Kinetic theory of the evaporative cooling of a trapped gas

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We apply kinetic theory to the problem of evaporative cooling of a dilute collisional gas in a trap. Assuming ''sufficient ergodicity'' (phase-space distribution only a function of energy) and s-wave collisions with an energy-independent cross section, an equation for the evolution of the energy distribution of trapped atoms is derived for arbitrary trap shapes. Numerical integration of this kinetic equation demonstrates that during evaporation the gas is accurately characterized by a Boltzmann distribution of atom energies, truncated at the trap depth. Adopting the assumption of a truncated Boltzmann distribution, closed expressions are obtained for the thermodynamic properties of the gas as well as for the particle and energy loss rates due to evaporation. We give analytical expressions both for power-law traps and for a realistic trapping potential (Ioffe quadrupole trap). As an application, we discuss the evaporative cooling of trapped atomic hydrogen gas.

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I. INTRODUCTION

Thermal escape, or evaporation, of particles from a trapped gas has long been of interest in the astrophysical context of stars escaping from globular clusters [1]. In the laboratory, the realization of systems of electromagnetically confined ultracold atomic gases [2] has sparked new interest in this process.

Evaporative cooling of a trapped gas is based on the preferential removal of atoms with an energy higher than the average energy and on thermalization by elastic collisions. For a gas confined in a trap with finite depth ϵ_t, atoms with energy ϵ greater than ϵ_t can leave the trap by reaching a pumping surface or by passing over a potential barrier. Since this reduces the average energy of the atoms remaining in the trap, the gas will be driven by thermalizing interatomic collisions towards a new equilibrium state at a lower temperature. These collisions also promote atoms to energies higher than ϵ_t, thus keeping the evaporation going. As the temperature of the trapped gas drops, the number of atoms that are able to leave the trap is exponentially suppressed, approximately like $\exp(-\epsilon_t/kT)$. Eventually the cooling rate is balanced by a competing heating mechanism, or becomes negligibly small. In order to force the cooling to proceed at a constant rate, the evaporation threshold ϵ_t may be lowered as the gas cools. Since evaporation leads, under suitable conditions, to efficient compression in phase space, it may be used as a tool for realizing quantum degeneracy in a weakly interacting atomic system.

Evaporative cooling was proposed as a means to attain Bose-Einstein condensation (BEC) in atomic hydrogen [3–5]. First observations of evaporative cooling were made by Hess *et al.* [6] with magnetically trapped atomic hydrogen (H↑); further experiments [7–9] improved this technique. An optical version of forced evaporative cooling of H↑ was demonstrated by Setija *et al.* [10]. Recently, evaporative cooling has also been applied to magnetically trapped alkali vapors [11,12].

In a very exciting development, Anderson *et al.* used evaporative cooling to achieve Bose-Einstein condensation in rubidium vapor [13]. This method was also used in the BEC experiments of Bradley *et al.*, with lithium [14].

II. THEORY

In this paper we apply kinetic theory to the problem of evaporative cooling. This approach provides a justification for the common use of a truncated Boltzmann distribution of atom energies to describe an evaporating gas [3–5,15–19] and leads to explicit expressions for the evaporation rate. Our aim is to understand the evaporative cooling process, rather than to provide a detailed analysis of any existing experiment. Consequently, we introduce a number of assumptions that, although reasonable in relation to ongoing experiments, are not, of course, universally applicable. Our basic assumption is ''sufficient ergodicity:'' we assume that the distribution of atoms in phase space (position and momentum) depends only on their energy. This would be the case, for example, in a trap with ergodic single-particle motion. We suppose, however, that even if the trap does not possess this property the phase-space distribution still obeys ''sufficient ergodicity'' to a good approximation as a consequence of the interatomic collisions.

Our model of evaporation is that every atom with a total energy ϵ greater than the trap depth ϵ_t is removed before it collides with another atom. We will not investigate here the influence of restrictions on escape of energetic atoms, which will reduce the evaporative cooling power. In this respect our theory is one of ''full-power evaporation,'' evaporation limited only by the rate at which elastic collisions promote atoms to the escape energy.

Efficient removal of atoms with $\epsilon > \epsilon_t$ can be realized in practice by confining a dilute gas in a potential well $U(\mathbf{r})$ that gives rise to sufficiently ergodic motion of the atoms. The motion is sufficiently ergodic if most trajectories of atoms with a total energy greater than ϵ_t leave the trap before colliding with another atom. Clearly, the trapped gas should

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be well in the Knudsen regime—the collisional mean free path of the atoms should be much larger than the size of the gas cloud (this is the case in present-day experiments on trapped gases). To maximize the escape probability, we can arrange a perfect absorber coinciding with the $U(\mathbf{r})=\epsilon_t$ equipotential surface. The absorber may be a material surface or a thin shell in space where light [20,21] or microwaves [20] resonantly pump trapped atoms to nontrapped states. The precise mechanism is unimportant for our model. Surkov, Walraven, and Shlyapnikov [22] have discussed how nonergodic motion of the atoms can lead to suppression of evaporative cooling.

We restrict our discussion to evaporation of a classical gas: the motion of the atoms is classical, which means the theory is restricted to temperatures much higher than the quantum level spacing of an atom in the trapping potential. In addition, the gas is assumed to be statistically classical:

$$n\Lambda^3 \ll 1, \tag{1}$$

where n is the atom density and $\Lambda=(2\pi\hbar^2/mkT)^{1/2}$ is the thermal de Broglie wavelength (m is the atom mass and T is the temperature).

The main interest in the theory is in the application to a dilute gas of elastically colliding bosons. For $\Lambda \gg R_0$, the range of the interatomic potential, the quantum mechanical scattering is solely s wave. We work in the low-temperature limit, for which the scattering is s wave with an energy-independent cross section $\sigma=8\pi a^2$, where a is the scattering length.

Strictly speaking, a thermal distribution of atom energies is not possible in a trap of finite depth. For finite ϵ_t the approach to thermal equilibrium is accompanied by the emptying of the trap by evaporation. However, if the average energy per trapped atom is much smaller than the evaporation threshold ($kT \ll \epsilon_t$), then most interatomic collisions lead to redistribution of the energy among the atoms and thus to a thermal quasiequilibrium of the trapped gas.

