Quantum suppression of cold atom collisions

R. Côté,
Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, Massachusetts 02138

E. J. Heller
Harvard-Smithsonian Center for Astrophysics and Department of Physics, 17 Oxford Street, Cambridge, Massachusetts 02138

A. Dalgarno
Department of Astronomy and Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, Massachusetts 02138

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Very-low-energy collisions between two atoms are usually suppressed, in that the probability of close approach of the atoms becomes greatly reduced as the collision energy vanishes, even if the potential is completely attractive (with the exception of the Coulomb interaction). The suppression is a quantum effect, related to the Wigner threshold law. It is gauged by comparing the ratio of the probability of being inside the well to the probability of being outside for both the classical and quantum regimes. As the asymptotic kinetic energy vanishes, the approaching atoms reach a minimum distance of typically 20 or 30 a.u. Here we study attractive interaction potentials of the form $-\alpha/r^n$, and give some numerical results for accurate $X\ ^1\Sigma_g^+$ and $a\ ^3\Sigma_u^+$ states of Li_2 and Na_2 molecules. We show that in some circumstances it is possible to use Wentzel-Kramers-Brillouin theory in the suppression regime (where it fails) and to correct for its failure with a simple factor.

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I. INTRODUCTION

Collisions of atoms at ultralow temperatures are a critical issue in Bose-Einstein condensation, high precision atomic measurements, coherent atomic sources, and the operation of atomic traps. In this paper we draw attention to a simple but dramatic effect which suppresses contact between atoms at very low energies and which may help in the control of trap dynamics. The effect (sometimes called ''quantum reflection'') is well known in the collision of an atom with a surface. At very low energies, the atom never enters the attractive well and is instead reflected at long range even for an interaction that is purely attractive at the large distances where reflection occurs [1–5]. This conclusion can be modified when many-body effects are included. The suppression may be relevant to collisions of atoms with superfluid Helium surfaces, where it leads to a reduction in the chances of atom-surface sticking at low energies [6,7].

A correct quantum calculation of low-energy atom collisions necessarily incorporates the suppression effects [8]. For example, the collision suppression effect is intimately related to the well-known Wigner threshold law for s-wave inelastic scattering [9]. It is nonetheless instructive to compare the classical, semiclassical, and quantum descriptions in order to clarify the nature of the suppression and to develop an understanding of the subtle consequences of suppression in many-body collision systems. In the context of atomic collisions, this point of view was taken earlier by Julienne and Mies [10], and further developed in Ref. [11]. As in the case of the tunnel effect, diffraction, and Anderson localization, quantum collision suppression is a concept that derives its utility by comparison with classical mechanics.

The word ''suppression,'' like tunneling, has come to be used for a variety of related phenomena. Suppression entails some form of exclusion of amplitude from certain regions. The collisional suppression we consider here does not, however, shut down inelastic processes at low energy. Indeed, the threshold $\sqrt{E}$ suppression of the radial wave function translates into the usual result that threshold inelastic cross sections diverge as $1/\sqrt{E}$, leading to inelastic rates that become constant at low temperature.

Our purpose here is to extend previous studies of quantum suppression, to make simple physical pictures of the suppression (which can be found also in Ref. [11]), to develop a simple correction factor that can be applied to the semiclassical description of scattering at low energies, and to report the results of explicit calculations for the ^{7}Li-^{7}Li and ^{23}Na-^{23}Na systems based on accurate molecular potential-energy curves.

II. THEORY OF THE SUPPRESSION

A. Qualitative picture

Suppose the atomic interaction potential is attractive at large distances with a repulsive wall at small distances. In classical scattering at low energies E, the head-on approach of the two atoms takes place slowly but the atoms continue their journey toward a collision that occurs when they reach the repulsive wall. The atoms hit the wall with a probability of unity. In quantal scattering, the probability of the atoms penetrating into the attractive well and continuing to the repulsive wall diminishes to zero as $E\rightarrow 0$. Even in s-wave head-on collisions, the two atoms do not approach closely. This statement requires modification for potentials decreasing as r^{-2} or slower and for the case when a bound state of the potential exists at zero energy. The suppression is a quantum-mechanical reflection of the amplitude by the as-

ymptotic tail of the potential. It may be demonstrated by the simple case of the attractive square well. If D is the well depth, μ is the reduced mass of the particle, and a is the width of the well, the s-wave function inside the well normalized to unit incoming flux is given in the limit of vanishing wave number k by

$$u(r)=\frac{2}{k'\cos(ka)}\sqrt{\frac{\mu}{\hbar}}k^{1/2}\sin(k'r), \tag{1}$$

where $k'=\sqrt{2\mu D/\hbar^2}$. Treating the sine wave as two traveling waves, the ratio R of the flux inside the well to the flux outside, which classically is unity, is instead

$$R=\frac{k'k}{k'^2\cos^2(k'a)+k^2\sin^2(k'a)}. \tag{2}$$

Normally, if $\cos(k'a)\neq 0$,

$$R\rightarrow\frac{k}{k'\cos(k'a)}, \tag{3}$$

which means the inside flux is suppressed as $\sqrt{E}$ as $E\rightarrow 0$. It might seem that the square well is peculiar because of its abrupt edge, but even a smooth potential becomes very sharp on the scale of a wavelength as $E\rightarrow 0$.

