Ultracold Atom-Atom Collisions in a Nonresonant Laser Field

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Using a recently developed approach for treating the three-dimensional anisotropic scattering we find considerable influence of a nonresonant laser field with intensity $I \geq 10^5$ W/cm^2 on the Cs-Cs ultracold collisions. Strong dependence on the laser wavelength λ_L is shown at the optical region as λ_L becomes shorter than the critical value $\lambda_0 \sim 3000$ nm (of the atomic de Broglie wave λ) defining the region $\lambda_0 \leq \lambda$ of the s-wave domination in the absence of the external field. Dependence on the laser polarization is also essential. The found effect can be applicable for controlling atom-atom interactions at ultralow temperatures.

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Ultracold collisions represent a very active research area at the intersection of several actual themes in atomic, molecular, and optical physics, and in condensed matter [1]. One of the important issues here is the study of possible controlling the atom-atom interaction of quantum gases for Bose-Einstein condensation (BEC) created thus far at ultralow temperatures [2]. Thus, several groups have discussed different possibilities for changing the atom-atom scattering length using near resonant lasers [3], radio frequency fields [4], Feschbach resonances induced by a magnetic field [5], and static electric fields [6,7]. However, it was shown [6,7] that in the presence of an external dc field the problem can be essentially anisotropic, developing strong coupling of the s wave with higher partial waves even at the zero-energy limit. That unusual scattering requires a special numerical technique.

In this Letter we consider the physics of ultracold atom-atom collisions in a nonresonant laser field

$$\mathbf{E} = (E/\sqrt{1+\gamma^2})[\,\mathbf{e}_z \cos(\mathbf{k}_L\mathbf{r} - \omega_L t) + \mathbf{e}_y \gamma \sin(\mathbf{k}_L\mathbf{r} - \omega_L t)], \tag{1}$$

where the wave vector $\mathbf{k}_L = k_L\mathbf{e}_x = \omega_L/c\mathbf{e}_x = 2\pi/\lambda_L\mathbf{e}_x$ is directed along the x axis and the polarization is defined by the ellipticity $0 \leq \gamma \leq 1$. In the quasistatic limit $k_L, \omega_L \to 0$ ($\lambda_L \to \infty$), we approach the case of the constant field $\mathbf{E} = E\mathbf{e}_z$ considered in Refs. [6,7]. In the present work the influence of the finiteness of the laser wavelength λ_L and the laser polarization on the scattering amplitude is analyzed. At that, we do not use the usual partial-wave technique. The method was suggested in Ref. [8] for solving nonseparable two-dimensional scattering problems. Here we extend the scheme to the three-dimensional scattering problem describing the relative atom-atom dynamics in an external field. Following [9] we use the basis of N spherical harmonics $Y_\nu(\hat{\mathbf{r}}_j)$ [$\nu = (lm) = 1, 2, \ldots, N$] defined on N grid points of the two-dimensional angular grid $\hat{\mathbf{r}}_j = \{\theta_j, \phi_j\}_1^N$ for reducing the initial Schrödinger equation to the system of differential equations

$$\sum_{j'}^{N}\left\{\left[-\frac{\partial^2}{\partial r^2} + 2MV(r,\hat{\mathbf{r}}_j) - k^2\right]\delta_{jj'} + \frac{1}{r^2}\sum_{\nu}^{N} Y_\nu(\hat{\mathbf{r}}_j)l(l+1)(Y^{-1})_{\nu j'}\right\}\psi(r,\hat{\mathbf{r}}_{j'}) = 0. \tag{2}$$

The values of the wave function $\psi(\mathbf{r})$ at the grid points of the angular space $\psi(r,\hat{\mathbf{r}}_j)$ are utilized in the spirit of the discrete-variable representation [10] or Lagrange-mesh method [11]. It drastically simplifies the calculations as against the usual partial-wave analysis. In fact, the atom-atom interaction $V(\mathbf{r})$, depending on the interatomic radius r and the relative atom-atom orientations $\hat{\mathbf{r}}_j$ with respect to the field $\mathbf{E}$, is a diagonal matrix in (2) and the diagonal elements $V(r,\hat{\mathbf{r}}_j)$ are simply the values of the potential $V(\mathbf{r})$ at the angular grid points. The only nondiagonal term is the angular part of the kinetic energy operator ($\sim 1/r^2$) where the coefficients $(Y^{-1})_{\nu j}$ are the matrix elements of the inverse of the matrix $Y_\nu(\hat{\mathbf{r}}_j)$. To the angular grid $\hat{\mathbf{r}}_j$ is associated a Gauss quadrature [9]. The high efficiency and flexibility of the scheme have been developed in calculations of bound states for strongly anisotropic interections $V(\mathbf{r})$ (the hydrogen atom in crossed magnetic and electric fields) [9,12].

