Evaluation of the $^{52}$Cr-$^{52}$Cr interaction via spin-flip scatterings

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In order to evaluate $g_0$, the interaction strength of a pair of $^{52}$Cr atoms with total spin $S = 0$, a specially designed $s$-wave scattering of the pair has been studied theoretically. Both the incident atom and the target atom trapped by a harmonic potential are polarized previously but in reverse directions. Due to spin-flip, the outgoing atom may have spin component $\mu$ ranging from -3 to 3. The outgoing channels are classified by $\mu$. The effect of $g_0$ on the scattering amplitudes of each of these $\mu$-channels has been predicted.

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The chromium atoms $^{52}$Cr are special due to having a larger spin $F = 3$ and a larger magnetic moment $6\mu_B$. Since the experimental realization of the chromium condensation [1], the interest in this field has been increasing. The $^{52}$Cr condensate is a new kind of matter aggregation having the magnetic dipole-dipole interaction $V_{dd}$ more than twenty times stronger than that of the alkalis family. A direct consequence of $V_{dd}$ is the coupling of the spatial and spin degrees of freedom so that the conversion of spin angular momentum into orbital angular momentum can be realized. Thereby new physical phenomena (say, creation of vortex) might appear. In addition to $V_{dd}$, the atom-atom interaction depends strongly on the total spin $S$ of the pair, and is in general written as $V_{12} = \delta(r_1 - r_2) \sum g_S P^S + V_{dd}$, where $g_S$ is the strength and $P^S$ is the projection operator of the $S$-spin-channel ($S = 0, 2, 4$ and $6$). Up to now, $g_2$, $g_4$, and $g_6$ have been determined, but $g_0$ has not yet [2, 3, 4, 5]. However, many features of the condensate depend on this parameter (say, the phase-diagram of the ground state depends strongly on $g_0$ [4, 6, 7, 8]. The dependence is also explicit in spin-evolution [9]). Therefore, the determination of $g_0$ is important for a thorough and clear description of the condensates. This paper is one along this line.

The effect of $g_0$ can be exposed via two-body scatterings. We study the scattering of a very slowly incident $^{52}$Cr atom by another $^{52}$Cr atom trapped previously in a potential $U(r)$. The energy of collision is so low that the trapped atom is not able to be excited, and only the $s$-wave of the incoming one is involved. The scattering should be so designed that related observables are sensitive to $g_0$. The following points are proposed to meet the goal.

(i) When $M_S$, the Z-component of the total spin $S$ of the pair, is non-zero, $g_0$ plays no role. Therefore, the two-body system must be designed to have $M_S = 0$. We therefore assume that the spin-state $\lambda\mu$ of the incident particle has $\mu = 3$, while that of the target particle in the trap has $\mu = -3$. This is different from the design of [2], where both particles have $\mu = -3$. With their design, they have successfully determined the values of $g_2$, $g_4$, and $g_6$. However, $g_0$ cannot be thereby determined.

(ii) In general, for a scattering by a potential $U(r)$, the cross-section depends on the parameters of the potential very sensitively. For an example, we study the case of a finite harmonic potential $U_p(r) = \frac{\lambda}{2}\omega^2(r^2 - r_0^2)$ if $r \leq r_0$, or $U_p(r) = 0$ if $r > r_0$. The parameter $r_0$ measures the width and depth of the potential. In what follows $\omega$ and $\lambda \equiv \sqrt{\frac{\hbar}{m\omega}}$ are used as units of energy and length, respectively. When a single $^{52}$Cr atom with an incident kinetic energy $k^2/2$ is scattered by this potential, the $s$-wave cross-section $\sigma_U$ against the parameter $r_0$ is shown in Fig.1, where $k = 0.1$. One can see, if $r_0$ is given in a narrow domain around 2.512, $\sigma_U$ would be much larger. In the follows two kinds of potentials will be used, and their parameters will be selected in the narrow domains that lead to large $\sigma_U$.
where \( S \) is the orbital angular momentum of the \( i \)-th atom, and \( r = r_2 - r_1 \). It can be proved that \( V_{dd} \) must cause an additional spatial relative rotation of the two particles in d-wave as shown in the appendix. However, if the total orbital angular momentum \( L \) can be kept zero (say, due to a constraint in energy), the effect of \( V_{dd} \) would be strictly suppressed, and therefore can be neglected. The neglect of \( V_{dd} \) would greatly facilitate the calculation shown below. This is different from the design of \([2]\), where a magnetic field is applied. It is reminded that, if higher partial waves are introduced by \( V_{dd} \), they are accompanied by large-S components due to the conservation of the total angular momentum. Among these components those with a large-\( M_S \) will lead to a decrease of energy due to the Zeeman effect. Therefore, the increase of rotation energy can be partially canceled by the additional Zeeman energy. Consequently, the magnetic field would help \( V_{dd} \) to cause a stronger mixing to include higher partial waves, and the effect of \( V_{dd} \) thereby becomes remarkable. This is the case of \([2]\).