Our assumption that the phase-space density is only a function of the single-particle energy leads, as we show below, to a radical simplification of the Boltzmann equation for the trapped atoms (Sec. IV). We find, through numerical integration of the resulting kinetic equation, that the energy distribution of an evaporating gas is, to a good approximation, a Boltzmann distribution truncated at the trap depth (Sec. V). This distribution is rather appealing, and has been used in the past as a starting point for descriptions of evaporation (e.g., [15,17,19]). Our calculations justify the use of this distribution.

Once the truncated Boltzmann distribution is adopted, a thermodynamic description of the sample follows naturally. We state a number of useful results in Sec. VI. We also show (Sec. VII) how the particle and energy loss rates due to evaporation are described by simple expressions. Comparison of the predictions of the truncated Boltzmann approximation with results of the direct integration of the kinetic equation is made in Sec. VIII. In Sec. IX we consider as a specific application the system of magnetically trapped spin-polarized atomic hydrogen.

It is worth contrasting our kinetic approach with the approach of Davis, Mewes, and Ketterle [19], which models evaporation as a truncation of the distribution function followed by relaxation to thermal equilibrium in an infinitely deep trap. The latter approach essentially treats evaporation as a throttling process, calculating the final state after the gas has recovered thermal equilibrium. Our approach considers the nonequilibrium evaporating gas directly, which allows us to calculate explicitly the rate of evaporation, determined by the collisions between the trapped atoms.

Preliminary results of the investigations leading to the present paper appeared in [16,18,23].

III. TRAP PROPERTIES

As a consequence of the assumption of ''sufficient ergodicity,'' all relevant information about the trapping potential $U(\mathbf{r})$ is contained in the energy density of states

$$\rho(\epsilon)\equiv(2\pi\hbar)^{-3}\int d^3r\,d^3p\,\delta(\epsilon-U(\mathbf{r})-p^2/2m), \tag{2}$$

defined so that $\rho(\epsilon)d\epsilon$ is equal to the number of single-particle eigenstates in the trapping potential having energies between ϵ and $\epsilon+d\epsilon$. The momentum integral may be evaluated to give

$$\rho(\epsilon)=\frac{2\pi(2m)^{3/2}}{(2\pi\hbar)^3}\int_{U(\mathbf{r})\le\epsilon} d^3r\sqrt{\epsilon-U(\mathbf{r})}. \tag{3}$$

For our purposes we therefore classify traps according to their energy density of states. The simplest class of traps are characterized by a power-law density of states (PL traps):

$$\rho(\epsilon)=A_{\mathrm{PL}}\epsilon^{1/2+\delta}. \tag{4}$$

This covers, for example, square ($\delta=0$), harmonic ($\delta=3/2$), and spherical-quadrupole ($\delta=3$) traps. It also includes the case of spherically symmetric power-law traps, with $U(r)\sim r^{3/\delta}$, and power-law traps of the form $U(\mathbf{r})\sim|x|^{1/\delta_1}+|y|^{1/\delta_2}+|z|^{1/\delta_3}$ with $\delta=\Sigma_i\delta_i$ [24].

We are particularly interested in the trapping potential given by

$$U(\mathbf{r})=\sqrt{\alpha^2(x^2+y^2)+(U_0+\beta z^2)^2}-U_0, \tag{5}$$

which describes to a good approximation the potential in an Ioffe quadrupole (IQ) trap [25], often used for magnetostatic trapping of neutral atoms [6,26,27]. Near the origin, for energies much smaller than U_0, the potential is harmonic. Clearly, potential (5) does not give rise to ergodic motion since it has axial symmetry. However, it is only an approximation to a true IQ trap. In reality there are small higher-order contributions which break the axial symmetry and lead to coupling of the degrees of freedom, as is discussed in detail in [28].

Using approximation (5) we find that the density of states of an IQ trap is given by the sum of cubic and quadratic terms:

$$\rho(\epsilon)=A_{\mathrm{IQ}}(\epsilon^3+2U_0\epsilon^2), \tag{6}$$

where $A_{\mathrm{IQ}}=(2m\pi^2)^{3/2}/[(2\pi\hbar)^3 2\alpha^2\beta^{1/2}]$. Both for $\epsilon \gg U_0$ and for $\epsilon \ll U_0$ the density of states of an IQ trap is equivalent to that of a PL trap.

Another practical quantity is the potential-energy density of states

$$\tilde{\rho}(U') \equiv \int d^3r\, \delta(U' - U(\mathbf{r})). \tag{7}$$

This function is useful when calculating sample properties averaged over the confining potential. Integrals of the form $\int d^3r F(U(\mathbf{r}))$ can be converted to the one-dimensional integral $\int dU \tilde{\rho}(U) F(U)$.

Note that a trap with $\tilde{\rho} \sim U^{\delta-1}$ may be identified as a PL trap with energy density of states (4). Using the approximation (5) for the trapping potential, the potential-energy density of states for an IQ trap is

$$\tilde{\rho}(U) = \frac{4\pi}{\alpha^2 \beta^{1/2}} (U^{3/2} + U_0 U^{1/2}). \tag{8}$$

IV. KINETIC EQUATION

In this section we derive an equation for the evolution of the energy distribution of the trapped gas. Generally, a trapped gas is described by its phase-space distribution function $f(\mathbf{r},\mathbf{p})$. We normalize this so that the total number of trapped particles $N = (2\pi\hbar)^{-3} \int d^3r d^3p f(\mathbf{r},\mathbf{p})$.

