Calculation of the interspecies *s*-wave scattering length in an ultracold Na-Rb vapor

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(Received 19 February 2003; revised manuscript received 22 July 2003; published 20 October 2003)

We report the calculation of the interspecies scattering length for the sodium-rubidium (Na-Rb) system. We present improved hybrid potentials for the singlet $X^1\Sigma^+$ and triplet $a^3\Sigma^+$ ground states of the NaRb molecule, and calculate the singlet and triplet scattering lengths a_s and a_t for the isotopomers $^{23}Na^{87}Rb$ and $^{23}Na^{85}Rb$. Using these values, we assess the prospects for producing a stable two-species Bose-Einstein condensate in the Na-Rb system.

DOI: 10.1103/PhysRevA.68.042708 PACS number(s): 34.20.Cf, 03.75.Kk, 05.30.Jp, 32.80.Pj

I. INTRODUCTION

The *s*-wave scattering length a plays a central role in the description of atom-atom collisions at ultralow temperatures ($T \ll 1$ mK). In this regime, the cross section for elastic collisions, $\sigma_{el} \sim \pi a^2$, and the cross section for inelastic spin-exchange collisions, $\sigma_{ex} \sim \pi(a_t - a_s)^2$, are both expressed in terms of a [1]. The scattering length is also a critically important parameter in the physics of Bose-Einstein condensates (BECs). For a bosonic atomic species *i*, a BEC is stable only if $a_i > 0$. In addition, efficient evaporative cooling demands that $\sigma_{el} \gg \sigma_{ex}$ [2]. *A priori* calculations of a are thus of fundamental interest, and the quest for BEC in alkali-metal atoms has spurred on efforts to calculate the scattering length in many atomic species.

A majority of the work on scattering lengths has concentrated on interactions between like alkali-metal atoms. However, the recent production of Bose-Fermi mixtures in ^{6}Li-^{23}Na [3], ^{6}Li-^{7}Li [4,5], and ^{40}K-^{87}Rb [6] and dual-species BEC in ^{41}K-^{87}Rb [7] has renewed interest in binary mixtures of ultracold gases. In these systems, the interspecies scattering length a_{12} is the basic quantity parametrizing the interactions between component atomic species. a_{12} determines the efficiency of sympathetic cooling *enroute* to the formation of quantum degenerate mixtures, and in the case of two-species BECs (TBECs), a_{12} determines the stability and miscibility of these mixtures [8]. However, relatively few calculations of interspecies scattering lengths exist [9,10]. This is due, in part, to the incomplete characterization of diatomic interaction potentials for many pairs of alkali-metal atoms.

In this paper we calculate the scattering lengths for the Na-Rb system. We construct the NaRb potential from a combination of spectroscopic data and precise long-range interaction parameters, and use a simple method for calculating the singlet and triplet scattering lengths for the isotopomers $^{23}Na^{87}Rb$ and $^{23}Na^{85}Rb$. The Na-Rb system is interesting in part because its an obvious candidate for TBEC. Both of the component species have been condensed and the condensates have been studied in detail [11]. The Na-Rb TBEC has been treated theoretically, and its properties are sensitive to the value of the interspecies scattering length a_{Na-Rb} [8].

This paper is divided into four sections. In Sec. II, we discuss methods for calculating a_{Na-Rb}, and address the source of errors involved in these calculations. In Sec. III, we introduce two hybrid potentials for the NaRb molecule, and contrast our potentials with previous results. In Sec. IV, we present our calculations for a_{Na-Rb}, and discuss the feasibility of producing a TBEC in the Na-Rb system.

II. SCATTERING LENGTH

If the potential $V(r)$ is known for all r, then the scattering length a can be calculated [12]. The procedure is to numerically integrate the radial Schrodinger equation for low collision energies to large values of r. At large r the numerical wave function $u(r)$ is "matched" to an asymptotic form $\chi(r)$ by requiring that $(\partial/\partial r)\ln u(r) = (\partial/\partial r)\ln \chi(r)$ at the match point $r = r_m$. The asymptotic wave function can be written as

$$\chi_{l=0}(r) \sim \frac{1}{k}[\sin(kr) + \tan(\delta_o)\cos(kr)], \tag{1}$$

where k is the atomic wave vector and δ_o is the *s*-wave phase shift. In the limit that $k \to 0$, the wave function asymptotically approaches a straight line as $r \to \infty$. The scattering length is given by the r intercept of this line [13], and can be formally defined in terms of the *s*-wave phase shift as