With the above consideration, for numerical calculations, two potentials are introduced. One is the finite harmonic well \( U_p(r) \) with the parameter \( r_0 \) mentioned above, the other is the Gaussian potential \( U_a(r) = -4e^{-(r/a)^2} \) with the parameter \( a \). The propagation number of the incoming atom \( k \leq 0.2 \) so that the related kinetic energy \( k^2/2 \) is much smaller than the energy gap of the ground state, and the maximal effective classical angular momentum of the incident particle \( \hbar k r_0 \) is smaller than \( \hbar \). With these choices the target atom can not be excited, and only the s-waves of both atoms are involved, and the total orbital angular momentum \( L \) remains to be zero as required.

When \( V_{dd} \) is dropped, \( S \) and \( M_S \) are good quantum numbers. Let the total wave function \( \Psi \) be a composition of different \( S \)-component,

\[
\Psi = \sum_{S} C_S \Psi_S = \sum_{S} C_S \frac{1}{r_1 r_2} \Phi_S(r_1, r_2)(12) S M_S \tag{2}
\]

where \( S \) is from 0 to 6 and \( M_S = 0 \) as designed. Each \( \Psi_S \) should satisfy the Schrödinger equation, while the coefficients \( C_S \) are determined by how the incoming channel would be. Since only s-waves are involved, the angular degrees of freedom are irrelevant. Thus the Schrödinger equation for \( \Phi_S \) reads

\[
[E + \frac{\alpha^2}{2 r_1^2} + \frac{\beta^2}{2 r_2^2} - U(r_1) - U(r_2)] \Phi_S(r_1, r_2) = 0 \tag{3}
\]

Where the total energy \( E = \varepsilon_g + k^2/2 \), and \( \varepsilon_g \) is the ground state energy (negative) of the target particle. Incidentally, \( \varepsilon_g \) and the associated wave function \( \phi_g \) are easy to be obtained. In order to facilitate numerical calculation, the \( \delta \)-function is replaced by \( e^{-\beta r^2}/(\pi/\beta)^{3/2} \), where \( \beta \) is chosen to be a very large number to assure a very short range. We choose \( \beta = 1/(0.06)^2 \), and we found that the effect of the change of \( \beta \) in a reasonable domain is slight. When \( S \) is even, \( \Phi_S \) must be symmetric with respect to the interchange of \( r_1 \) and \( r_2 \), whereas when \( S \) is odd, it must be anti-symmetric.

For \( k = 0.1 \) and \( U = U_p \), we know from Fig.1 that the optimal \( r_0 \) leading to the largest \( \sigma_U \) is 2.512. Accordingly, three cases with \( r_0 = 2.5, 2.512 \), and 2.53 are chosen to see the effect of the variation of \( r_0 \) around its optimal value. We define a domain (0.5) for both \( r_1 \) and \( r_2 \). Then, Eq.(3) is solved numerically in the domain. The crucial point is the embedment of boundary conditions. Obviously, we have \( \Phi_S(0, r_2) = \Phi_S(r_1, 0) = 0 \). Furthermore, it is reminded that, due to the constraint in energy, if one atom is far away, the other one would remain in the trap in the ground state (the outgoing \( S \)-wave of both atoms is not possible). Therefore, when \( r_2 \) is sufficiently large, \( U(r_2) = 0 \), \( V_{12} = 0 \), and \( \Phi_S(r_1, r_2) \) would tend to \( \phi_g(r_1)(b_S \cos(kr_2) + a_S \sin(kr_2)) \), where the second factor is the common form of s-waves. Both \( b_S \) and \( a_S \) are real numbers, and the unitarity is thereby assured. When \( r_2 = 5 \), the second factor is just a constant denoted by \( h_S \). Now we arrive at the second pair of boundary conditions, namely, \( \Phi_S(r_1, 5) = \phi_g(r_1) h_S \) and \( \Phi_S(5, r_2) = -\phi_g(r_2) h_S \). Where, \( h_S \) can be arbitrary given because the eventual results do not depend on it as shown below. The factor \((-1)^S\) is needed to assure the correct permutation symmetry.