The evolution of the phase-space distribution function of a classical gas is described by the familiar Boltzmann equation [29]

$$\left(\frac{\mathbf{p}}{m} \cdot \boldsymbol{\nabla}_{\mathbf{r}} - \boldsymbol{\nabla}_{\mathbf{r}} U \cdot \boldsymbol{\nabla}_{\mathbf{p}} + \frac{\partial}{\partial t} \right) f(\mathbf{r},\mathbf{p}) = \mathscr{I}(\mathbf{r},\mathbf{p}). \tag{9}$$

The collision integral $\mathscr{I}$, for s-wave collisions with an energy-independent cross section, is given by

$$\mathscr{I}(\mathbf{r},\mathbf{p}_4) = \frac{\sigma}{(2\pi\hbar)^3 2\pi m} \int d^3p_3 d\Omega' q \{ f(\mathbf{r},\mathbf{p}_1) f(\mathbf{r},\mathbf{p}_2) - f(\mathbf{r},\mathbf{p}_3) f(\mathbf{r},\mathbf{p}_4) \}. \tag{10}$$

Here $\mathbf{p}_3$ and $\mathbf{p}_4$ are the momenta of two atoms before collision; the relative momentum is then $\mathbf{q} = (\mathbf{p}_3 - \mathbf{p}_4)/2$. The momenta after collision are $\mathbf{p}_1 = \mathbf{P}/2 + \mathbf{q}'$ and $\mathbf{p}_2 = \mathbf{P}/2 - \mathbf{q}'$, where $\mathbf{P} = \mathbf{p}_3 + \mathbf{p}_4$, $q' = q$ and Ω' specifies the direction of $\mathbf{q}'$ with respect to $\mathbf{q}$.

Our assumption of ''sufficient ergodicity,'' i.e., that the phase-space distribution of particles is a function only of the single-particle energy ϵ, allows us to write

$$f(\mathbf{r},\mathbf{p}) = \int d\epsilon\, \delta(U(\mathbf{r}) + p^2/2m - \epsilon) f(\epsilon). \tag{11}$$

Quantum mechanically, we can interpret the function $f(\epsilon)$ as the occupation number for trap eigenstates with energy ϵ. The number of atoms with energy between ϵ and $\epsilon + d\epsilon$ is $\rho(\epsilon) f(\epsilon) d\epsilon$.

As in the case of a homogeneous gas [30–32], specialization to a distribution that depends only on energy leads to a drastic simplification of the Boltzmann equation. We apply to both sides of (9) the operation $(2\pi\hbar)^{-3} \int d^3r d^3p\, \delta(U(\mathbf{r}) + p^2/2m - \epsilon)$. On the left-hand side the gradient terms sum to zero, leaving $\rho(\epsilon) \dot{f}(\epsilon)$, where $\dot{f} \equiv \partial f / \partial t$. On the right-hand side we express the distributions in the collision integral as functions of energy using (11). The resulting equation may be written

$$\rho(\epsilon_4) \dot{f}(\epsilon_4) = \frac{2\pi\sigma}{(2\pi\hbar)^6 m} \int d\epsilon_1 d\epsilon_2 d\epsilon_3 \{ f(\epsilon_1) f(\epsilon_2) - f(\epsilon_3) f(\epsilon_4) \} \int d^3r d^3P dq q^3 du du' \prod_{i=1}^{4} \delta(U(\mathbf{r}) + p_i^2/2m - \epsilon_i), \tag{12}$$

where u (u') is the cosine of the angle between $\mathbf{P}$ and $\mathbf{q}$ ($\mathbf{q}'$), $p_{1,2}^2 = P^2/4 + q^2 \pm Pqu$, and $p_{3,4}^2 = P^2/4 + q^2 \pm Pqu'$. We may now easily perform the integrations over u and u' and, subsequently, over q and the orientation of $\mathbf{P}$, to give

$$\rho(\epsilon_4) \dot{f}(\epsilon_4) = \frac{16\pi^2 \sigma m^2}{(2\pi\hbar)^6} \int d\epsilon_1 d\epsilon_2 d\epsilon_3 \{ f(\epsilon_1) f(\epsilon_2) - f(\epsilon_3) f(\epsilon_4) \} \delta(\epsilon_1 + \epsilon_2 - \epsilon_3 - \epsilon_4) \int_{U(\mathbf{r}) \leq \epsilon_{\min}} d^3r \int_{P_{\min}(\mathbf{r})}^{P_{\max}(\mathbf{r})} dP, \tag{13}$$

where $\epsilon_{\min} = \min(\epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4)$. The integration over $\mathbf{r}$ is restricted to energetically accessible regions, the integration over P to values possible given the momenta $p_i(\mathbf{r})$ of the atoms of energy ϵ_i at position $\mathbf{r}$. Assuming, without loss of generality, that $\epsilon_{\min} = \epsilon_1$ and, hence, $p_1 = \min(p_1, p_2, p_3, p_4)$ and using the fact that in that case $P_{\min} = p_2 - p_1$ and $P_{\max} = p_1 + p_2$, we easily find that $\int dP = 2\{2m[\epsilon_{\min} - U(\mathbf{r})]\}^{1/2}$. Using definition (2) of the energy density of states we thus arrive at the following kinetic equation for the evolution of the ergodic distribution function $f(\epsilon)$ in a trap:

$$\rho(\epsilon_4) \dot{f}(\epsilon_4) = \frac{m\sigma}{\pi^2 \hbar^3} \int d\epsilon_1 d\epsilon_2 d\epsilon_3\, \delta(\epsilon_1 + \epsilon_2 - \epsilon_3 - \epsilon_4) \rho(\min[\epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4]) \{ f(\epsilon_1) f(\epsilon_2) - f(\epsilon_3) f(\epsilon_4) \}. \tag{14}$$

It is noteworthy that this expression is applicable to a homogeneous gas as a special case. Then the energy is all kinetic and the density of states $\rho(\epsilon) \propto \epsilon^{1/2}$; the kinetic equation in this case can be inferred from equations appearing in the recent BEC literature [30,32].

V. NUMERICAL SOLUTION

To investigate the evolution of the distribution function of an evaporating trapped gas, we solve the kinetic equation (14) numerically. We suppose that atoms with energy $\epsilon > \epsilon_t$ are efficiently removed, so that $f(\epsilon) = 0$ for these energies. Our initial condition is chosen such that $f(\epsilon)$ is constant for $\epsilon < \epsilon_t$, corresponding to infinite temperature.