One of the exceptions to the suppression is the possibility of a bound state existing exactly at threshold ($E=0$). This is seen in the formula for R when $\cos(k'a)=0$. If such a threshold bound state is pushed up or down only slightly, suppression is restored, but to see it one has to get very close to $E=0$. This effect is easily explored with the help of Eq. (2).

Another instructive example is a simple one-dimensional step-down potential. This potential naturally has no complications from bound-state resonances. In the case of a smooth step down $V(r)=A-A/[1+\exp(r)]$ it can be shown that the transmission probability of a plane wave over the ''cliff'' of energy E incident from the left is, for small E,

$$T=4\sqrt{2}\pi\coth(\pi\sqrt{2A})\sqrt{E}, \tag{4}$$

where $m=\hbar=1$. (This can be deduced from a discussion in Ref. [12].) Classically, the transmission probability is always unity at any positive energy. The fundamental cause of the suppression is seen in this example as the reduction of transmission past a purely attractive ledge. The ratio of the quantum to the classical probability for finding the particle to the right of the step vanishes as $\sqrt{E}$.

B. Classical and semiclassical theory

Classically, the ratio of the probability density per unit distance of finding the particles inside and outside the well is equal to the inverse ratio of the speeds. If v_∞ is the incident velocity and v is the velocity at the deepest point of the well, the ratio is given by

$$K_{\rm cl}=\frac{v_\infty}{v}=\left(\frac{E}{E+D}\right)^{1/2}, \tag{5}$$

which for low values of $k=2\mu v/\hbar$ becomes

$$K_{\rm cl}=\frac{\hbar k}{\sqrt{2\mu D}}\left(1-\frac{\hbar^2k^2}{4\mu D}+\cdots\right). \tag{6}$$

In the semiclassical description, the amplitude is decomposed into incoming and outgoing terms, each of which has the square root of the classical probability density as a prefactor. The two terms combine to give interference oscillations but after squaring the wave function and averaging over the oscillations the classical probability density is recovered. The semiclassical or Wentzel-Kramers-Brillouin (WKB) scattering wave function in a potential $V(r)$ is

$$u_{\rm WKB}(r)=\frac{C}{\sqrt{p(r)}}\sin[\phi(r)+\pi/4], \tag{7}$$

where

$$p(r)=\left\{\frac{2\mu}{\hbar^2}[E-V(r)]\right\}^{1/2}, \tag{8}$$

$$\phi(r)=\frac{1}{\hbar}\int_{r_0(E)}^{r}p(r')dr', \tag{9}$$

and $r_0(E)$ is the inner distance of closest approach and C is a normalization constant.

Near the equilibrium distance r_e of an attractive well, the wave function $|u^{\rm in}_{\rm WKB}|$ will reach a local maximum; this local maximum will act as a reference amplitude for comparison with the external amplitude. Suppose this maximum is reached at $r^*_{\rm in}$; then $\sin[\phi(r^*_{\rm in})+\pi/r]=\pm 1$ and,

$$u^{\rm in}_{\rm WKB}=u_{\rm WKB}(r^*_{\rm in})=\frac{C}{\sqrt{p(r^*_{\rm in})}}, \tag{10}$$

where, because energy is close to zero, we may take $p(r^*_{\rm in})=\sqrt{-2mV(r^*_{\rm in})}$. At large distance we have

$$u^{\rm out}_{\rm WKB}=\frac{C}{\sqrt{\hbar k}}\sin(kr+\eta_{\rm WKB}), \tag{11}$$

where $\eta_{\rm WKB}$ is the semiclassical approximation to the phase shift. The semiclassical density ratio is

$$K_{\rm sc}=\frac{|u^{\rm in}_{\rm WKB}|^2}{|u^{\rm out}_{\rm WKB}|^2}=\frac{\hbar k}{p_e}=\left(\frac{E}{E+D}\right)^{1/2}, \tag{12}$$

identical to the (incorrect) classical result. Thus suppression requires a breakdown of the WKB approximation, as first pointed out by Julienne and Mies [10,11].