To solve the scattering problem, we approximate the radial part of the kinetic energy operator in (2) with the finite differences and specify the boundary condition at the right edge of the radial grid r_ρ ($\rho = 0, 1, \ldots, m$) as

$$\psi(r_m,\hat{\mathbf{r}}_j) + q(k)\psi(r_{m-1},\hat{\mathbf{r}}_j) = g(k,\hat{\mathbf{k}}_n) \tag{3}$$

following the idea of [13] to utilize the scattering asymptotic at two last edge points $\rho = m-1$ and m:

$$f(k,\hat{\mathbf{k}}_n,\hat{\mathbf{k}}_j) = \exp\{-ikr_\rho\}\psi(r_\rho,\hat{\mathbf{r}}_j) - r_\rho \exp\{i(\mathbf{k}\mathbf{r}_\rho - kr_\rho\}. \tag{4}$$

In fact, by eliminating the scattering amplitude

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$f(k, \hat{\mathbf{k}}_n, \hat{\mathbf{k}}_j)$ from two asymptotic equations (4) we obtain the condition (3) with the coefficients

$$q(k) = -\exp\{ik(r_m - r_{m-1})\},$$
$$g(k, \hat{\mathbf{k}}_n) = r_m \exp\{i\mathbf{k}\mathbf{r}_m\} - r_{m-1}\exp\{i(\mathbf{k}\mathbf{r}_{m-1} + k(r_m - r_{m-1})\}. \quad (5)$$

The reduction to the finite-difference boundary-value problem permits one to apply powerful computational methods. Specifically, we use LU decomposition which is stable and efficient in our case. Solving the problem (2) and (3) for the initial wave vector $\mathbf{k} = (k, \hat{\mathbf{k}}_n)$ (possible orientations of $\hat{\mathbf{k}}$ are created by the angular grid $\hat{\mathbf{k}}_n = \{\theta_n \phi_n\}_1^N$) first we calculate the vector function $\psi(r_\rho, \hat{\mathbf{r}}_j)$ and then, by using the asymptotic (4), nth row of the scattering amplitude matrix $f(k, \hat{\mathbf{k}}_n, \hat{\mathbf{k}}_j)$ describing the transitions $(k, \hat{\mathbf{k}}_n) \to (k, \hat{\mathbf{k}}_j)$, where $j = 1, \ldots, N$.

We have analyzed with this approach the Cs-Cs ground state collisions in the laser field (1) using the two-terms atom-atom potential $V(r, \hat{\mathbf{r}}_j) = V(r) + V_E(r, \hat{\mathbf{r}}_j)$ with the spherically symmetric field-independent part $V(r) \underset{r\to\infty}{\longrightarrow} -C_6 r^{-6}\zeta(r - r_C)$ suggested in [14]. The model potential $V(r)$ was applied for evaluating effects of a static field in Ref. [6]. It was noted [6] that with this model one can reproduce the results close to the actual scattering data and generate a broad spectrum of values for the scattering length a_0 by slightly changing the cutoff radius r_C. For the anisotropic field-dependent interaction $V_E(r, \hat{\mathbf{r}}_j)$ we have used the dipole-dipole induced interatomic potential [15]

$$V_E(r, \hat{\mathbf{r}}_j) = -\frac{\alpha^2(\omega_L)E^2}{2(1+\gamma^2)r^3}\left\{\frac{3(z_j^2 + \gamma^2 y_j^2)}{r^2} - 1 - \gamma^2\right\} \times \cos(k_L x_j)\{\cos(k_L r) + (k_L r)\sin(k_L r)\} \times \zeta(r - r_C), \quad (6)$$

yielding the strong coupling at the large interatomic separation $r \to \infty$. We define the region $r \geq r_C$ of the potential $V_E(r, \hat{\mathbf{r}}_j)$ action by the cutoff function $\zeta(r - r_C)$ introduced in Ref. [14] for matching the long-range part in $V(r)$. Here we consider a low-frequency nonresonant case with a constant coefficient $\alpha(\omega_L)$ coinciding with the static dipole polarizability $\alpha(0)$ of the Cs atom and keep in (6) only the main terms with respect to $(k_L r)$ [15]. (A time average over the period of the laser $T = 2\pi/\omega_L$ has been performed.)