The computational procedure is straightforward. We discretize the energy scale between zero and ϵ_t into n bins of width $\Delta\epsilon = \epsilon_t/n$. The ith bin ($i = 1, \ldots, n$) is represented by the energy $\epsilon_i = (i - 1/2)\Delta\epsilon$. Then, with $\rho_i \equiv \rho(\epsilon_i)$ and $f_i \equiv f(\epsilon_i)$, the discretized kinetic equation is

$$\rho_i \dot{f}_i = \frac{m\sigma}{\pi^2\hbar^3}(\Delta\epsilon)^2 \sum_{k,l} \rho_h \{f_k f_l - f_i f_j\}, \tag{15}$$

where $j = k + l - i$ and $h = \min(i,j,k,l)$. This equation is integrated using a Euler method. The number of bins is 64, although essentially the same result is obtained with $n = 32$ or even 16.

Figure 1 shows the distribution at several times (identified by the number of collisions that have been experienced by atoms in the trap). It is clear from this simulation that the calculated distribution is well fit at all times by a simple exponential. We find this behavior for values of the PL exponent δ from zero (square well) to three (linear confinement, e.g., by a spherical quadrupole trap). It was also noticed by Kochanski in computer simulations of trapped atomic hydrogen [33].

Thus, evaporation preserves, to a good approximation, the thermal nature of the distribution. The true distribution

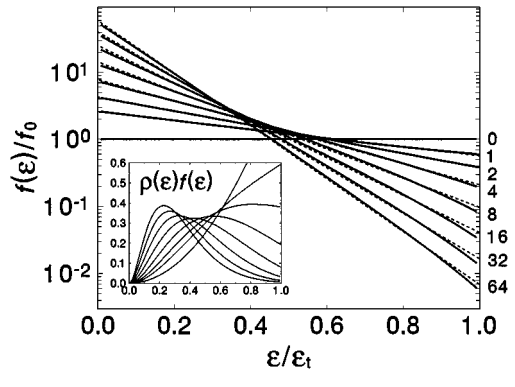

FIG. 1. Evolution of the distribution function $f(\epsilon)$ during evaporative cooling in a harmonic potential of fixed depth ϵ_t, comparing the calculated distribution (solid) to the best-fit Boltzmann form (dashed). For $\epsilon > \epsilon_t$, $f(\epsilon) = 0$. Each curve is labeled at the right by the total number of collisions per atom (the integral of the instantaneous collision rate per atom). The inset shows the energy distribution $\rho(\epsilon) f(\epsilon)$ (calculated distribution only).

$f(\epsilon)$ of the evaporating gas may be accurately described by a Boltzmann distribution truncated at the depth of the trap:

$$f(\epsilon) = n_0 \Lambda^3 e^{-\epsilon/kT} \Theta(\epsilon_t - \epsilon). \tag{16}$$

Here $\Theta(x)$ is the Heaviside step function: $\Theta(x) = 0$ for $x < 0$ and $\Theta(x) = 1$ for $x \geq 0$. The distribution (16) is specified by two (time-dependent) parameters $n_0\Lambda^3$ (occupation number of the low-energy states in the trapping potential) and kT (characteristic energy for variation of occupation number with energy). The physical interpretation of n_0 and T will be discussed below.

In the following sections we *assume* that $f(\epsilon)$ is given by the truncated Boltzmann (quasi-thermal) distribution (16) and consider the consequences. In Sec. VIII we will compare the rate of evaporative cooling predicted by this approximation with the rate that we obtain directly by numerical solution of the kinetic equation.

VI. THERMODYNAMICS

In this section we discuss the thermodynamic properties of an ideal gas with a truncated Boltzmann energy distribution. This is important in connection with evaporative cooling, since the truncation resulting from the finite depth of the trap can lead to important modifications to quantities such as the internal energy of the gas.

The truncated Boltzmann distribution (16) leads, via (11), to the phase-space distribution

$$f(\mathbf{r},\mathbf{p}) = f_0(\mathbf{r},\mathbf{p})\Theta(\epsilon_t - U(\mathbf{r}) - p^2/2m), \tag{17}$$

where

$$f_0(\mathbf{r},\mathbf{p}) = n_0\Lambda^3 \exp[-(U(\mathbf{r}) + p^2/2m)/kT] \tag{18}$$

has the form of the phase-space distribution of a classical ideal gas in thermal equilibrium in the potential field $U(\mathbf{r})$. In an infinitely deep trap we could integrate over momentum states to obtain the well-known thermal density distribution

$$n_\infty(\mathbf{r}) = n_0 \exp[-U(\mathbf{r})/kT]. \tag{19}$$

In this case n_0 would be equal to the particle density at the minimum of the trap.

For a trap of finite depth ϵ_t we find, integrating $f(\mathbf{r},\mathbf{p})$ over momentum states, the density distribution

$$n(\mathbf{r}) = n_\infty(\mathbf{r})[\mathrm{erf}\sqrt{\kappa} - 2\sqrt{\kappa/\pi}\exp(-\kappa)], \tag{20}$$

with $n_\infty(\mathbf{r})$ given by (19) and $\kappa(\mathbf{r}) \equiv [\epsilon_t - U(\mathbf{r})]/kT$. The quantity in square brackets is the incomplete gamma function $P(3/2,\kappa)$ [34]. The change of the density distribution due to the truncation in phase space is illustrated in Fig. 2. Note that the density distribution as defined by (20) is still characterized by a "temperature" T and a "density" n_0. However, n_0 is no longer the central density, $n(0) < n_0$, and strictly speaking T cannot be interpreted as the thermodynamic temperature of the system. In the case of a truncated distribution T and n_0 are convenient parameters characterizing an essentially nonequilibrium distribution. Nevertheless, $n_0\Lambda^3$ remains a proper measure of phase-space density, even

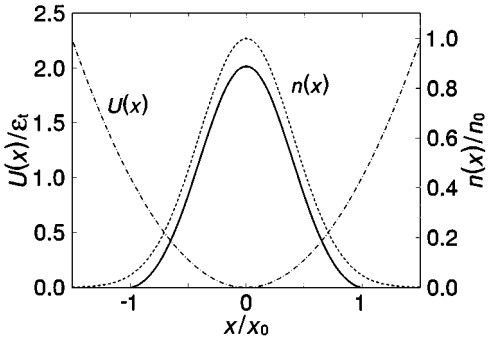

FIG. 2. The full thermal density distribution $n_\infty(x)$ (dashed) and the density distribution $n(x)=n_\infty(x)P(3/2,\kappa)$ (solid), associated with a Boltzmann distribution truncated at ϵ_t, along the x axis as a function of coordinate x for $kT=\epsilon_t/3$ in a potential well harmonic in all directions. Also shown (dot-dashed) is the potential along the x axis, $U(x)$. The coordinate x_0 is defined by $U(x_0)=\epsilon_t$.