C. Breakdown of the semiclassical theory

The semiclassical WKB approximation is accurate when the wavelength undergoes little change in a wavelength. Thus we need the condition

$$\epsilon_{\rm WKB}=\hbar\frac{|p'(r)|}{p(r)^2}\ll 1 \tag{13}$$

for WKB to work. We show in Fig. 1 the WKB error $\epsilon_{\rm WKB}$ for the Morse potential

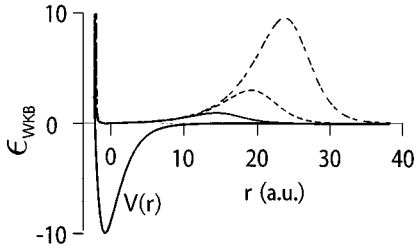

FIG. 1. A plot of the WKB error term as a function of coordinate for three low energies: $E=0.05$ a.u. (solid), $E=0.005$ a.u. (dashed), and $E=0.0005$ a.u. (dash-dot).

$$V(r)=10[1-\exp(-r)]^2-10, \tag{14}$$

(with $m=\hbar=1$) for three different energies, $E=0.05$, 0.005, 0.0005. A similar figure was given by Julienne and Mies [10] for the collision of two He(^3S) atoms. The error increases with lower energy and extends to larger radii, pointing to the region where the suppression originates. Proceeding outward at small r and passing through the inner turning point (at which the WKB approximation fails but is easily corrected), the wave function enters the well. Inside the entire well region well the WKB wave function is accurate. As it moves towards the asymptotic region, it breaks down for low energies, but eventually regains its accuracy as it reaches still larger distances. Because of the breakdown region, the asymptotic WKB solution has the wrong amplitude and phase. This error is the harbinger of the suppression phenomenon.

D. Quantum suppression

The partial-wave equation for zero-angular-momentum scattering of a particle of mass μ by a potential $V(r)$ is

$$\frac{d^2u(r)}{dr^2}+\left[k^2-\frac{2\mu V(r)}{\hbar^2}\right]u(r)=0, \tag{15}$$

such that $u(0)=0$. It is convenient to normalize $u(r)$ to the asymptotic form

$$u^{\text{out}}(r)\sim\frac{\sin(kr+\eta)}{\sin\eta}, \tag{16}$$

so that in the zero energy limit

$$u^{\text{out}}(r)\sim 1-r/a, \tag{17}$$

where a is the scattering length. The quantum ratio of the probability densities is given by

$$K_{\text{qm}}=\frac{|u^{\text{in}}(r^*_{\text{in}})|^2}{|u^{\text{out}}(r^*_{\text{out}})|^2}\equiv|u^{\text{in}}|^2\sin^2\eta, \tag{18}$$

where we have used a large exterior reference radius r^*_{out} such that $\sin(kr^*_{\text{out}}+\eta)=\pm 1$, and where we have dropped the argument (r^*_{in}). Provided that the potential falls off faster than r^{-5}, we can use effective range theory [13] to write Eq. (18) as

$$K_{\text{qm}}=|u^{\text{in}}|^2\frac{k^2}{k^2+\left(\frac{1}{a}-\frac{1}{2}\rho k^2\right)^2}, \tag{19}$$

$$=a^2|u^{\text{in}}|^2k^2[1+ak^2(\rho-a)+\cdots], \tag{20}$$

where ρ is the effective range. The ratio of the quantum-mechanical probability of entering the well to the semiclassical probability Eq. (5) is given by

$$P=\frac{K_{\text{qm}}}{K_{\text{sc}}}\approx\frac{2\mu}{\hbar^2}a^2|u^{\text{in}}|^2\sqrt{D+E}\sqrt{E}\times\left[1+\frac{2\mu Ea}{\hbar^2}(\rho-a)+\ldots\right], \tag{21}$$

as $E\to 0$.

We now demonstrate that the amplitude of the inner wave function is independent of E as $E\to 0$. Following Gribakin and Flambaum [14], we obtain an analytical expression for $u^{\text{in}}(r)$ by solving the s-wave scattering Eq. (15). We use the WKB approximation for scattering in an attractive potential that varies at large distances as $-\alpha r^{-n}$. At $E=0$ the condition Eq. (13) for the validity of the WKB approximation in this case is

$$r\ll\left(\frac{2\gamma}{n}\right)^{2/(n-2)}, \tag{22}$$

where $\gamma=\sqrt{2\mu\alpha/\hbar^2}$. For ^{7}Li, $n=6$ and $\gamma=4213$ a.u., hence we must have $r\ll 37a_0$ to be in the ''safe'' zone for WKB. The ^{7}Li potential-energy curve retains its long-range form into separations r^* much less than $37a_0$, so that there is a large region of r where the WKB approximation is valid and the potential varies as r^{-6}. The WKB approximation is also valid within the potential well and we can write the zero-energy wave function in the form

