Quantum-diffractive background gas collisions in atom-trap heating and loss

S. Bali, K. M. O'Hara, M. E. Gehm, S. R. Granade, and J. E. Thomas
Physics Department, Duke University, Durham, North Carolina 27708-0305
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We derive a simple formula for the heating rate that arises from quantum-diffractive background gas collisions in atom traps. This result appears to explain the residual heating rates reported for recent experiments with a Cs vapor-loaded, far-detuned optical trap at $\simeq 10^{-9}$ Torr [Phys. Rev. Lett. **81**, 5768 (1998)]. Diffractive collisions may determine the minimum heating rates achievable in shallow all-optical or magnetic atom traps operating at low temperature and high density. [S1050-2947(99)50307-7]

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It is well known that background gas collisions cause exponential decay in atom traps. For magneto-optical traps (MOTs), where the well depth U_0 is of order 1 K, the loss rate can be calculated using a classical small-angle scattering approximation [1]. A cold ($\simeq 1$ mK) atom leaves the trap when the scattering angle θ exceeds a threshold angle θ_0 such that the collisional energy change of the trapped atom, $\Delta E(\theta > \theta_0)$, exceeds U_0. By contrast, in relatively shallow traps, for example, in far off resonance traps [2,3] or magnetic traps [4], typical well depths range from less than 1 mK to 10 mK. In this case, the classical small-angle approximation predicts that the ejection cross section grows without limit as the well depth decreases, since collisions at an ever-increasing range are effective in expelling atoms.

However, when the scattering angles required to eject atoms from the trap are sufficiently small, they fall into the diffractive cone of the scattering amplitude, where a classical small-angle approximation is not valid [5]. In this case, a quantum-mechanical treatment of the scattering cross section is needed. In the limit of very shallow traps, the maximum attainable cross section is the total collision cross section, as determined by the optical theorem [6]. The total cross section includes both classical and diffractive scattering contributions.

It is known that small-angle collisions with $\theta \leqslant \theta_0$ can leave atoms in the trap and cause heating. This heating mechanism has been explored numerically, including classical and diffractive contributions, by Monroe *et al.* [5]. In deep traps, part of the heating rate can arise from classical glancing-angle scattering. However, in shallow traps, the heating rate arises entirely from quantum-diffractive scattering. These small residual heating rates from background gas collisions may limit the maximum attainable phase-space density in current low-temperature trap experiments. To our knowledge, explicit formulas for the expected heating rates in this regime have not been published previously.

In this paper, we calculate the heating rate that arises from diffractive collisions of background gas atoms with atoms in shallow traps. A trap is shallow (deep) if U_0 is small (large) compared to the diffractive energy scale defined below. We show that the heating rate, Eq. (16), is inherently quantum mechanical and can be written in terms of the total trap loss rate, the well depth, and the natural scale of the energy imparted in a diffractive collision.

We begin by reviewing the basic features of diffractive collisions. For a trapped atom of velocity $\vec{v}_a$ and a background perturbing gas atom of velocity $\vec{v}_p$, the initial relative velocity is $\vec{v}_r = \vec{v}_a - \vec{v}_p$. During a collision, the relative velocity changes by $\Delta\vec{v}_r$, leading to a change in the velocity of the trapped atom

$$\Delta\vec{v}_a = \frac{\mu}{M}\Delta\vec{v}_r, \tag{1}$$

where M is the trapped atom mass and μ is the reduced mass. Assuming elastic collisions, $|\Delta\vec{v}_r|^2 = 2\,v_r^2(1-\cos\theta)$, where θ is the scattering angle between the final and initial relative velocity. For the small-angle scattering of interest here, we take $|\Delta\vec{v}_r| \simeq v_r\theta$. Hence, $|\Delta\vec{v}_a| \simeq \mu v_r \theta/M$.