Now, the values of \( \Phi_S(r_1, r_2) \) at all the borders are specified. Thus the problem is to solve an elliptic partial differential equation under the Dirichlet condition. Numerical solutions can therefore be obtained by using standard programs of difference equations. For \( S = 2, 4, \) and 6, \( g_s \) have been known. Using \( h \omega \) and \( \lambda \) as units, \( g_2 = -0.134 \times 10^{-3} \sqrt{\omega} \), \( g_4 = 1.11 \times 10^{-3} \sqrt{\omega} \), and \( g_6 = 2.14 \times 10^{-3} \sqrt{\omega} \). For \( S = 0 \), \( g_S \) will be given at a number of values from \(-2 g_6 \) to \( 2 g_6 \). When \( S \) is odd, \( g_S \) is simply zero. Examples of \( \Phi_S \) are given in Fig.2. One can see in Fig.2a that the two atoms can be very close to each other in the trap if \( S \) is even, but can not if \( S \) is odd as shown in 2b. Obviously, \( \Phi_S(r_1, r_2) \) is symmetric (anti-symmetric) in 2a (2b) as expected.

Once \( \Phi_S \) has been solved numerically, we can extract \( b_S \) and \( a_S \) from its asymptotic form. It is reminded that the incoming particle has \( \mu = 3 \), and the target particle has \( \mu = -3 \). To meet this requirement, we choose \( C_S = C_S 0, 3, -3/\(a_S - i b_S\)) \). With this choice, in the asymptotic region (say, \( r_1 \) is large while \( r_2 \) is small), the total wave function appears as

\[
\Psi \rightarrow \frac{1}{r_1 r_2} \phi_g(r_2) \left[ \sin(kr_1) \chi_3(1) \chi_{-3}(2) \right]
+ \sum_{\mu} f_\mu \exp(ikr_1) \chi_\mu(1) \chi_{-\mu}(2) \tag{4}
\]
where $$f_\mu = \sum_S C_{3,3,\mu}^{3,0} b_S a_S - i b_S C_{3,\mu,3,\mu}^{0}$$

where both even and odd S are included in the summation. $$f_\mu$$ is the s-wave scattering amplitude of the $$\mu$$-channel (i.e., the outgoing particle has spin component $$\mu$$, while the inner one has $$-\mu$$). The asymptotic form with a large $$r_2$$ is similar. From (4) we know that, in addition to the scattering by the potential, spin-flips might occur due to the spin-dependent interaction $$V_{12}$$. Incidentally, since $$C_S$$ contains the factor $$(a_S - ib_S)$$ and both $$a_S$$ and $$b_S$$ are proportional to $$h_S$$, $$\Psi$$ depends not at all on the set of constants $$b_S$$ chosen before.

We are interested in how the s-wave cross section of a $$\mu$$-channel $$\sigma_\mu \equiv 4\pi|f_\mu|^2/k^2$$ is affected by $$g_0$$. It was found that $$\sigma_3$$ (elastic channel without spin-flip) is much larger than other $$\sigma_\mu$$. When the cross section of pure potential-scattering $$\sigma_U$$ is considered as a unit, the ratio $$\sigma_3/\sigma_U$$ against $$g_0$$ is plotted in Fig.3. Four points are noted:

(i) The magnitude of $$\sigma_3$$ is in general close to $$\sigma_U$$. In particular, if $$g_0$$ is close to $$g_2$$, $$\sigma_3$$ would be very close to $$\sigma_U$$.

(ii) $$\sigma_3$$ depends sensitively on the potential parameter, because $$\sigma_U$$ does. It implies that an appropriate choice of parameters is crucial.