$$a = -\lim_{k \to 0} \frac{\tan(\delta_o)}{k}. \tag{2}$$

For low collision energies, r_m should be large to ensure that the numerical wave function attains its asymptotic behavior. The total integration time can be reduced by calculating the corrections to the asymptotic wave function at smaller values of the match point $r = r_m$. For example, Marinescu has shown [14] that the wave function for large r may be written as $\chi(r) = \alpha\epsilon_\alpha(r) + \beta\epsilon_\beta(r)$, where the functions $\epsilon_{\alpha,\beta}(r)$ are solutions to the differential equations $\epsilon''_{\alpha,\beta}(r) = [2\mu V(r)/\hbar]\epsilon_{\alpha,\beta}(r)$ subject to the boundary conditions $\epsilon_\alpha(r) \to r$ and $\epsilon_\beta(r) \to 1$ as $r \to \infty$. This equation cannot be solved exactly. However, if an analytic expression for the long-range potential is known, then the functions $\epsilon_{\alpha,\beta}(r)$ may be estimated to arbitrary precision using a method of successive approximations. The scattering length is then

given by $a=-\beta/\alpha$, which can be found by applying the usual continuity condition at $r=r_m$.

The uncertainty in the calculated value of a depends upon the reliability of the potential $V(r)$. Gribakin and Flambaum [15] have shown that for diatomic potentials which fall off at long range as $-C_6/r^6$, the scattering length is given by

$$a=a_o[1-\tan\{\Phi(E=0)-\pi/8\}], \tag{3}$$

where a_o is a''mean scattering length,'' and $\Phi(E)$ is the semiclassical phase, defined as

$$\Phi(E)=\int_{r_{inner}}^{\infty}\sqrt{\frac{2\mu(E-V(r))}{\hbar^2}}dr, \tag{4}$$

where r_{inner} is the inner classical turning point of the potential at energy E and μ is the reduced mass of the colliding atoms. As can be seen from Eq. (3), the scattering length is infinite if $\Phi(E=0)=(5/8+n)\pi$, where $(n=1,2,3,\ldots)$. This situation occurs if the nth vibrational state of the potential $V(r)$ is barely bound at $E=0$. In general, $V(r)$ will not admit a barely bound state. However, variations of the potential within its estimated uncertainties will shift the energies of its bound states, and states lying closest to dissociation experience the largest shifts. A bound state may even be introduced or removed from the well, depending on the size of the potential shift and the proximity of a bound or virtual level to the dissociation energy. As states are added or removed from the well, the scattering length passes through $\pm\infty$. Therefore, if the interatomic potential is not known well enough to predict whether or not a barely bound state exists, then a cannot be specified within finite bounds.

Because of the extreme sensitivity of a to the binding energy of the highest vibrational state of the interatomic potential $V(r)$, the most precise calculations of a in alkali-metal atoms typically rely on the spectroscopy of bound states near dissociation. Two-color photoassociation or Raman spectroscopy is used to resolve these lines to high precision [16]. In the absence of near-dissociation spectroscopy, the scattering length may still be calculated, but the accuracy and precision of such a calculation is limited by the accuracy and precision of the interatomic potential $V(r)$. In the case of alkali-metal dimers, spectroscopy is sparse and near-dissociation spectroscopy is nonexistent. However, the potential $V(r)$ may still be ''assembled'' from RKR (Rydberg-Klein-Rees) [17] data and well-known analytic expressions for short- and long-range potentials to create a ''hybrid'' potential valid for all r. In assigning error bars to a, care must be taken to ensure that variations of the hybrid potential within its estimated uncertainties do not introduce or remove bound states from the well. For example, uncertainties in the C_6 coefficient of NaK allowed for additional bound states in its hybrid potential, and frustrated attempts to determine the scattering length for some isotopomers [9]. Fortunately, this is not the case for NaRb, as shown below.

III. NaRb POTENTIALS

Compared to many alkali-metal dimers, the ground states of the NaRb molecule are relatively well known. Rovibrational states to within 5% of dissociation have been observed in both the triplet $a^3\Sigma^+$ [18] and singlet $X^1\Sigma^+$ potential wells [19,20]. The rotationless interatomic potentials $V_s(r)$ and $V_t(r)$, corresponding to the $X^1\Sigma^+$ and $a^3\Sigma^+$ states, respectively, have been determined through RKR analysis, and a direct fit to the singlet spectrum [20] using a modified Lennard-Jones (MLJ) [21] parametrization has also been performed. *Ab initio* ground-state potential curves for NaRb have been calculated [22]. However, these curves are not very accurate, so we do not use them in constructing our interatomic potentials.