In a diffractive collision, the scale of the scattering angle is $\theta \simeq \theta_d$, where the diffraction angle is of order $\theta_d = \lambda_{dB}/(\pi R) = 2/(kR)$. Here, $k = 2\pi/\lambda_{dB} = \mu v_r/\hbar$ is a thermal wave vector. R is the range of the collision potential, which is related to the total scattering cross section σ. In the hard-sphere approximation, $\sigma \simeq 2\pi R^2$. Half of the total cross section arises from classical scattering with a geometrical cross section πR^2. An additional πR^2 arises from diffraction [7]. With the small-angle approximation to Eq. (1), the trapped-atom velocity change in a diffractive collision is then $|\Delta\vec{v}_a| \simeq 2\hbar/(MR)$. An interesting feature of this result is that the perturber properties enter only through the range of the potential R [8,9]. For a trapped atom moving at a low velocity compared to the velocity change imparted by the collision ($|\vec{v}_a| \ll |\Delta\vec{v}_a|$), the natural scale for the diffractive energy change of a trapped atom is $\epsilon_d = M(\Delta\vec{v}_a)^2/2$. ϵ_d depends only on the total scattering cross section σ and the trapped atom mass M,

$$\epsilon_d = \frac{4\pi\hbar^2}{M\sigma}. \tag{2}$$

Table I shows typical values for ϵ_d for trapped alkali-metal-background alkali-metal self-collisions. Such collisions occur in all atom traps and are dominant in vapor loaded traps. The total cross sections are determined from the Van der Waals constants, as described below, assuming that the background atoms are at room temperature, 300 K. The

TABLE I. Total collision cross sections σ, total collision rate γ_C [γ_C/n_p (10^{-9} cm^3/sec)], and diffractive energy changes ϵ_d for background gas collisions with alkali-metal atoms in shallow traps. Note that we assume ^{87}Rb in calculating ϵ_d for Rb. For ^{7}Li-Li, $\epsilon_d=94.3$ mK; for ^{7}Li-He, $\epsilon_d=535$ mK; and for ^{7}Li$-H_2$, $\epsilon_d=363$ mK. The background temperature is taken to be $T=300$ K. C_6 constants are given in atomic units (a.u.)$=e^2a_0^5$, where e is the electron charge and a_0 is the Bohr radius.

Atom	C_6 (a.u.)	σ (Å^2)	γ_C/n_p	ϵ_d (mK)
^{6}Li-Li	1390	920	8.8	110
Na-Na	1470	1230	6.0	21.4
K-K	3810	2000	7.5	7.7
Rb-Rb	4430	2500	6.3	2.8
Cs-Cs	6330	3140	6.4	1.4
^{6}Li-He	21.9	162	1.9	624
Na-He	25.1	171	2.0	154
K-He	34.5	194	2.3	80.2
Rb-He	36.6	198	2.3	35.1
Cs-He	44.9	215	2.5	21.2
^{6}Li$-H_2$	82.5	239	4.0	423
Na-H_2	91.0	249	4.1	106
K-H_2	130	286	4.7	54.3
Rb-H_2	140	295	4.9	23.6
Cs-H_2	170	320	5.3	14.3

diffractive-energy change ranges from $\epsilon_d=1.4$ mK for Cs-Cs collisions to 110 mK for Li-Li collisions, showing that diffractive collisions can impart substantial energy compared to the energy of atoms in low-temperature traps. For traps at very low pressure, He and H_2 are likely to be the dominant background gases. Table I shows that the small cross sections for these perturbers result in large values of ϵ_d.