First, to test the convergence of the scheme and to have a possibility of direct comparison with the previous calculation [6] we analyze the static regime $k_L = 0$ ($\lambda_L = \infty$), $\gamma = 0$ with the field-dependent part $2V_E(r, \hat{\mathbf{r}}_j, k_L = \gamma = 0)$. We have considered two different model interactions $V(r)$(defined by the different r_C): a resonant interaction generating $a_0 = -2120$ a.u. ($r_C = 23.1245$ a.u.) and a nonresonant case with $a_0 = 1.98$ a.u. ($r_C = 23.19$ a.u.). The total cross sections have been calculated by the numerical integration over the scattering angles $\hat{\mathbf{k}}_j$ and averaging over the possible initial orientations $\hat{\mathbf{k}}_n$,

$$\sigma(k) = \frac{1}{4\pi}\sum_{n,j}^{N} |f^B(k, \hat{\mathbf{k}}_n, \hat{\mathbf{k}}_j)|^2 w_n w_j,$$
$$f^B(k, \hat{\mathbf{k}}_n, \hat{\mathbf{k}}_j) = (1/\sqrt{2})[f(k, \hat{\mathbf{k}}_n, \hat{\mathbf{k}}_j) + f(k, \hat{\mathbf{k}}_n, -\hat{\mathbf{k}}_j)], \quad (7)$$

where w_n and w_j are the weights of a Gauss quadrature. We have symmetrized the amplitude f^B to compare with the case of two colliding bosonlike Cs atoms [6]. The boundary of integration was chosen rather far, at $r_m = 10^4$ a.u., to obtain the convergent result for the amplitudes at zero-energy limit. The calculations have been performed on the three-dimensional grids $\{r_\rho, \theta_j, \phi_j\}_{\rho,j=1}^{m,N}$ with $N = 3\times3 = 9$, $5\times5 = 25$, and $7\times7 = 49$ angular and $m = 10^4$ radial grid points defined in [9,16], respectively. The result presented in Fig. 1 demonstrates the fast convergence over N for both cases with $a_o = -2120$ and 1.98 a.u. in all the range of the field alteration. The achieved accuracy has the order of $\sim10^{-4}$ for $f(k, \hat{\mathbf{k}}_n, \hat{\mathbf{k}}_j)$ as $N \geq 25$. We compare our result with a partial-wave analysis [6] available for the resonant case $a_0 = -2120$ a.u. Both results converge one to another as $N \geq 25$ for all the $E \leq 700$ kV/cm except the small region $E > 600$ kV/cm of the strongly anisotropic scattering [6].

In the limiting case of the static field $\mathbf{E} = E\mathbf{e}_z$ the ϕ variable may be separated. However, for a finite value of the laser wavelength λ_L we have the nonseparable three-dimensional problem. Figure 2 illustrates the analysis of the Cs-Cs scattering in the presence of the laser field of intensities $I = cE^2/(8\pi) \leq 1.5 \times 10^9$ W/cm^2 with varying λ_L. A rather regular atom-atom interaction $V(r)$ generating $a_0 = 1.98$ a.u. was considered. It was found that dependence on the λ_L becomes essential as