$$u^{\text{in}}(r)=\frac{C}{\sqrt{p_0(r)}}\sin\left(\frac{1}{\hbar}\int_{r_0}^{r}dr'p(r')+\pi/4\right),\quad r>r_0, \tag{23}$$

where $r_0=r_0(0)$ is the inner classical turning point and $p_0=\sqrt{-2\mu V(r)}$. The normalization constant C is chosen so that both $u^{\text{in}}(r)$ and $u^{\text{out}}(r)$ match at r^*. By extending the Gribakin and Flambaum analysis (see Appendix), we find that

$$C=\frac{\sqrt{\hbar}}{\cos(\Phi-r^*-\pi/4)}\left\{\frac{\Gamma(1+\nu)}{\sqrt{\pi\nu}(\gamma\nu)^\nu}\cos(r^*-\pi\nu/2-\pi/4)-\frac{\Gamma(1-\nu)(\gamma\nu)^\nu}{a\sqrt{\pi\nu}}\cos(r^*+\pi\nu/2-\pi/4)\right\}, \tag{24}$$

where $\nu=1/(n-2)$, $x=2\gamma\nu r^{-1/2\nu}$, and $\Phi=\phi(r^*)+x^*$ evaluated at zero energy. Then near the equilibrium distance r_e,

$$u^{\text{in}}=-\frac{\sqrt{\hbar}}{a}\frac{\Gamma(1-\nu)(\gamma\nu)^\nu}{\sqrt{\pi\nu}(2\mu D)^{1/4}}\frac{\sin(\pi\nu)}{\cos(\Phi-\nu\pi/2)}. \tag{25}$$

TABLE I. Phase shift and inner amplitude as a function of the kinetic energy.

	$X^1\Sigma_g^+$		$a^3\Sigma_u^+$	
$\log_{10}E$	η	$\lvert u^{\rm in}_{\rm exact}\rvert$	η	$\lvert u^{\rm in}_{\rm exact}\rvert$
		Li_2		
−9.0	−0.132 945	0.032 457 6	0.055 288	0.310 242 8
−10.0	−0.041 795	0.032 966 9	0.019 194	0.290 084 0
−11.0	−0.013 206	0.033 025 2	0.006 130	0.288 043 1
−12.0	−0.004 176	0.033 031 3	0.001 940	0.287 835 3
		Na_2		
−9.0	−0.240 411	0.029 065 6	−0.500 465	0.040 283 7
−10.0	−0.072 210	0.032 119 0	−0.158 352	0.044 769 2
−11.0	−0.022 644	0.032 565 3	−0.050 039	0.045 276 0
−12.0	−0.007 153	0.032 615 9	−0.015 822	0.045 329 7

Equation (25) shows that with the normalization Eq. (17), $u^{\rm in}(r^*_{\rm in})$ is independent of E at low E. Therefore, the ratio P of the quantum mechanical to the semiclassical probability of finding the particle in the inner well tends to zero as $E^{1/2}$, a result that is consistent with the conclusions of Clougherty and Kohn [4] for atom-surface scattering, including (in their case) inelastic processes. Inserting Eq. (25) into Eq. (21) we can write P as

$$P=P_0E^{1/2}\left[1+\frac{2\mu Ea}{\hbar^2}(\rho-a)+\cdots\right], \tag{26}$$

with

$$P_0=\left(\frac{2\mu}{\hbar^2}\right)^{1/2}\frac{[\Gamma(1-\nu)]^2(\gamma\nu)^{2\nu}}{(2\mu D)^{1/2}}\,\frac{\sin^2(\pi\nu)}{\cos^2(\Phi-\pi\nu/2)}. \tag{27}$$

The lone exception is a zero-energy bound state, where the factor $\cos(\Phi-\nu\pi/2)$ vanishes as the scattering length a blows up as $E\to 0$, giving an energy dependence to Eq. (25). The wave function accumulates in the inner well at threshold resonances because once amplitude is "captured," it is difficult to escape. For some purposes it is useful to think of the suppression effect as a penetrable barrier potential that normally reflects amplitude, except if there is a quasibound state (resonance) inside the barrier.

III. SCATTERING: THE ALKALI-METAL ATOMS

In this section we calculate the suppression effect for ^{7}Li-^{7}Li and ^{23}Na-^{23}Na, collisions for which accurate potential-energy curves have been constructed [15]. The partial wave equations were solved by numerical integration. In Table I, we give the magnitude $\lvert u^{\rm in}\rvert$ of the inner wave function evaluated near the deepest point of the wells for the four potential-energy curves. As predicted, the wave function is nearly independent of the energy of relative motion. In Table II we compare the magnitude $\lvert u^{\rm in}\rvert$ of the inner wave function determined numerically from Table I for $\ln E=10^{-12}$ a.u. with the results of the analytical formula Eq. (25), for $E=0$. The agreement demonstrates the utility of Eq. (26). In Figs. 2 and 3, we compare the numerical and analytical results for the suppression factor in the form $R=P^{-1}$. The calculated R includes the second terms of the expansion Eq. (26). The agreement is close. Both sets of results demonstrate the dramatic rise in suppression as the energy decreases below 10^{-10} a.u. or, equivalently, 30 μK.