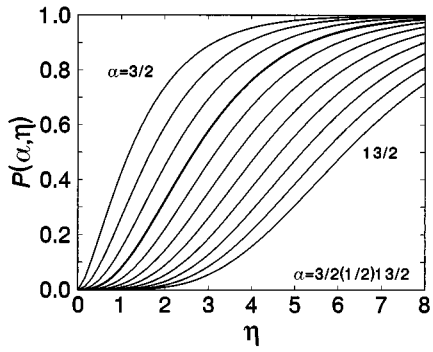

FIG. 3. Incomplete gamma function $P(a,\eta)$ as a function of η for a series of relevant a values. The truncation correction factor ζ/ζ_∞ for the reference volume V_e is $P(3/2+\delta,\eta)$. The thick curve, $a=3$, corresponds to the harmonic trap.

if ϵ_t is comparable to kT. The density distribution (20) was used by Helmerson, Martin, and Pritchard [27] in their analysis of experiments with magnetically trapped sodium atoms.

A. Reference volume and partition function

It is useful to introduce the reference volume V_e of the sample, which relates the reference density n_0 to the total number of trapped particles [35]:

$$V_e \equiv N/n_0 . \tag{21}$$

The relationship

$$V_e = \Lambda^3 \zeta \tag{22}$$

follows immediately from the definition of the single-atom partition function ζ for a trapped ideal gas (see, e.g., [29]):

$$\zeta = (2\pi\hbar)^{-3} \int d^3r d^3p \exp[-(U(\mathbf{r})+p^2/2m)/kT]. \tag{23}$$

The integration is restricted to the volume in phase space where $U(\mathbf{r})+p^2/2m \leq \epsilon_t$. Using definition (2) of the energy density of states, we can write

$$\zeta = \int_0^{\epsilon_t} d\epsilon \rho(\epsilon) \exp(-\epsilon/kT). \tag{24}$$

For a PL trap (4) we have

$$\zeta = \zeta_\infty P(3/2+\delta, \eta), \tag{25}$$

where

$$\zeta_\infty = A_{\mathrm{PL}} \Gamma(3/2+\delta)(kT)^{3/2+\delta} \tag{26}$$

is the partition function for an infinitely deep trap, $\eta \equiv \epsilon_t/kT$, and $P(a,\eta)$ is the incomplete gamma function [34], which increases monotonically from zero at $\eta=0$ to unity as $\eta \to \infty$.

In view of its importance for truncated distributions in PL traps, we plot in Fig. 3 the incomplete gamma function $P(a,\eta)$. For $a=3/2+\delta$ this is the correction factor ζ/ζ_∞ for the reference volume. For reasonable values of δ $(0<\delta<3)$ it is typically for $\eta<8$ that truncation effects become important.

Making use of the density of states (6), ζ for an IQ trap is readily obtained:

$$\zeta = \zeta_\infty^0 \left[P(4,\eta) + \frac{2}{3}\frac{U_0}{kT} P(3,\eta) \right], \tag{27}$$

with

$$\zeta_\infty^0 \equiv 6 A_{\mathrm{IQ}} (kT)^4, \tag{28}$$

the partition function for an infinitely deep IQ trap with $U_0=0$.

B. Internal energy and heat capacity

The internal energy E of a trapped gas characterized by a phase-space distribution function $f(\epsilon)$ is given by

$$E = \int d\epsilon \epsilon \rho(\epsilon) f(\epsilon). \tag{29}$$

For a truncated Boltzmann distribution the internal energy can be expressed in terms of the single-particle partition function:

$$E = NkT^2 \frac{1}{\zeta}\frac{\partial \zeta}{\partial T}. \tag{30}$$

One can easily show from (22) and (30) that the internal energy $E=(3/2+\gamma)NkT$, where $\gamma \equiv (T/V_e)(\partial V_e/\partial T)$. In the limit of a deep trap ($\eta \to \infty$) the position and momentum integrals in expression (23) for the partition function may be separated, allowing us to identify $(3/2)NkT$ as the kinetic energy and γNkT as the potential energy. For finite η, however, the two terms cannot be identified as pure kinetic energy and potential-energy contributions even though their sum is the total energy.

Using (25) we easily obtain the internal energy E in a PL trap with evaporation threshold ϵ_t:

$$E = E_\infty R(3/2+\delta, \eta) < E_\infty , \tag{31}$$

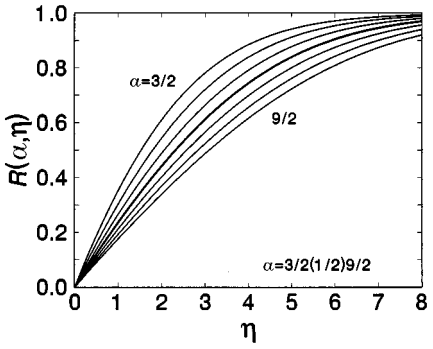

FIG. 4. Ratio of incomplete gamma functions $R(a,\eta)\equiv P(a+1,\eta)/P(a,\eta)$ as a function of η for a series of relevant a values. The truncation correction factor E/E_∞ for the internal energy of a gas in a PL trap is $R(3/2+\delta,\eta)$. The thick curve, $a=3$, corresponds to the harmonic trap.

where $E_\infty=(3/2+\delta)NkT$ is the internal energy of a sample of N atoms in thermal equilibrium in an infinitely deep trap and $R(a,\eta)\equiv P(a+1,\eta)/P(a,\eta)$. Note that the internal energy per atom depends only on the temperature T, the exponent δ, and the truncation parameter η; i.e., it is independent of the size and the exact shape of the trap. In Fig. 4 the correction factor E/E_∞ associated with truncation is plotted as a function of η for several values of δ.

