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Semiclassical theory of collision-induced loss from optical traps

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A semiclassical analysis of the losses in an optical trap due to radiative collisions is presented. We use WKB theory to calculate the overlap between the ground- and excited-state wave functions. The results may be written as an absorption line shape and a survival on the excited state, with an excited-state velocity determined by energy conservation. In the region around resonance for the transition, the results reduce to those presented in previous analyses.

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I. INTRODUCTION

The study of collisions that cause the escape of atoms from optical traps is an important part of the new field of ultracold atom collisions (for an overview of research in this area see Julienne, Smith, and Burnett [1]). Investigations of trap-loss processes have been conducted both experimentally and theoretically. The two basic mechanisms by which kinetic energy may be gained are

$$A(S)+A(S)+\hbar\omega \rightarrow A_2^*(e,P_{3/2}+{}^2S)$$

$$\rightarrow A(S)+A(S)+\hbar\omega'+\varepsilon_{\rm RE}\ , \quad (1)$$

$$\rightarrow A({}^2P_{1/2})+A(S)+\varepsilon_{\rm FS}\ . \quad (2)$$

The mechanism in Eq. (1) is called radiative escape and transfers an energy $\varepsilon_{\rm RE}=\hbar(\omega-\omega')$ to the ground-state atoms. The second mechanism results from fine-structure splitting of the molecular potentials and transfers an amount of kinetic energy $\varepsilon_{\rm FS}$ equal to the ${}^2P_{3/2}$-${}^2P_{1/2}$ splitting. Experiments have been performed for a cesium trap by Sesko *et al.* [2] and for a sodium trap by Prentiss *et al.* [3], which observe these mechanisms.

The first analytical treatment of trap loss was made by Gallagher and Pritchard [4]. Their analysis was entirely classical, but it did contain the essential physics of the trap-loss process. Essentially, they showed how atoms moving along varying molecular potentials during a collision could give rise to the mechanisms Eqs. (1) and (2). The physics was modelled in terms of an absorption profile into an excited state and a survival along this state into the center of the collision.

This theory was then improved by Julienne and Vigué [5], who included the effect of a discrete sum over allowable angular momenta and who developed the multichannel quantum-defect theory (MCDT) to treat the close-range problem quantum mechanically. This new theory now agreed with ordinary collision theory at high temperatures. However, it still treated the longer range problem classically in terms of a survival and an absorption line shape. There also remained an ambiguity as to whether the initial velocity on the excited state should be specified according to energy conservation or according to the Franck-Condon principle (i.e., the local velocity does not change on making the transition to the excited state). For absorption of photons off resonance, these two choices give rise to different results. Inside the classical framework there is no way to justify *a priori* which choice is correct. More recently, Band and Julienne [6] have introduced an optical Bloch equation method to model the preparation of the atoms at long range. However, there is still an ambiguity in determining the velocity of the incoming atom along the excited-state potential.

The purpose of this paper is to address this problem and develop a semiclassical derivation that justifies the models used by Gallagher and Pritchard and by Julienne and Vigué. In doing this we can resolve the question of energy conservation versus the Franck-Condon principle.

We begin in Sec. II by considering the problem of radiative escape [Eq. (1)] in a one-dimensional optical trap. We do not include the complication of angular momentum, as in the complete analysis of Julienne and Vigué. However, this may be added to our basic method without difficulty. To determine the overlap between ground- and excited-state wave functions we use WKB wave functions and the principle of stationary phase. This allows us to determine the energy distribution of the excited state as well as the emission rate into final momentum states. The final expression can be written as an integral (over the point of excitation) of a line shape and a survival term, as in Gallagher and Pritchard [4] and Julienne and Vigué [5]. However, unless the excitation is close to the resonance for the transition (where the interatomic potential matches the laser detuning), the form of these terms does not reduce to those used by Julienne and Vigué. In general, they are more complicated but they clearly show that energy conservation is the more fundamental principle in determining excited-state survival. The only regime where both energy conservation and the Franck-Condon principle apply is around resonance, in which case neither is preferred and we return to the ambiguity discussed above.