IV. PHOTOABSORPTION AND THE FACTORIZATION APPROXIMATION

Photoabsorption of radiation by colliding alkali-metal atoms has been the subject of considerable experimental and theoretical attention [18,19]. Provided the intensity of the radiation field is not high, the concepts behind the suppression factor P suggests an approximate factorization

$$\sigma_{\rm abs}=P\sigma_{\rm WKB}, \tag{28}$$

TABLE II. Inner amplitude $\lvert u^{\rm in}\rvert$ determined from Eq. (25) for zero-energy ($n=6,\nu=\frac{1}{4}$) compared to the Table I numerical results $\lvert u^{\rm in}_{\rm exact}\rvert$ at $\ln E=10^{-12}$. All quantities are in atomic units.

	Li_2		Na_2	
	2μ = 12 798.391		2μ = 41 907.7602	
	α = 1388		α = 1472	
	γ = 4213.274		γ = 7854.185	
Quantity	$X^1\Sigma_g^+$	$a^3\Sigma_u^+$	$X^1\Sigma_g^+$	$a^3\Sigma_u^+$
a	36.9	−17.2	34.94	77.3
ρ	66.5	1014.8	187.5	62.5
D	$3.880\,46\times10^{-2}$	$1.519\,063\times10^{-3}$	$2.743\,835\,9\times10^{-2}$	$7.931\,798\times10^{-4}$
Φ	$42\pi+0.204\,218$	$11\pi+1.389\,241$	$66\pi+0.5506$	$15\pi+2.8548$
$\lvert u^{\rm in}\rvert$	0.0325 2	0.2885 2	0.0318	0.0455
$\lvert u^{\rm in}_{\rm exact}\rvert$	0.0330 3	0.2878 4	0.032 62	0.045 33
$P_0=R_0^{-1}$	3 632.673	12 275.733	9 343.428	15 967.447

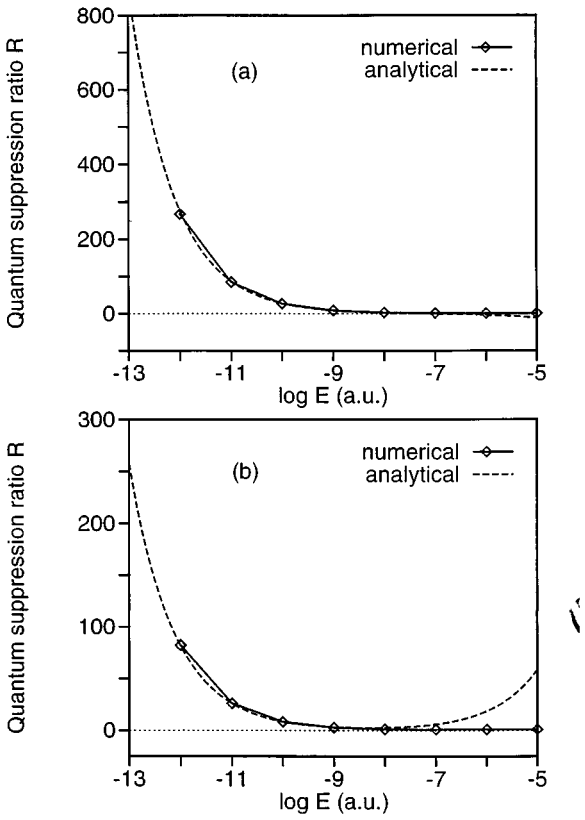

FIG. 2. Suppression ratio R for the $X\ ^1\Sigma_g^+$ and $a\ ^3\Sigma_u^+$ states of $^7Li_2$.