Using (27) we find that the internal energy in an IQ trap with evaporation threshold ϵ_t is given by

$$E=\frac{12P(5,\eta)+6(U_0/kT)P(4,\eta)}{3P(4,\eta)+2(U_0/kT)P(3,\eta)}NkT. \tag{32}$$

The internal energy E_∞ for a deep trap ($\epsilon_t\gg kT$) is obtained by setting the P to unity. Then, for $kT\ll U_0$ the average energy $E_\infty\approx 3NkT$, reflecting the fact that for $U_0>0$ the potential is harmonic near its minimum. The internal energy per particle, even for a trap of finite depth, is independent of $A_{\rm IQ}$ and hence of α and β. The temperature dependence is completely determined by the trap parameter U_0 and the trap depth ϵ_t.

The heat capacity is another useful quantity:

$$C\equiv\left(\frac{\partial E}{\partial T}\right)_N=\left(\frac{3}{2}+\gamma+T\frac{\partial\gamma}{\partial T}\right)Nk. \tag{33}$$

For a PL trap, the heat capacity

$$C=C_\infty R(3/2+\delta,\eta)\{(5/2+\delta)R(5/2+\delta,\eta) -(3/2+\delta)R(3/2+\delta,\eta)\}, \tag{34}$$

where $C_\infty=(3/2+\delta)Nk$.

VII. EVAPORATION

To calculate the evaporation rate in the truncated Boltzmann approximation we simply substitute the truncated distribution (16) into the kinetic equation (14) and integrate over untrapped energy states to find the rate of change of the number of trapped atoms:

$$\dot N_{\rm ev}=-\int_{\epsilon_t}^{\infty}d\epsilon_4\rho(\epsilon_4)\dot f(\epsilon_4). \tag{35}$$

For $\epsilon_4>\epsilon_t>\epsilon_1,\epsilon_2$ the minimum energy of a particle participating in a collision is $\epsilon_3=\epsilon_1+\epsilon_2-\epsilon_4$ (the energy of the particle left in the trap) and thus

$$\dot N_{\rm ev}=-\frac{m\sigma}{\pi^2\hbar^3}\int d\epsilon_1 d\epsilon_2 d\epsilon_3\rho(\epsilon_3)f(\epsilon_1)f(\epsilon_2). \tag{36}$$

The domain of integration is determined by the requirement that energies ϵ_1 and ϵ_2 are less than ϵ_t while ϵ_4 is not $(\epsilon_1+\epsilon_2-\epsilon_3>\epsilon_t)$. In this domain $f(\epsilon)$ is a simple exponential and the integral may be easily evaluated to give

$$\dot N_{\rm ev}=-n_0^2\sigma\bar v e^{-\eta}V_{\rm ev}, \tag{37}$$

where $\bar v\equiv(8kT/\pi m)^{1/2}$ and the effective volume for elastic collisions leading to evaporation

$$V_{\rm ev}=\frac{\Lambda^3}{kT}\int_0^{\epsilon_t}d\epsilon\rho(\epsilon)[(\epsilon_t-\epsilon-kT)e^{-\epsilon/kT}+kTe^{-\eta}]. \tag{38}$$

The rate of change of the internal energy of the gas due to evaporation is found from the energy carried away by the evaporated atoms:

$$\dot E_{\rm ev}=-\int_{\epsilon_t}^{\infty}d\epsilon_4\epsilon_4\rho(\epsilon_4)\dot f(\epsilon_4). \tag{39}$$

After some manipulation, similar to the calculation of $\dot N_{\rm ev}$, we find

$$\dot E_{\rm ev}=\dot N_{\rm ev}\left\{\epsilon_t+\frac{W_{\rm ev}}{V_{\rm ev}}kT\right\}, \tag{40}$$

where the volume $W_{\rm ev}=V_{\rm ev}-X_{\rm ev}$, with

$$X_{\rm ev}=\frac{\Lambda^3}{kT}\int_0^{\epsilon_t}d\epsilon\rho(\epsilon)[kTe^{-\epsilon/kT}-(\epsilon_t-\epsilon+kT)e^{-\eta}]. \tag{41}$$

The volume $X_{\rm ev}$ is positive; thus, the mean energy carried away by an evaporating atom is between ϵ_t and ϵ_t+kT.

Equations (37), (38), (40), and (41) describe the evaporation dynamics in a relatively simple closed form for an arbitrary potential.

For a PL trap we find characteristic volumes

$$V_{\rm ev}=\Lambda^3\zeta_\infty[\eta P(3/2+\delta,\eta)-(5/2+\delta)P(5/2+\delta,\eta)] \tag{42a}$$

$$X_{\rm ev}=\Lambda^3\zeta_\infty P(7/2+\delta,\eta), \tag{42b}$$

with ζ_∞ given by (26).

For an IQ trap of the form (5) $V_{\rm ev}$ and $W_{\rm ev}$ may be expressed as linear combinations of incomplete gamma functions. Here we write the volumes out in full:

$$V_{\rm ev}=\Lambda^3\zeta_\infty^0\{\eta-5+\xi\eta(2\eta/3-8/3)+e^{-\eta}\times[\eta^4/24+\eta^3/3+3\eta^2/2+4\eta+5+\xi\eta(\eta^3/9+2\eta^2/3+2\eta+8/3)]\}, \quad (43a)$$

$$W_{\rm ev}=\Lambda^3\zeta_\infty^0\{\eta-6+\xi\eta(2\eta/3-10/3)+e^{-\eta}\times[\eta^5/120+\eta^4/12+\eta^3/2+2\eta^2+5\eta+6+\xi\eta(\eta^4/36+2\eta^3/9+\eta^2+8\eta/3+10/3)]\}, \quad (43b)$$

with $\xi\equiv U_0/\epsilon_t$ and ζ_∞^0 given by (28).

For an IQ trap (or PL trap with $1/2+\delta$ an integer) both the particle and the energy loss rate can be written as the sum of an algebraic term in η times $e^{-\eta}$, which is the leading term, and an algebraic term in η times $e^{-2\eta}$, which is a correction due to the truncated nature of the evaporating distribution. In previous descriptions of evaporation (see, for example, [15,17]) the $e^{-2\eta}$ terms were not taken into account. In the present context, neglect of these terms corresponds to calculating the rate of population of the high-energy tail of the Boltzmann distribution including collisions involving the atoms that would be present in this tail in thermal equilibrium.