In general, the energy change of a trapped atom is $\Delta E=M[(\vec{v}_a+\Delta\vec{v}_a)^2-\vec{v}_a^2]/2$. For very cold atoms with initial energies E_a near the bottom of the well, $E_a=M\vec{v}_a^2/2\ll U_0$, and the threshold angle θ_0 is approximately independent of $\vec{v}_a$. Then, we can make an isotropic assumption and take $\langle\vec{v}_a\cdot\Delta\vec{v}_a\rangle\simeq 0$ so that $\Delta E\simeq M(\Delta\vec{v}_a)^2/2$. Using Eq. (1) in the small-angle approximation yields

$$\Delta E(\theta)=\frac{1}{2}\frac{\mu^2}{M}v_r^2\theta^2. \quad (3)$$

For an atom to be ejected from the trap, we require $\theta\geq\theta_0$, while for heating, we require $\theta\leq\theta_0$, where the threshold angle θ_0 is determined by $\Delta E(\theta_0)=U_0$. The well depth then defines θ_0 according to

$$U_0=\frac{1}{2}\frac{\mu^2}{M}v_r^2\theta_0^2=\epsilon_d\frac{\theta_0^2}{\theta_d^2}. \quad (4)$$

For shallow wells, where $U_0\ll\epsilon_d$, we have $\theta_0<\theta_d$. In this case, the collisions that cause heating are entirely in the diffractive regime, where a classical small-angle approximation is invalid.

The collision rate to scatter into a solid angle $d\Omega$ is $n_pv_r(d\sigma/d\Omega)d\Omega$, where $d\sigma/d\Omega$ is the differential scattering cross section and n_p is the background gas density. For a scalar interaction potential, $d\sigma/d\Omega=|f(\theta)|^2$, where $f(\theta)$ is the scattering amplitude. Using Eq. (4) to determine θ_0 in terms of the well depth, the loss rate is given by

$$\gamma_C=n_pv_r\int_{\theta_0}^{\pi}2\pi\,d\theta\sin\theta\,|f(\theta)|^2. \quad (5)$$

When the thermalization time of the atoms in the trap is short compared to the observation time, the total energy transferred to the trapped atoms by collisions with the background gas heats the stored atoms, raising their average energy. The corresponding average heating rate per atom for $\theta_0\ll 1$ can be written in the small-angle approximation as

$$\dot{Q}=n_pv_r\int_0^{\theta_0}2\pi\,d\theta\,\theta\,|f(\theta)|^2\Delta E(\theta). \quad (6)$$

In the classical limit, where $kR\theta\gg 1$, the scattering amplitude can be evaluated in the stationary phase approximation [10]. The differential cross section then is given by the classical formula $|f(\theta)|^2=[b(\theta)/\sin\theta]db/d\theta$, where $\theta(b)$ is the scattering angle for impact parameter b.

To determine the heating rate for diffractive collisions, we use a standard approximation for the scattering amplitude that is valid in the diffractive region. Using the semiclassical partial-wave phase shifts for a power-law potential $V(r)=-C_n/r^n$, yields [7]

$$|f(\theta)|_d^2\simeq\left(\frac{k\sigma}{4\pi}\right)^2q(n)\left[1-c(n)\frac{k^2\sigma}{8\pi}\theta^2+\cdots\right]. \quad (7)$$

Here, the optical theorem determines $\mathrm{Im}\,f(0)=k\sigma/(4\pi)$, where σ is the total scattering cross section. The factor $q(n)$ arises because $f(0)$ has a real part, in general. For $n>3$, $q(n)=1+\tan^2[\pi/(n-1)]$. Reference [7] gives $c(n)$ for $n>5$, with $c(\infty)=1$ and $c(6)=2.07$.

We evaluate the heating rate for diffractive collisions in the limit of a shallow well, so that $U_0\ll\epsilon_d$, and $\theta_0\ll\theta_d$. In this case, with $\sigma\simeq 2\pi R^2$, Eq. (7) shows that $|f(\theta)|^2\simeq|f(0)|^2$ is nearly constant, since $\theta^2k^2\sigma/(8\pi)\simeq\theta^2/\theta_d^2\ll 1$. Using Eqs. (4) and (6) then yields a simple result for the diffractive contribution to the heating rate,

$$\dot{Q}_d=\frac{q(n)}{4}n_p\,v_r\,\sigma(v_r)\frac{U_0^2}{\epsilon_d(v_r)}. \quad (8)$$

Here, we explicitly include the dependence of the total cross section σ on the relative speed.