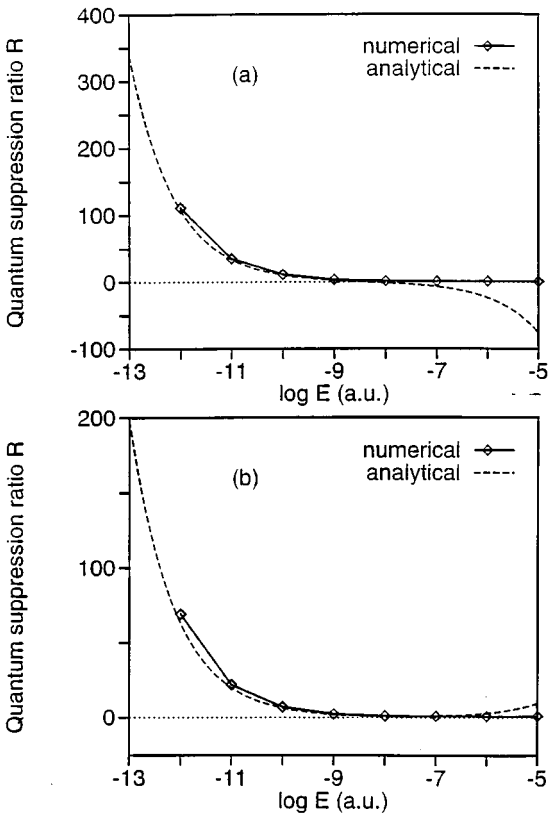

FIG. 3. Suppression ratio R for the $X\ ^1\Sigma_g^+$ and $a\ ^3\Sigma_u^+$ states of $^{23}Na_2$.

where $\sigma_{\rm abs}$ is the quantum cross section, P is the probability of entering the well and $\sigma_{\rm WKB}$ is the cross section obtained with WKB wave functions. The factorization should be successful provided no threshold resonances occur. Such a factorization is also clearly discussed in the work of Julienne and Mies [10]. Because of the quantum suppression, a kinematical estimate of the frequency of approach into the well may be seriously misleading. We explore the case of photoabsorption by a pair of ^{7}Li atoms colliding in the $X\ ^1\Sigma_g^+$ and $a\ ^3\Sigma_u^+$ states of $^7Li_2$, assuming s-wave scattering. The potentials and transition dipole moments are summarized by Côté *et al.* [15]. The dipole matrix element that controls the absorption probability is

$$D_v(E)=\int_0^\infty dr u_v(r)D(r)u_E(r), \tag{29}$$

where $D(r)$ is the dipole transition moment, $u_v(r)$ is the final vibrational state wave function and $u_E(r)$ is the initial wave function describing a pair of free atoms with an energy E of relative motion. Then

$$|D_v(E)|^2=P|D_v^{\rm WKB}(E)|^2, \tag{30}$$

where

$$D_v^{\rm WKB}(E)=\int_{r_0}^\infty dr u_E^{\rm WKB}(r)D(r)u_v(r). \tag{31}$$

In Fig. 4(a), we compare the quantum and the uncorrected and corrected semiclassical values of $|D_v(E)|^2$ for $v=68$ as a function of E for the singlet $X\ ^1\Sigma_g^+-A\ ^1\Sigma_u^+$ transition. The correction is substantial and it brings the semiclassical calculations into agreement with the quantum results for energies up to 10^{-7} a.u. Beyond $E=10^{-5.5}$, the WKB approximation is valid and no correction is needed. The simple expansion Eq. (26) does not work for the intervening energy range.

Similar conclusions apply to the triplet transition $a\ ^3\Sigma_u^+-1\ ^3\Sigma_g^+$, although the agreement is poorer [see Fig. 4(b)]. The poorer performance arises because the classical distance of closest approach $r_0(E)$ in the $a\ ^3\Sigma_u^+$ state lies inside the well of the excited state and the WKB truncation of the initial free-wave function to the left of the turning point may eliminate a contribution the matrix element. Also, the outer turning point of $u_v(r)$ is at quite large r, and overlaps with $u_E^{\rm WKB}(r)$ in a region where the WKB error term is considerable.

The quantum suppression correction can be used for energies up to the mK range, a range well above that which experiments are currently able to reach. Quantum suppression is an important effect in atomic collisions taking place in weak perturbative fields.

The collision suppression in this context of a secondary process (photoassociation) is connected to the Wigner threshold law for x-wave inelastic scattering [9], which predicts a $\sqrt{E}$ behavior very near threshold. That law, deduced originally with R-matrix theory, can be viewed as a manifestation