It is noteworthy that the volumes $V_{\rm ev}$ and $X_{\rm ev}$ characterizing the evaporation dynamics may be calculated directly from the trap potential $U(\mathbf{r})$, without reference to the density of states. Since evaporation is a local phenomenon, we may consider each volume element d^3r as a square well [PL trap with $\delta=0$, well depth $\epsilon_t-U(\mathbf{r})$, and $\Lambda^3\zeta_\infty=d^3r$]. Then it is straightforward to derive

$$V_{\rm ev}=\int d^3r e^{\kappa-\eta}[\kappa P(3/2,\kappa)-(5/2)P(5/2,\kappa)] \quad (44a)$$

$$X_{\rm ev}=\int d^3r e^{\kappa-\eta}P(7/2,\kappa) \quad (44b)$$

where $\kappa(\mathbf{r})\equiv[\epsilon_t-U(\mathbf{r})]/kT$. The integrals in (44) are one dimensional if the potential-energy density of states (7) is known.

VIII. COMPARISON OF RESULTS

In this section we compare the predictions of the results based on the assumption of a truncated Boltzmann approximation (Secs. VI and VII) with the direct integration of the kinetic equation (Sec. V).

With the gas characterized by its ''temperature'' T and the total number of trapped atoms N, the evolution of the state of the gas follows from

$$\dot{E}=C\dot{T}+\mu\dot{N}, \quad (45)$$

where C is the heat capacity (33) and $\mu\equiv(\partial E/\partial N)_T=E/N$ is akin to a chemical potential. The differential equations describing the evolution of T and N are

$$\dot{T}=\frac{\dot{E}_{\rm ev}-\mu\dot{N}_{\rm ev}}{C} \quad (46)$$

and

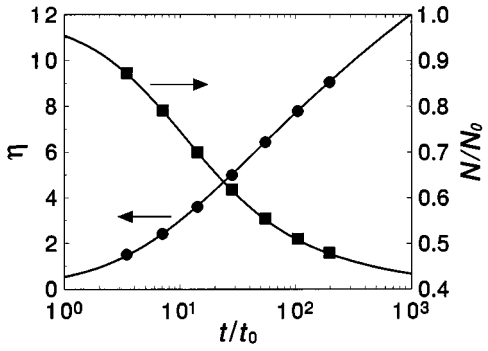

FIG. 5. Truncation parameter η (circles) and fraction of atoms remaining in trap N/N_0 (squares) as a function of reduced time t/t_0 after initiating evaporation from infinite temperature. Curves are obtained by integration of the differential equations resulting from the truncated Boltzmann approximation, symbols by fitting to the distribution obtained by numerical solution of the kinetic equation.

$$\dot{N}=\dot{N}_{\rm ev}, \quad (47)$$

where $\dot{N}_{\rm ev}$ and $\dot{E}_{\rm ev}$ are the known functions of T and N obtained in Sec. VII. We consider a harmonic trap (PL trap with $\delta=3/2$). In Fig. 5 the number of atoms in the trap N and the truncation parameter η (inverse temperature) are plotted as a function of time after initiating evaporation from infinite temperature. The characteristic time t_0 is given by $1/t_0=(12/\pi)(N_0/V)(2\epsilon_t/m)^{1/2}\sigma$, where N_0 is the initial number of trapped atoms and V is the volume enclosed by the $U(\mathbf{r})=\epsilon_t$ surface. The curves are obtained by numerical integration of the differential equations, and the points are obtained by fitting an exponential to the evolving energy distribution given by the kinetic equation. The good agreement justifies the assumption of a truncated Boltzmann distribution during evaporation.

It is worth emphasizing the difference between evaporation and thermalization. We have found that evaporation does not lead to large deviations of the distribution from a Boltzmann form. This is in contrast to the recovery of thermal equilibrium in an infinitely deep trap after the atoms in the high-energy tail are removed. Using the kinetic equation we find that in this case restoration of the truncated tail leads to significant deviations that persist even after the (approximately) four atomic collision times required for thermalization [30].

IX. COOLING ATOMIC HYDROGEN

In magnetically trapped atomic hydrogen [36], evaporative cooling must compete with heating due to magnetic relaxation; this gives rise to fundamental limits on the temperatures attainable by evaporative cooling. In this section we address the problem of calculating the evolution of the temperature and density of the trapped gas and will discuss the temperatures that may be obtained. We employ the truncated Boltzmann approximation.

Relaxation events can produce atoms both in trapped and in untrapped spin states. We assume here that *all* products

leave the gas cloud: the atoms in untrapped spin states according to their nature and the atoms in trapped spin states because they are too energetic. Even so, relaxation leads to heating. Because it is a two-body process, with rate proportional to the square of the gas density, relaxation occurs preferentially at the high-density center of the gas cloud, removing atoms with lower-than-average potential energy.

The rate of change of the number of trapped atoms due to spin relaxation,

$$\dot{N}_{\rm rel} = -n_0^2 G V_{2e}, \tag{48}$$

where the rate constant G is assumed to be independent of temperature, and the effective volume for binary collisions

$$V_{2e}(T) = \int d^3r [n(\mathbf{r})/n_0]^2, \tag{49}$$

with $n(\mathbf{r})$ given by (20). The associated rate of change of internal energy,

$$\dot{E}_{\rm rel} = \dot{N}_{\rm rel}(3/2+\gamma_2)kT, \tag{50}$$

where $\gamma_2(T) = (T/2V_{2e})\partial V_{2e}/\partial T$. The evolution of the trapped gas is given by differential equations obtained from (46) and (47) by replacing $\dot{N}_{\rm ev}$ by $\dot{N}_{\rm tot} = \dot{N}_{\rm ev} + \dot{N}_{\rm rel}$ and $\dot{E}_{\rm ev}$ by $\dot{E}_{\rm tot} = \dot{E}_{\rm ev} + \dot{E}_{\rm rel}$.