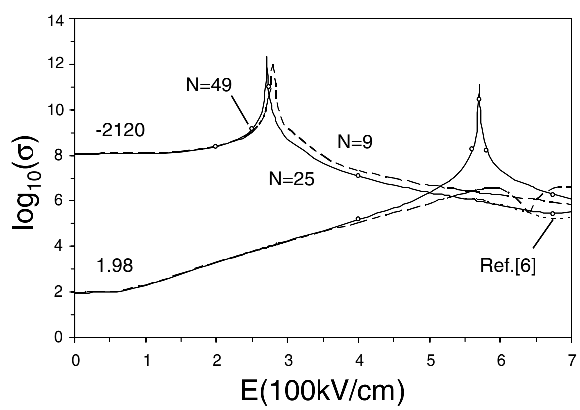

FIG. 1. The logarithm of the total scattering cross sections calculated at $k = 5.5 \times 10^{-6}$ a.u. ($T = 37.4$ pK) as a function of the electric field in the static regime $k_L = 0$ ($\lambda_L = \infty$) for two different interatomic potentials labeled by the value of the scattering length a_0 in the absence of the field. The convergence with respect to N is shown: $N = 9$ (dashed curves), $N = 25$ (solid curves), and $N = 49$ (open circles). The result of Ref. [6] (dotted curve) is also given for the case $a_0 = -2120$ a.u. (Atomic units are used for cross sections and scattering lengths.)

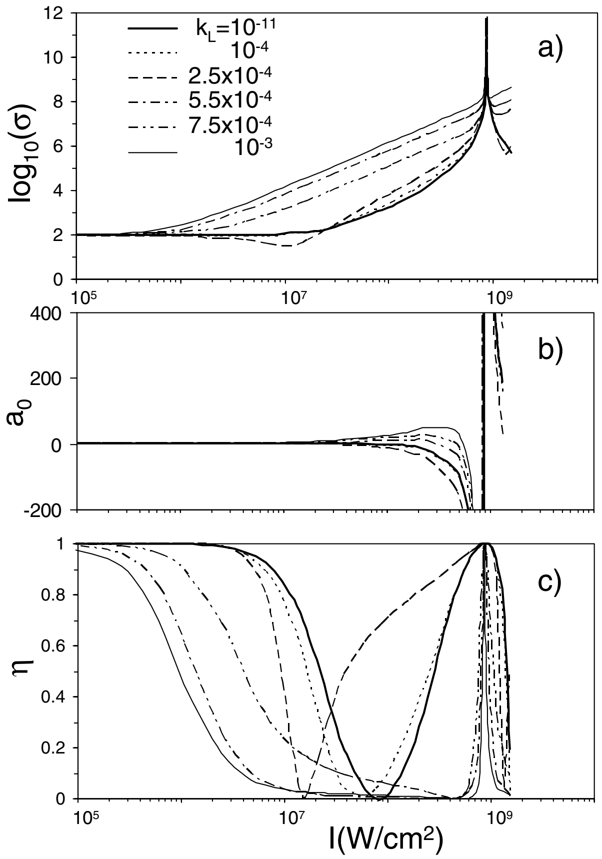

FIG. 2. The dependence of the logarithm of the total cross section $\sigma(k, k_L, I)$ (a), the scattering length $a_0(k, k_L, I)$ (b), and the anisotropy parameter $\eta(k, k_L, I)$ (c) on the field intensity $I = cE^2/8\pi$ for a few laser wave numbers k_L. The calculations were performed at $k = 5.5 \times 10^{-6}$ a.u. ($T = 37.4$ pK) and $\gamma = 0$. (The calculated values are given in atomic units.)

$\lambda_L = 2\pi/k_L \leq 6.28 \times 10^4$ a.u. ($k_L \geq 10^{-4}$ a.u.) already for the fields of intensities $I = cE^2/(8\pi) \geq 10^5$ W/cm^2 ($E \geq 15$ kV/cm). Note that we do not use the partial-wave analysis; i.e., the scattering amplitude $f(k, \hat{\mathbf{k}}_n, \hat{\mathbf{k}}_j)$ is calculated directly on the angular grids $\{\hat{\mathbf{k}}_n\}_1^N, \{\hat{\mathbf{k}}_j\}_1^N$. However, for investigating the anisotropy effects it is convenient to introduce the s-wave scattering length by transforming the calculated amplitude to the conventional lm representation

$$a_0(k) = -[1/(4\sqrt{2}\pi)] \times \sum_{n,j}^{N} f^B(k, \hat{\mathbf{k}}_n, \hat{\mathbf{k}}_j) Y_{00}(\hat{\mathbf{r}}_n) Y_{00}^*(\hat{\mathbf{r}}_j) w_n w_j \underset{k\to 0}{\longrightarrow} a_0 \quad (8)$$