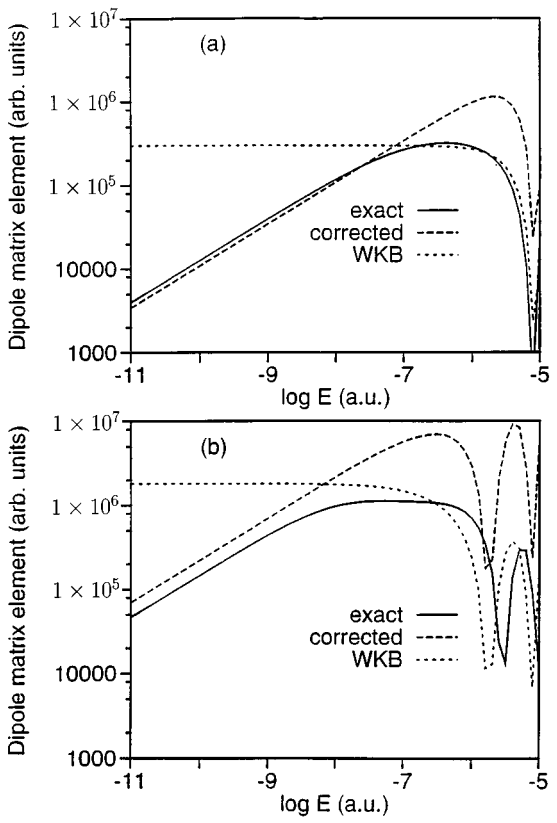

FIG. 4. Dipole matrix elements $|D_v(E)|^2$, $|D_v(E)|^2_{\rm corr}$, and $|D_v^{\rm WKB}(E)|^2$ for the level $v=68$ of (a) the singlet transitions and (b) the triplet transitions of $^7Li_2$.

of the suppression: if an inelastic process requires penetration into the interaction region, then it will be suppressed by the reflection at large distance, subject to the usual caveats regarding threshold bound states. Indeed $\sqrt{E}$ behavior for photoassociation for *s* waves was seen in calculations in Ref. [19] and ascribed to the Wigner law.

V. SUMMARY AND OUTLOOK

We have reviewed the suppression effect and provided some perspective on what it is and when to expect it. (The exceptions are Coulomb potentials and threshold resonances.)

We have shown that the effect of quantum suppression of collisions applies to *s*-wave low-energy atom-atom scattering using realistic potentials for ^{7}Li-^{7}Li and ^{23}Na-^{23}Na collisions at achievable energies. The suppression effect is well established in the field of surface collisions. Its manifestation in scattering theory is the Wigner threshold law for *s* waves, which we have reinterpreted here as quantum suppression of the collisions at very low energy. The suppression is in fact part of the story behind Wigner cusp k^{-1} threshold behavior.

At energies reached by present day traps, dramatic suppression exists which can affect secondary processes such as photoabsorption and trap loss, and accretion, i.e., formation of clusters by three-body collision. (We emphasize, however, that these effects are already included in a proper treatment of threshold inelastic processes.)

Bose-Einstein condensation, which is adversely affected by actual accretion, could be assisted by the existence of suppression of the inner part of the wave function at low temperatures, since this suppression is independent of the sign of the scattering length a. The wave-function suppression in the WKB breakdown region (typically at several tens of atomic units) may form the last line of defense against complete collapse of a negative scattering length Bose condensate. There is a caveat: large suppression sets in typically earlier (higher energy) for positive scattering length than for negative; this is a purely geometrical effect having to do with the less likely combination of large asymptotic amplitude and negative intercept for the extrapolated wave function.

We related the suppression to breakdown of the WKB approximation (see also Refs. [10,11]). A simple rule to estimate the validity of WKB is

$$\hbar\frac{|p'(r)|}{p(r)^2}\ll 1. \tag{32}$$

If this holds from the region of the well outward, then no suppression will occur.

The suppression behavior in more complex regions where multichannel couplings become relatively strong at low energies may be different [4] and remains to be explored in atom-atom interactions.

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APPENDIX: DERIVATION OF $|u_0^{\rm in}|$

Following Gribakin and Flambaum [14], we will find an analytical expression for $|u_0^{\rm in}|$. To do so, we solve the Schrödinger equation for *s*-wave zero-energy scattering particle

$$\frac{d^2u(r)}{dr^2}-U(r)u(r)=0,\ \text{where}\ \ U(r)=\frac{2m}{\hbar^2}V(r), \tag{A1}$$

with the boundary condition $u(0)=0$.

Assuming that the WKB approximation is valid within the potential well, we can write the wave function in the form

$$u(r)=\frac{C}{\sqrt{p_0(r)}}\sin\left(\frac{1}{\hbar}\int_{r_0}^{r}dr'\,p_0(r')+\frac{\pi}{4}\right)\ \text{for}\ r>r_0, \tag{A2}$$

where r_0 is the classical turning point and $p_0=\sqrt{-2mV(r)}$ is the local zero-energy momentum. At large distances, the potential varies as $-\alpha/r^n$ and the condition for the validity of the WKB approximation reads

$$r \ll \left(\frac{2\gamma}{n}\right)^{2/(n-2)}, \quad \text{where} \quad \gamma \equiv \frac{1}{\hbar}\sqrt{2m\alpha}. \tag{A3}$$