(iii) When the potential is narrower than the one leading to the optimal $$\sigma_U$$, if $$g_0$$ is smaller than $$g_2$$, a more negative $$g_0$$ would lead to a larger $$\sigma_3$$, while a more positive $$g_0$$ lead to a smaller $$\sigma_3$$ (refer to the dash curves of Fig.3). When the potential is broader, the effect of $$g_0$$ is in reverse (refer to the dash-dot-dot curves). However, when the parameter of the potential is optimized, a larger $$|g_0 - g_2|$$ would lead to a smaller $$\sigma_3$$ (refer to the bold curves).

(iv) The above qualitative feature does not depend on the details of the potential. This is explicit by comparing 3a and 3b, where distinct potentials are used. Thus, for selecting an appropriate potential, the crucial point is the understanding of the optimal parameter.

Incidentally, in all the cases of Fig.3 the ground state is deeply bound. For an example, when $$U_p(r)$$ has $$r_0 = 2.5$$, the ground state energy is -1.6294, while the first excited state is about 1 higher. Thus the gap is greatly larger than the bombarding energy $$k^2/2 \leq 0.02$$.

In Fig.4 $$\sigma_\mu/\sigma_3$$ against $$g_0$$ is plotted. Three points are noted:

(i) The cross-sections of spin-flip channels $$\sigma_\mu$$ are remarkably smaller than that of the non-spin-flip channel.

(ii) It is reminded that the three $$\Psi_S$$ with odd S are free from atom-atom interaction, therefore they have the same $$b_S/(a_S - ib_S)$$. Since $$\sum_S C_{3,3,\mu}^{0} C_{3,\mu,3,\mu}^{0} = (\delta_{\mu,3} - \delta_{\mu,-3})/2$$, where the summation covers only the three odd S, it is straight forward to prove $$f_{-\mu} = f_\mu$$ if $$\mu \neq \pm 3$$. Hence, the cases with $$\mu = -2$$ and -1 can not be seen in the figure.
(iii) Besides the non-spin-flip channel, the most important spin-flip channels would be the $\mu = \pm 2$ channels if $g_0$ is negative. However, if $g_0$ is positive, $\mu = 0$ channel would be a little more important, while $\sigma_{\pm 2}$ is the smallest. In particular, when $g_0 \approx g_0/2$, $\sigma_{\pm 2}$ is close to zero.

The features of Fig.4 are quite popular. When different potentials with different parameters are used, the qualitative features remain unchanged. This is shown in Fig.5 to be compared with Fig.3a. Note that, when $k$ varies, the optimal parameters of the potentials would vary accordingly.

In summary, a specific s-wave scattering of a pair of $^{52}$Cr atoms has been designed and studied theoretically. Different from the design of [2], both atoms are polarized but in reverse directions previously and no magnetic field is applied. The effect of $g_0$ on the scattering amplitudes without and with spin-flip has been predicted. Whether $g_0$ is smaller or larger than $g_2$ is found to be crucial to the qualitative features. In order to determine the unknown $g_0$, associated experiments are desirable.

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**APPENDIX A: MATRIX ELEMENTS OF THE DIPOLE-DIPOLE INTERACTION**

In this appendix the matrix elements of the dipole-dipole interaction between the total spin-states $(12)_{SM}$ of a pair of spin-3 atoms are given.

Making use of the spherical components of the spin-operator $F_1$ and $F_2$, we have

$$
\langle (12)_{S'M'} | V_{dd} | (12)_{SM} \rangle = -\frac{C_d}{3^2}252\sqrt{4\pi}C_{1,0,1,0}^0 \sqrt{2S' + 1}
$$

$$
\left\{ \begin{array}{c}
1 & 1 & 2 \\
3 & 3 & S' \\
3 & 3 & S'
\end{array} \right\} C_{2,M-M',S',M'}^S \sqrt{2} \hat{r} (A1)
$$

where the Clebsch-Gordan and 9-j symbols [10] are introduced, and $S + S'$ must be even. From this formula it is clear that $V_{dd}$ must cause a spatial relative rotation in d-wave together with a change of $S$ (the choices of $S'$ is $[S-2]$, $S$, and $S+2$).

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