Since both $\dot{N}_{\rm ev}$ and $\dot{N}_{\rm rel}$ are quadratic in the density n_0, the effect of scaling n_0 (or, equivalently, N) is merely to change the time scale. It is also useful to define the characteristic temperature T_* at which an atom has equal probability to experience an inelastic or an elastic collision (in a full thermal distribution), given by

$$kT_* = \frac{\pi m G^2}{16\sigma^2}. \tag{51}$$

In this paper we will consider H↑ in low magnetic fields, for which the relaxation rate constant $G \simeq 10^{-15}\,\mathrm{cm^3 s^{-1}}$. The scattering length $a \simeq 0.072$ nm and hence $T_* \simeq 1.4$ nK. The results apply equally well, however, to situations with other values of G or even to other atoms with different σ and m. Only the temperature T_* is different and the temperatures quoted below should simply be rescaled.

Rather than presenting the time evolution of the gas, we will discuss a few characteristics of such evolutions. One such characteristic is the minimum temperature, attained in the long-time limit. Setting $\dot{T} = 0$, this is given as a function of η by

$$\left(\frac{T}{T_*}\right)^{1/2} = \frac{\sqrt{2}(\gamma - \gamma_2 + x)V_{2e}e^{\eta}}{(\eta - 3/2 - \gamma - x)V_{\rm ev} + W_{\rm ev}}, \tag{52}$$

evaluated with $x = 0$. Another characteristic is the temperature at which the phase-space density $n_0\Lambda^3$ reaches its maximum value. This is given by the same formula but with $x = (3/2+\gamma+T\partial\gamma/\partial T)/(3/2+\gamma)$. At lower temperatures evaporative cooling will be accompanied by decreasing phase-space density. A final characteristic of interest is the temperature at which the density n_0 reaches its maximum value. This temperature is found by setting $x = (3/2+\gamma+T\partial\gamma/\partial T)/\gamma$.

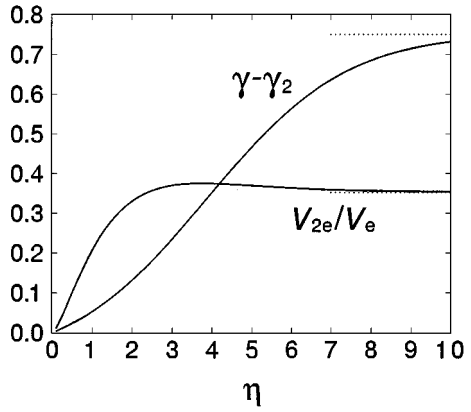

FIG. 6. Quantities characterizing two-body decay in a harmonic trap: V_e/V_{2e} and $\gamma - \gamma_2$ as a function of the truncation parameter η. For large η these approach $1/2\sqrt{2}$ and 3/4, respectively.

We consider here H↑ in a harmonic trap. Unfortunately, it appears that even in this case the important quantities V_{2e} and γ_2 are not expressible in a simple form and must, for strongly truncated distributions, be evaluated numerically from (20). Figure 6 shows V_{2e}/V_e and $\gamma - \gamma_2$ as functions of η. The characteristic temperatures given by (52) are plotted in Fig. 7 as functions of η. Also plotted for $\eta > 7$ are the same functions calculated without correcting any quantity for truncation effects (i.e., with incomplete gamma functions everywhere set to unity). Note that it is possible to cool with increasing $n_0\Lambda^3$ even at very low T, although at the cost of a strongly truncated distribution. Cooling with increasing density n_0 is only possible for $T > 2\ \mu K$. Our treatment of evaporative cooling based on kinetic theory supports the conclusion drawn in previous works [3–5,15] that BEC can be attained in magnetically trapped atomic hydrogen. We find that, interestingly, this conclusion remains valid even for small η values.

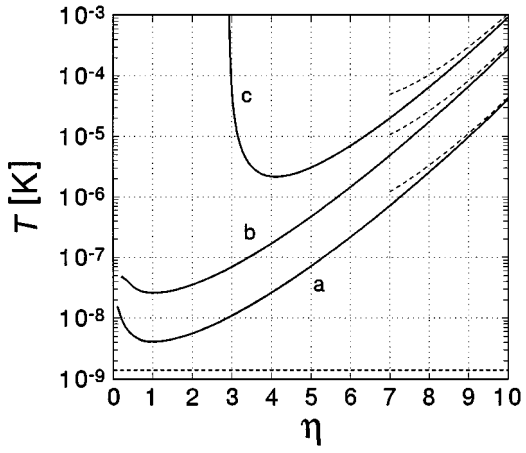

FIG. 7. Characteristic temperatures for evaporative cooling with dipolar decay of H↑ in a harmonic trap, as functions of η. Curve a: asymptotic temperature. Curve b: lowest temperature for cooling with increasing phase-space density $n_0\Lambda^3$. Curve c: lowest temperature for cooling with increasing reference density n_0. Also shown (dashed) are the same curves without corrections due to truncation of the distribution. The horizontal dashed line is the scale temperature T_*.

X. CONCLUSION

We have presented a detailed kinetic treatment of evaporative cooling of a dilute trapped gas. From the Boltzmann equation an expression is derived for the evolution of the energy distribution function of the gas. Numerical integration of this kinetic equation lends support to the common assumption of quasiequilibrium during evaporative cooling. Subject to this assumption, we obtain useful expressions describing the thermodynamics and evaporation of a gas in a trap of finite depth. Closed expressions are obtained for a variety of important trap geometries. Our theory is directly applicable to the design and analysis of experiments aiming at Bose-Einstein condensation of atomic hydrogen or other ultracold gases. A useful direction for future work would be to include stimulated emission factors in the kinetic equation and study how the gas evaporatively cools into the quantum degeneracy regime, thereby generalizing the calculations of [30–32] to the case of an inhomogeneous, trapped gas.

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$$P(a,\eta)\equiv\frac{1}{\Gamma(a)}\int_0^\eta dt t^{a-1}e^{-t}.$$
[35] The reference volume V_e is smaller than the familar effective volume $\int d^3r n(\mathbf{r})/n(0)$ by a factor $P(3/2,\eta)$. The two volumes are thus equal in the limit of a deep trap ($\eta\rightarrow\infty$).
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