For a shallow well where $\theta_0\ll\theta_d$, the corresponding loss rate is obtained by evaluating Eq. (5) in the limit $\theta_0\simeq 0$. In this case, the integral over θ yields essentially the total cross section and

$$\gamma_C\simeq n_p\,v_r\,\sigma(v_r). \quad (9)$$

For a power-law potential, the total scattering cross section for collisions with room-temperature perturbers can be evaluated using semiclassical phase shifts [7]. The cross section scales with the relative speed as $\sigma(v_r)$

$=\sigma(u_p)(v_r/u_p)^{-2/(n-1)}$. Equations (8) and (9) are averaged over the thermal distribution of background gas speed. We assume an isotropic Maxwellian distribution with a $1/e$ width $u_p \equiv \sqrt{2\,k_B T/m_p}$ for a background atom of mass m_p at temperature $T=300$ K, so that $v_a \ll u_p$. Then,

$$\left\langle \left(\frac{v_r}{u_p}\right)^{1-\beta}\right\rangle = \frac{2}{\sqrt{\pi}}\Gamma\left(2-\frac{\beta}{2}\right). \tag{10}$$

The loss rate then is given by

$$\gamma_C = \frac{2}{\sqrt{\pi}}\Gamma\left(2-\frac{1}{n-1}\right) n_p u_p \sigma(u_p). \tag{11}$$

The heating rate from diffractive collisions is

$$\dot{Q}_d = g(n)\,\gamma_C \frac{U_0^2}{\epsilon_d}. \tag{12}$$

Here, Eq. (2) gives ϵ_d with $\sigma \equiv \sigma(v_r = u_p)$ from Ref. [7] and

$$g(n) = \frac{q(n)}{4}\,\frac{\Gamma\left(2-\frac{2}{n-1}\right)}{\Gamma\left(2-\frac{1}{n-1}\right)}. \tag{13}$$

For a Van der Waals interaction, $n=6$, the total scattering cross section [7] is

$$\sigma(u_p) = 7.57 b_6^2(u_p),$$

$$b_6(u_p) = 1.033\left(\frac{C_6}{\hbar u_p}\right)^{1/5}. \tag{14}$$

The corresponding loss rate rate is

$$\gamma_C = 1.05\, n_p u_p \sigma(u_p). \tag{15}$$

Finally, the heating rate for a shallow well with $E_a \ll U_0 \ll \epsilon_d$ is given by

$$\dot{Q}_d = 0.37\gamma_C \frac{U_0^2}{\epsilon_d}. \tag{16}$$

For comparison, in the hard-sphere limit, $n \to \infty$, Ref. [7] shows that $\sigma \to 2\pi b_\infty^2$, where $b_\infty = R$ is independent of v_r. The corresponding loss rate differs from Eq. (15) only in the numerical factor $1.05 \to 2/\sqrt{\pi}$. For the heating rate, Eq. (16), $0.37 \to 1/4$ in the hard-sphere limit.

Using the Van der Waals C_6 constants given in Ref. [11], we obtain the total cross sections $\sigma(u_p)$ from Eq. (14) for a room-temperature background gas at $T=300$ K. The corresponding diffractive energies are given by Eq. (2). These are summarized in Table I for trapped alkali-metal-background alkali-metal self-collisions. Table I also summarizes the results for He and H_2 background gases, using C_6 constants from Ref. [12].