At large r, the NaRb interatomic potential is accurately represented by a sum of two independent contributions, the exchange and dispersion energies. The dispersion energy is given by a well-known expansion in powers of r^{-1}:

$$V_{disp}(r)=-\left(\frac{C_6}{r^6}+\frac{C_8}{r^8}+\frac{C_{10}}{r^{10}}\right). \tag{5}$$

The coefficients C_n may be calculated from a knowledge of atomic polarizabilities [23]. The exchange interaction is calculated using the surface integral method of Smirnov and Chibisov [24], which yields

$$V_{ex}(r)=\pm J(A,B,\alpha,\beta,r)r^{(2/\alpha)+(2/\beta)-[1/(\alpha+\beta)]-1}e^{-(\alpha+\beta)r}, \tag{6}$$

where $\alpha^2/2$ and $\beta^2/2$ are the ionization energies (in atomic units) of each atom, and r is assumed to be in units of Bohr radii. The function $J(A,B,\alpha,\beta,r)$ can be expanded in a power series $\Sigma_n(J_n r^n(\alpha-\beta)^n)/n!$ whose coefficients J_n are expressed as integrals that must be solved numerically. The complete long-range potential is then given by

$$V_{LR}(r)=V_{disp}(r)\pm V_{ex}(r). \tag{7}$$

The exchange energy is positive (negative) for the triplet (singlet) state. As $r\to\infty$, the long-range interaction potential is dominated by the well-known van der Waals potential $-C_6/r^6$. The exchange interaction is expected to become important inside the LeRoy radius R_{LeRoy} [25], beyond which the potential is well approximated by the dispersion energy alone. For NaRb, $R_{LeRoy}\sim 11$ Å.

The NaRb molecular potentials can be modeled by smoothly joining RKR data to the long-range interaction potentials. Zemke and Stwalley (Z-S) have constructed such hybrid potentials for the $a^3\Sigma^+$ and $X^1\Sigma^+$ states of the NaRb molecule [26]. More complete spectra of the NaRb singlet state [20] and a more precise estimate of the C_6 coefficient for NaRb [27] have since become available, allowing us to construct new hybrid potentials for both the NaRb $X^1\Sigma^+$ and $a^3\Sigma^+$ states. For $r<11$ Å, we use the recent MLJ potential to model the $X^1\Sigma^+$ state. Our potential for the $a^3\Sigma^+$ state is identical to the Z-S triplet potential for $r<13.5788$ Å. Our long-range potential differs from that used by Z-S in a number of ways. We use the C_8 and C_{10} dispersion coefficients

TABLE I. Our chosen values for the parameters of the NaRb long-range potential $V_{LR}(r)$.

Parameter	Value
C_6 [a]	1.293×10^{7}
C_8 [b]	3.4839×10^{8}
C_{10} [b]	1.1552×10^{10}
α_{Na} [c]	0.61458
β_{Rb} [c]	0.55409
A_{Na} [d]	0.76752
B_{Rb} [d]	0.56945
J_0 [e]	1.4197×10^{-2}
J_1 [e]	6.0963×10^{-4}
J_2 [e]	1.9537×10^{-3}

[a]C_6 given in units of cm^{-1} Å^6. See Ref. [27].
[b]C_8 and C_{10} given in units of cm^{-1} Å^8 and cm^{-1} Å^{10}, respectively. See Ref. [28].
[c]The quantities are expressed in atomic units. See Ref. [29].
[d]The constants A and B are related to the size of the wave function of each atom in the region of interaction. See Ref. [30].
[e]We found that the exchange energy was adequately represented in our region of interest by the first three terms of the expansion $V_{ex}\sim\Sigma_n(J_n r^n(\alpha-\beta)^n)/n!$. Here we use atomic units. See Ref. [24].

recommended by Marinescu and Sadeghpour [28], but choose for C_6 the highly precise value calculated by Derevianko *et al.* [27]. For the exchange energy, we used the heteronuclear expression of Smirnov and Chibisov given by Eq. (6). Both the singlet MLJ and triplet RKR potential curves are joined smoothly to our long-range potential as given by Eq. (7). Our complete long-range potential is given in Table I.