In the case of lithium, taking $n=6$ we get $r \ll 37.5a_0$ (^{7}Li: $\gamma = 4213.3$ a.u.). We suppose that the potential curve takes its asymptotic form $-\alpha r^{-n}$ at a shorter distance, in which case the differential equation becomes

$$\frac{d^2u(r)}{dr^2} + \frac{\gamma^2}{r^n}u(r) = 0. \tag{A4}$$

Defining a new function $u = \sqrt{r}\phi$ and a new variable x, we can rewrite Eq. (A4) into a Bessel equation (see O'Malley, Spruch, and Rosenberg [16]) whose general solution is given in terms of a combination of Bessel and Neumann functions,

$$u_>(r) = \sqrt{r}[AJ_\nu(x) - BN_\nu(x)], \quad r > r^*, \tag{A5}$$

where $\nu \equiv 1/(n-2)$ and $x \equiv 2\gamma\nu r^{-1/2\nu}$. For $n>3$, $\nu<1$ and we can use the expansion of $J_\nu(x)$ and $N_\nu(x)$ for $r \to \infty$ (or $x \ll 1$) to obtain the asymptotic form of $u_>(r)$

$$u_>(r) = C_1 r + C_2, \tag{A6}$$

where

$$C_1 = \frac{B}{(\gamma\nu)^\nu}\frac{1}{\sin(\pi\nu)\Gamma(1-\nu)}, \tag{A7}$$

$$C_2 = \frac{(\gamma\nu)^\nu}{\Gamma(1+\nu)}[A - B\cot(\pi\nu)]. \tag{A8}$$

To determine the constants A and B, we must match the analytical solution to the WKB solution at r^*. Since r^* has been chosen to satisfy the condition (A3), we can assume that its value is not too large and that $x^* \gg 1$, in which case we can use the expansion of $J_\nu(x)$ and $N_\nu(x)$ for large x to evaluate $u_>(r)$ near r^* (see Butkov [17]). Then, we find

$$\frac{A}{B} = \tan\left(\Phi - \frac{\pi\nu}{2}\right), \quad \text{with} \quad \Phi \equiv \frac{1}{\hbar}\int_{r_0}^{\infty} dr' p(r'). \tag{A9}$$

The scattering length is simply given by

$$a = -\frac{C_2}{C_1} = \bar{a} f(\Phi), \tag{A10}$$

where

$$\bar{a} = \cos(\pi\nu)(\gamma\nu)^{2\nu}\frac{\Gamma(1-\nu)}{\Gamma(1+\nu)}, \tag{A11}$$

$$f(\Phi) = \left[1 - \tan\left(\Phi - \frac{\pi\nu}{2}\right)\tan(\pi\nu)\right]. \tag{A12}$$

We want to normalize $u(r)$ in such a way that

$$u(r) \simeq C_1 r + C_2 \to 1 - \frac{r}{a}. \tag{A13}$$

So one must divide the previous result by C_2 and write $u = u/C_2$. At r^* we have

$$u(r^*) = \frac{u_{\mathrm{WKB}}(r^*)}{C_2} = \frac{u_>(r^*)}{C_2}, \tag{A14}$$

which gives, after some algebra,

$$\frac{C}{C_2} = \frac{\sqrt{\hbar}}{\cos(\Phi - x^* - \pi/4)}\left\{P\cos\left(x^* - \frac{\pi\nu}{2} - \frac{\pi}{4}\right) - \frac{Q}{a}\cos\left(x^* + \frac{\pi\nu}{2} - \frac{\pi}{4}\right)\right\}, \tag{A15}$$

with

$$P \equiv \frac{\Gamma(1+\nu)}{\sqrt{\pi\nu}(\gamma\nu)^\nu} \quad \text{and} \quad Q \equiv \frac{\Gamma(1-\nu)(\gamma\nu)^\nu}{\sqrt{\pi\nu}}, \tag{A16}$$

where we used the expressions for a and C_2, the fact that $\Phi = \phi(r^*) + x^*$ and $p_0(r^*) = \hbar\gamma[r^*]^{-n/2}$, and also the expansion of $J_\nu(x)$ and $N_\nu(x)$ for $x^* \gg 1$.

For $n>3$, the quantity $|u_0^{\mathrm{in}}|$ can be evaluated from Eq. (A15). In fact, we have

$$u_0^{\mathrm{in}} \equiv \frac{1}{\sqrt{p_e}}\frac{C}{C_2}. \tag{A17}$$

Using the expression for a and Eq. (A15) for C/C_2, we can rewrite u_0^{in} as

$$u_0^{\mathrm{in}} \simeq -\frac{\sqrt{\hbar}}{a}\frac{\Gamma(1-\nu)(\gamma\nu)^\nu}{\sqrt{\pi\nu}(2\mu D)^{1/4}}\frac{\sin(\pi\nu)}{\cos(\Phi - \pi\nu/2)}. \tag{A18}$$

As mentioned before, the case $n=3$ is quite peculiar because in that case $\nu=1$ and the Gribakin and Flambaum scheme becomes ill defined.

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