Equation (16) is the primary result of this paper. The predicted heating rates can be compared to the residual heating rate of $\simeq 4$ μK/sec reported for a recent elegant experiment on Raman cooling in a Cs vapor-loaded, far-detuned optical trap [3]. In the experiments, the vapor pressure is chosen in the nTorr range to obtain a high trapped atom density and strong collisional coupling between the radial and axial directions. The collision time is estimated to be $\simeq 1$ ms and the radial-axial thermalization time is found to be 50 ms. Hence, we assume that after a background gas collision, all atoms that remain in the trap thermalize quickly compared to the observation time. The well depth is $U_0 = 0.16$ mK and the initial energy of the atoms is $\ll U_0$, so that Eq. (16) is applicable. The trap $1/e$ lifetime of 2 sec is limited by background gas collisions in the cell MOT used to load the optical trap so that $\gamma_C \simeq 0.5$ sec^{-1}. From Table I for Cs-Cs collisions, we obtain $\epsilon_d = 1.4$ mK. Using these parameters in Eq. (16) yields $\dot{Q}_d = 3.4$ μK/sec, in reasonable agreement with the observed residual heating rate of 4 μK/sec.

When the trap well depth U_0 is not small compared to ϵ_d, Eq. (6) is readily integrated by approximating the scattering amplitude, Eq. (7), as a Gaussian. The result shows that, in general, Eq. (16) must be corrected by a factor $\simeq 2\phi(x_0)/x_0^2$, where $x_0 \equiv c(n) U_0/\epsilon_d$ and $\phi(x_0) \equiv 1-(1+x_0)\exp(-x_0)$. The maximum diffractive heating rate expected for a deep well, where E_a and $\epsilon_d \ll U_0$, is easily determined from Eq. (6) in the same approximation:

$$\dot{Q}_d^{\max} = 2\pi \frac{\hbar^2}{M} n_p \langle v_r \rangle \frac{q(n)}{[c(n)]^2}, \tag{17}$$

where $\langle v_r \rangle = (2/\sqrt{\pi}) u_p = \sqrt{8\,k_B T/(\pi\, m_p)}$. For the Van der Waals case, $n=6$, we obtain

$$\dot{Q}_d^{\max} = 2.24 \frac{\hbar^2}{M} n_p \langle v_r \rangle. \tag{18}$$

In the hard-sphere limit, the factor $2.24 \to 2\pi$. An interesting feature of the maximum diffractive heating rate is that it depends only on the thermal speed and density of the background gas, and the mass M of the trapped atom. This arises because the collision rate is proportional to the cross section, while the diffractive energy change per collision is inversely proportional to the cross section. Hence, the cross section does not appear in the final result. In the deep-well approximation, diffractive collisions are ineffective in expelling atoms from the trap, and trap loss arises from classical small-angle scattering as calculated previously [1]. For Cs-Cs collisions, Eq. (18) yields a maximum diffractive heating rate in a deep well of $\dot{Q}_d^{\max} \simeq 62$ μK/sec/nTorr. Equation (18) predicts the *minimum* collision-induced heating rate for a deep well. Additional heating may arise from classical small-angle scattering.

In conclusion, we have explored the role of quantum diffractive background gas collisions in atom trap heating and loss. We have shown that diffractive collisions produce energy changes that are substantial compared to the depth of most magnetic and optical traps, so that the loss rate is determined by the total collision cross section. The calculated diffractive heating rates are inherently quantum mechanical and can be particularly important for vapor-loaded traps. Since the heating rates are quite small, they are most important for very-low-temperature traps. The calculated heating rates appear to explain the residual heating rates reported for a vapor-loaded optical trap [3]. This result suggests that the dominant nonoptical heating rates in very far-detuned all-optical traps may arise from background gas collisions and laser noise-induced trap fluctuations, as described recently [13,14].

Note added. We make the simple assumption that collisionally kicked atoms either cleanly leave the trap (if $\Delta E > U_0$) or remain and thermalize (if $\Delta E < U_0$). However, for sufficiently hot atoms, the thermalization time in the trap may be longer than the observation time, and Eqs. (16)–(18) may not be applicable. Recently it has come to our attention that loss and heating arising from background gas collisions are discussed by Cornell, Ensher, and Wieman [15]. There, an estimate of the heating rate also is given, and the issue of thermalization is discussed. Further, it is pointed out that for large and dense atomic samples, multiple scattering of collisionally kicked atoms may be important, since the maximum energy transferred to the sample by a background gas collision can exceed the well depth.

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