IV. RESULTS AND DISCUSSION

A. Na-Rb scattering lengths

To calculate the singlet or triplet scattering lengths, we choose the hybrid potential $V_s(r)$ or $V_t(r)$ and integrate the radial Schrodinger equation at $E=0$ from r_{inner} to the match point r_m using the Numerov algorithm [31]. The reduced mass μ is given by $M_{Na}M_{Rb}/(M_{Na}+M_{Rb})$, where M labels the atomic mass of either ^{23}Na, ^{85}Rb, or ^{87}Rb. We expect the isotopic correction to the internuclear potential $V(r)$ to be negligible [20]. Following Ref. [14], the scattering length is given by

$$a=\frac{u\epsilon'_\alpha-u'\epsilon_\alpha}{u\epsilon'_\beta-u'\epsilon_\beta}\Big|_{r=r_m}, \tag{8}$$

where $u(r)$ is the numerically integrated wave function, and the functions $\epsilon_{\alpha,\beta}(r)$ are determined from the long-range potential, as discussed in Sec. II. The primes denote derivatives with respect to r. We found that a fourth-order approximation to $\epsilon_\alpha(r)$ and $\epsilon_\beta(r)$ guaranteed convergence to a reliable value of a at a match point $r_m=100$ Å. Our results are summarized in Table II.

Because the scattering length is very sensitive to the details of the interatomic potential $V(r)$, it is important to ensure that our calculated values of a are stable with respect to changes in $V_{s,t}(r)$ within their known experimental or theoretical uncertainties. These include uncertainties in the value of the dissociation energy D_e, the inner and outer turning points of the RKR potentials, the binding energy of the observed vibrational states, and the coefficients of the long-range parameters. We estimate our errors by calculating the change in the semiclassical phase $\Phi(E=0)$ due to the error in each parameter of our potential. These "phase errors" $\Delta\phi$ are then summed in quadrature to give a total phase error $\Delta\phi_{total}$. We convert this value into a scattering length error using Eq. (3).

TABLE II. The scattering lengths found from our hybrid potentials for ^{23}Na^{85}Rb and ^{23}Na^{87}Rb.

Isotopomer	a_S	a_T
^{23}Na^{85}Rb	167^{+50}_{-30}	59^{+12}_{-9}
^{23}Na^{87}Rb	55^{+3}_{-3}	51^{+9}_{-6}

For the triplet state, the error in a was estimated with respect to changes in D_e, C_6, and the difference between RKR turning points $(r_{inner}-r_{outer})$. In the case of the singlet state, the MLJ parametrization allowed us to vary all parameters simultaneously in a statistically meaningful way. We treated the MLJ parameters as random variables with a well-defined mean and standard deviation. The phase $\Phi(E=0)$ was then calculated for a 100 "random" potentials. The phase error was determined by examining the distribution of phases. This phase error was used to calculate the error in a_s.

As shown in Table II, our error bars are small. This is, in some ways, a fortuitous result. Had a bound or virtual state been closer to dissociation, variations in the potential may have caused the phase to pass through a region where $a\to\infty$. Because the scattering lengths are relatively small, they are more stable with respect to changes in the corresponding potential. In addition, our hybrid potentials are reasonably well constrained. This is due, in part, to the observation of bound states relatively close to dissociation in the NaRb triplet well, which enabled Z-S to reduce the uncertainty in the dissociation energy to $\Delta(D_e)=\pm0.1$ cm^{-1}, and the very precise calculation of the C_6 coefficient by Derevianko [27].

One interesting consequence of the new singlet potential is the appearance of an additional bound state. We found that our complete potential for the $X^1\Sigma^+$ state supported 83 bound states, whereas the corresponding Z-S potential only supported 82 bound states. This can be understood by examining Fig. 1, which shows the energy difference between the Z-S singlet and MLJ potentials for 6 Å$<r<$16 Å. Because the MLJ potential is everywhere deeper, the wave vector $k(E=0)$ will be larger for all r. In semiclassical terms, the wave function will build up more phase Φ in this potential. In our case, $\Phi_{MLJ}-\Phi_{Z-S}>\pi$, so that another bound state appears in the MLJ molecular well. The energy differences between the two curves is due primarily to errors in the extrapolation procedure used by Z-S to connect the short- and long-range components of their hybrid singlet-state potential.