and the anisotropy parameter $\eta(k, k_L, I) = 8\pi a_0^2(k, k_L, I)/\sigma(k, k_L, I)$ such that $\eta \to 1$ as I and $k \to 0$. The calculated $a_0(k_L, I)$ and $\eta(k_L, I)$ are presented in Figs. 2(b) and 2(c). They show that the singularity developed in Fig. 2(a) in the total cross section at the field $I = 8.66 \times 10^8$ W/cm^2 ($E_r = 570$ kV/cm) is the s-wave resonance. It is also shown that with increasing k_L (decreasing λ_L) the s-wave width of the resonance becomes more narrow, but the total width remains practically unchanged due to increasing anisotropic effects.

Figure 3 presents the result of the analysis of the critical region $\lambda \geq \lambda_0$ ($k \leq k_0 = 2\pi/\lambda_0$) for the atomic de Broglie wavelengths λ where the Cs-Cs scattering is isotropic $\sigma(k) = 8\pi a_0$ [$\eta(k) = 1$] in the absence of the external field ($I = 0$). Applying the field of intensity $I > 10^5$ W/cm^2 alters the scattering dramatically: it becomes strongly anisotropic [$\eta(k, k_L, I) < 1$] even in the region $k \leq k_0 \simeq 10^{-4}$ a.u. ($\lambda \geq \lambda_0 \simeq 6.28 \times 10^4$ a.u.) where the s wave dominates at $I = 0$. The anisotropy parameter $\eta(k, k_L, I)$ can be changed by varying the laser parameters (I and λ_L) but remains, nevertheless, a constant, k-independent value in this specific region. Thus, the s-wave scattering length approximation does not work even for the zero-energy limit in the presence of a laser radiation for the special field intensities and the wavelengths. We already noted that the special effect of the strong lm coupling at zero-energy limit has been discussed in [6] for a static field. However, this regime demands an application of rather intense static (or quasistatic laser) fields: $\sim$1–3 $\times 10^5$ V/cm ($\sim 10^7$–10^8 W/cm^2) (see Figs. 1 and 2 and Ref. [6]). Figure 2 demonstrates that with decreasing the length λ_L of the laser wave the demand on the field intensity becomes essentially less strong $E \geq 10^4$ V/cm ($I \geq 10^5$ W/cm^2).

It should also be noted that the dependence on the λ_L becomes considerable already for rather long waves with $\lambda_L \leq 10^5$ a.u. ($k_L \geq 10^{-4}$ a.u.) (see Fig. 2). It is, however, not surprising because the wavelength λ_L of the laser radiation specifies the length of "modulation" of the long-range part (6) of the atom-atom interaction defining the scattering at ultralow energies. Thus, by decreasing the modulation length one can violate the quasistatic regime as λ_L approaches and becomes shorter the de Broglie wavelength λ. Figure 2 illustrates the ultracold collisions with $\lambda = 1.14 \times 10^6$ a.u. where the quasistatic regime is considerably violated as λ_L becomes shorter $2\pi/k_L \simeq 10^5$ a.u. Note also that the critical laser wavelength $\sim 10^5$ a.u. is close to the critical de Broglie wavelength

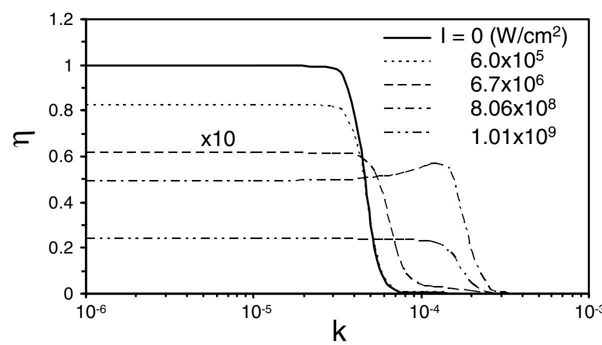

FIG. 3. The dependence of the anisotropy parameter $\eta(k, k_L, I)$ on the relative colliding momentum k (in a.u.) for a few different intensities I of the laser field. The calculations were performed for $k_L = 5.5 \times 10^{-4}$ a.u. ($\lambda_L = 604$ nm) and $\gamma = 0$.

