculated for two method. The numbers in brackets denote multiplicative powers.

| Isotope | WKB | Numerov |
|---------|-----|---------|
| $^{208}\text{Fr} - ^{208}\text{Fr}$ | 1.92617(-16) | 1.92528(-16) |
| 209 – 209 | 6.33833(-16) | 6.34022(-16) |
| 210 – 210 | 7.76874(-15) | 7.7886(-15) |
| 211 – 211 | 1.11438(-13) | 1.11430(-13) |
| 212 – 212 | 6.12083(-14) | 6.12111(-14) |
| 213 – 213 | 6.64271(-15) | 6.64287(-15) |
| 214 – 214 | 6.39060(-15) | 6.39503(-15) |
| 215 – 215 | 1.97909(-15) | 8.12064(-16) |
| 216 – 216 | 2.73785(-15) | 2.73760(-15) |
| 223 – 223 | 9.52820(-17) | 9.52802(-17) |
IV. CONCLUSIONS

The elastic scattering properties for the collision of the francium atoms in a limited range of moment \( k < \bar{a}^{-1} \approx 0.01 \text{a.u.} \) for francium-francium isotopes) at low temperatures are sensitive to the details of interaction potentials. Scattering properties such as scattering length, effective range and cross section have been computed using semi-classical and a numerical methods for the \( V(r) \) potentials as dependence of cutoff radius adjusted by comparing with the experimental potential for ultra-cold francium-francium isotopes collision. We investigated the convergence of these scattering properties as the depending of core radius and \( K^0 \) parameter using Quantum Defect Theory and analytical calculations derived by Radoslaw Szmytkowski for inverse problems. Cross section was obtained as \( \sim 10^{-15} \text{m}^2 \) at low energy. The phase shifts, an intermission parameter for scattering length and effective range, has linear manner at small momenta \( k < \bar{a}^{-1} \).

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