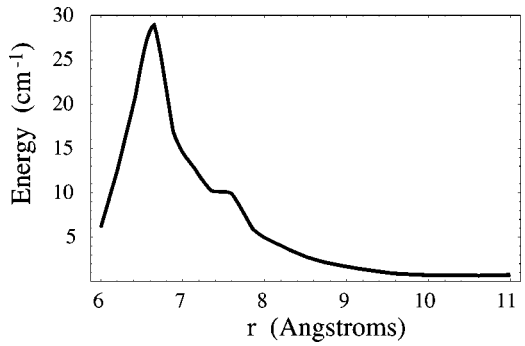

FIG. 1. A plot of the difference between the Z-S and MLJ $X^1\Sigma^+$ potentials .

B. Two-species Na-Rb BEC

Having calculated the Na-Rb scattering lengths, we now consider the properties of a mixture of Na and Rb condensates. The interactions in a Na-Rb TBEC are parametrized by three scattering lengths: a_{Na}, a_{Rb}, and a_{Na-Rb}. The values of a_{Rb} and a_{Na} are known to high precision, and are given in Table III. We consider a Na-Rb mixture in which the Na atoms are in the state $|F_{Na},m_{Na}\rangle$, and the Rb atoms are in the state $|F_{Rb},m_{Rb}\rangle$, where F is the total angular momentum of the atom and m is its projection on the quantization axis. We represent the two-atom state by the ket $|F_{Na},m_{Na};F_{Rb},m_{Rb}\rangle$. To calculate the scattering lengths we use the low-energy elastic approximation [34,35], which assumes that elastic collisions dominate the total cross section for collisions. This approximation gives for the scattering lengths

$$a=a_sP_s+a_tP_t, \tag{9}$$

where P_s and P_t are the probabilities of the atoms being in a singlet or triplet state, respectively. To calculate the probabilities P_s and P_t, we project the state $|F_{Na},m_{Na};F_{Rb},m_{Rb}\rangle$ onto the states $|S,m_S;I,m_I\rangle$, where S and I refer to the total electronic and nuclear spin of the two-atom system, respectively, while $m_{S,I}$ are their projections onto the quantization axis. This basis is useful for characterizing the system at smaller internuclear distances where the exchange energy dominates. In this region, F_{Na} and F_{Rb} are no longer ''good'' quantum numbers, and the singlet and triplet states are labeled by $S=0,1$, respectively.

To calculate the projections $C^{F_{Na},m_{Na},F_{Rb},m_{Rb}}_{S,m_S,I,m_I}=\langle S,m_S;I,m_I|F_{Na},m_{Na};F_{Rb},m_{Rb}\rangle$, we perform the angular-momentum recoupling of the four quantum numbers S_{Na}, I_{Na}, S_{Rb}, and I_{Rb} by making use of the Wigner 9-j symbols and standard Clebsch-Gordan algebra. We calculated the complete recoupling matrices U_{SI-FF} for both ^{23}Na^{85}Rb and ^{23}Na^{87}Rb, and extracted the probabilities P_s and P_t for all input channels $|F_{Na},m_{Na};F_{Rb},m_{Rb}\rangle$. The scattering length for an arbitrary input channel is then given by Eq. (9).

TABLE III. Recently determined scattering lengths for ^{23}Na, ^{85}Rb, and ^{87}Rb.

Species	a_s	a_t
^{23}Na [a]	19.1 ± 2.1	65.3 ± 0.9
^{85}Rb [b]	2795^{+420}_{-290}	-388 ± 3
^{87}Rb [b]	90.4 ± 0.2	98.98 ± 0.04

[a]See Ref. [32].
[b]See Ref. [33].

Knowledge of a enables us to calculate the cross section for elastic collisions, $\sigma_{el}=4\pi a^2$. Elastic collisions mediate the rethermalization of atoms during evaporative cooling and sympathetic cooling. Furthermore, knowledge of a_s and a_t allows us to characterize the inelastic losses in the system. The dominant two-body mechanism for the loss of atoms from a trap is spin-exchange collisions. In these types of collision, the internal spin states of one or both of the atoms changes. In the case of magnetically trapped samples, such collisions can cause atoms to be ejected from the mixture by sending them into nontrappable spin states. More generally, the atoms may be ejected if the spin reorientation energy is converted to kinetic energies greater than the depth of the (magnetic or optical) potential confining the mixture. In the elastic approximation we can write the cross section for such inelastic processes as [35]

$$\sigma_{ex}=M_{if}\pi(a_t-a_s)^2, \tag{10}$$

where M_{if} is a factor that depends on the asymptotic hyperfine states involved in the collision. Letting primes denote the asymptotic output channel, we have

$$M_{if}=\left[\sum_{m_S,I,m_I}(C_{S=0}C'_{S=0}-C_{S=1}C'_{S=1})\right]^2, \tag{11}$$

where C is the projection coefficient defined above, and the indices have been suppressed.