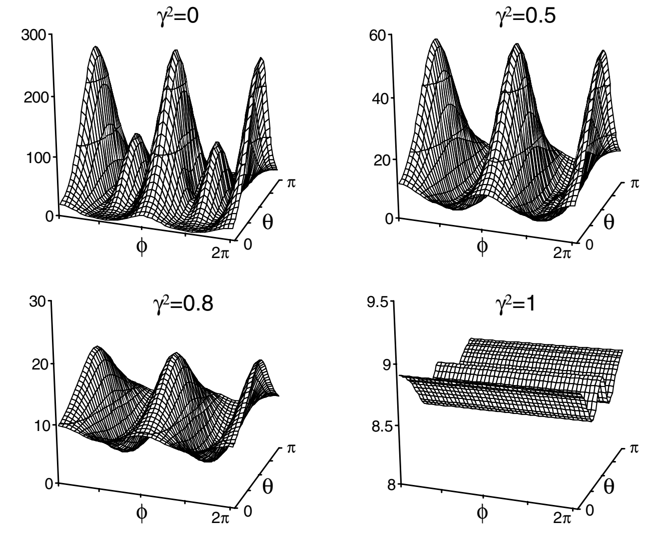

FIG. 4. The differential cross sections as a function of the scattering angles θ and ϕ for different polarizations. The calculations were performed for the field with $I = 1.07 \times 10^6$ W/cm^2 ($E = 28$ kV/cm), $k_L = 5.5 \times 10^{-4}$ a.u. ($\lambda_L = 604$ nm) at $k = 5.5 \times 10^{-6}$ a.u. ($T = 37.4$ pK). (Cross sections are given in atomic units.)

$\lambda_0 = 2\pi/k_0 \simeq 2\pi \times 10^4$ a.u. $\simeq 3300$ nm defining the range of the s-wave domination as $I = 0$ (see Fig. 3).

Figure 4 demonstrates strong dependence of the differential Cs-Cs cross sections on the laser polarization for the chosen I and λ_L. Here the averaging over the possible initial orientations of the interatomic axis was performed. The calculation has been done for the laser propagation along the z direction. In this case, by changing from the linear ($\gamma = 0$) to the circular ($\gamma = 1$) polarization the ϕ dependence in the scattering is excluded. The anisotropy effects are less important for the circular polarization ($\gamma = 1$). The differential cross section has two weak maximums (of the order of a few percent above the mean value) in the direction of the laser propagation (z axis) and on the plane of the polarization ($\theta = \pi/2$). With decreasing γ we observe the appearance of a new structure over the ϕ variable. The maximum anisotropy is developed for the linear polarization ($\gamma = 0$). The differential cross section is changing here from zero up to a maximal value about 300 a.u. in the direction of polarization (x axis). However, in spite of this strong anisotropy the correspondent total cross section deviates from the field free case only by a factor of 1.8 and the anisotropy parameter is equal $\eta = 0.613$ (see Fig. 2).

The performed analysis shows that applying a nonresonant optical laser with intensities $I \geq 10^5$ W/cm^2 one can change essentially the Cs-Cs scattering amplitude at ultracold collisions. At that, the usual scattering length approach $f^B(k, \hat{\mathbf{k}}_n, \hat{\mathbf{k}}_j) = -a_0$ does not work (except the regions of s-wave resonances) and one has to analyze the stability of BEC for unusual behavior of the amplitude $f^B(k, \hat{\mathbf{k}}_n, \hat{\mathbf{k}}_j) = f^B(\hat{\mathbf{k}}_n, \hat{\mathbf{k}}_j)$. Figure 4 illustrates that the amplitude may be strongly dependent on the relative atom-atom orientation with respect to the field and even changes the sign at some scattering angles. It would be interesting to include this effect into the theoretical models for BEC. We suppose that experimental investigations of the ultracold atom-atom collisions in the presence of intense optical lasers would be also valuable, maybe opening new physics here. Note also that earlier calculations [3] of the resonant laser effects in ultracold atom-atom collisions were limited by the framework of the s-wave scattering length and, with increasing the laser intensity, has to be extended to include important anisotropic effects.

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