The achievement of a miscible two-component BEC places a number of constraints on the three relevant scattering lengths. Efficient sympathetic cooling requires a large magnitude of a_{Na-Rb}. Collisional stability against spin-exchange collisions requires small values of σ_{ex}, which implies that the difference between a_s and a_t be small. Dynamical stability of the individual BECs requires $a_{Na}>0$ and $a_{Rb}>0$. In the Thomas-Fermi approximation, the criteria for stability implies the existence of a critical value of $|a_{Na-Rb}|=a_c$ above which the two-species condensate cannot coexist. The criteria is given by $|a_{Na-Rb}|\leqslant a_c=\gamma\sqrt{a_{Na}a_{Rb}}$, where $\gamma=\sqrt{M_{Na}M_{Rb}}/(M_{Na}+M_{Rb})$ [36]. For $a_{Na-Rb}\leqslant -a_c$ the attraction between the condensates overwhelms the repulsive interaction within each condensate and they collapse, while for $a_{Na-Rb}\geqslant a_c$ the mutual repulsion of the two condensates is too great for them to overlap at all.

The single-species scattering lengths are positive for both ^{23}Na-^{23}Na and ^{87}Rb-^{87}Rb collisions, which allows for single-species BEC in either atomic species. Using Eq. (9) and the scattering lengths given in Tables II and III, we calculate a_c for all asymptotic states in a ^{23}Na-^{87}Rb mixture. The near equality of a_s and a_t implies that σ_{el} will be approximately the same for all states, and that σ_{ex} will be

small. Therefore interspecies elastic collisions will dominate inelastic spin-exchange collisions. Using the mean values for the triplet and singlet scattering lengths given in Table II, we find that for all asymptotic two-atom states, $a > a_c$. Taking into account the known uncertainties in the various scattering lengths, we find that the inequality $a > a_c$ still holds. We therefore conclude that a stable, miscible TBEC in a ^{23}Na-^{87}Rb mixture is not possible.

Next, we consider the mixture ^{23}Na-^{85}Rb. This is an interesting case, since BEC has only been observed in ^{85}Rb by utilizing a Feshbach resonance to tune the scattering length of the $|F=2,m_F=-2\rangle$ state [37]. To simplify our analysis, we eliminate from consideration those states for which the ^{85}Rb single-species scattering length is negative. Of the remaining states, we choose states that are lossless with respect to both homo- and heteronuclear spin-exchange collisions. Because of the large positive singlet scattering length in ^{85}Rb, there is a large variation in a_{el} from state to state. If we use the mean values for the interspecies scattering lengths given in Table II, we again find no asymptotic states that satisfy the condition for TBEC stability. However, unlike the case of ^{23}Na-^{87}Rb, the inequality $a < a_c$ is satisfied for nine of the two-atom states within the bounds of the uncertainties of the various scattering lengths. Of these states, only the state $|F_{Na},m_{Na};F_{Rb},m_{Rb}\rangle = |1,-1;2,-1\rangle$ is magnetically trappable in the weak-field limit.

V. CONCLUSIONS

We have derived hybrid potentials for the $X^1\Sigma^+$ and $a^3\Sigma^+$ states of the NaRb molecule. We compare them to other recently derived potentials, and we discuss why our potentials are preferred. We have calculated the singlet and triplet scattering lengths from these potentials for both ^{23}Na^{85}Rb and ^{23}Na^{87}Rb. Using the elastic approximation, we have calculated the scattering length for all two-atom asymptotic hyperfine states for both isotopomers. The cross sections for elastic and inelastic spin-exchange collisions can be found using these values. Applying the Thomas-Fermi approximation criterion for TBEC stability, we find no two-atom asymptotic states for which a NaRb TBEC is stable. Further experimental studies of ultracold Na-Rb vapors, including efforts to produce a TBEC in the NaRb system, will help refine our knowledge of the interatomic potentials and test these conclusions.

ACKNOWLEDGMENTS

This work was supported in part by the U.S. Office of Naval Research, by the National Science Foundation, and by the U.S. Army Research Office.

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