In Sec. III to ascertain the impact of our expressions, we perform a numerical study of trap loss for cesium atoms. Julienne and Vigué have shown that significant loss occurs in the far wing of the absorption linewidth, where our theory suggests their expressions are perhaps inaccurate. The numerical results indicate that there is a difference of about 25% between the methods, which makes the energy-conserving result more compatible with the experiment of Sesko *et al.* [2].

Finally, in the conclusion, we discuss the assumptions made in our model and the impact our results have on the theory of Julienne and Vigué. Essentially, we consider that their theory is valid for far off-resonant absorption if they incorporate our expression for the line shape. We also discuss quantum-mechanical methods for the trap-loss process, which would fully resolve this problem.

II. WKB METHOD FOR RADIATIVE TRAP LOSS

In this section we develop a quantum theory for one-dimensional trap loss. The trap is specified by a standing-wave laser field tuned to the red of the frequency of the atomic transition. The intensity of the laser field is assumed sufficiently small that the atoms are not saturated. This is true if a standard optical molasses configuration is in operation.

We consider the loss from the trap as resulting from a series of two-body collisions causing the mechanism in Eq. (1). For each binary collision, one atom is fixed as the origin and the other atom moves directly towards this center at the relative velocity of the two atoms. There is now a two-step process for atoms initially in the ground state. First, at some interatomic separation, the moving atom absorbs a photon and moves into the excited state of the atom pair. This atom is then accelerated towards the other atom as it moves along the molecular potential, which describes the interaction between the atoms. Eventually, the excited atom will spontaneously emit and return to the ground state for the pair. The entire process is represented diagrammatically in Fig. 1. If the atom survives in the excited state sufficiently close into the collision, then the final momentum p_f is given enough extra energy [$\varepsilon_{\rm RE}$ in Eq. (1)] to escape from the trap. In Fig. 1 we have assumed that, over the range of interatomic separation where the process occurs, the ground-state potential $V_g(R)$ is flat. This is justified for the long-range collisions we are considering. At short range there are the usual strong repulsive interactions, which we consider only to reflect the final momentum p_f. The excited molecular potential is assumed to be the $1/R^3$ resonant dipole-dipole potential, as in the theory of Julienne and Vigué. This means that the problem of long-range retardation is avoided. The effect of the retarded $1/R$ and $1/R^2$ potentials in collisions between laser-cooled atoms is discussed in Smith and Burnett [7].

At any time the wave function representing the colliding atoms can be described as a superposition of ground- and excited-state wave functions. Therefore, the complete wave function may be expanded as

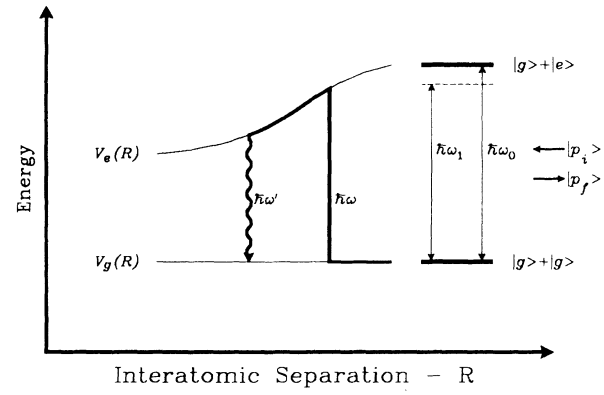

FIG. 1. Diagram showing the radiative escape (RE) mechanism for collisional trap loss. The kinetic energy gained is $\varepsilon_{\rm RE}=\hbar(\omega-\omega')$. The asymptotic ground- and excited-state energy levels are displayed. These energy levels are perturbed by the interatomic potentials $V_e(R)$ and $V_g(R)$. ω_1 is the frequency of the standing wave trapping field, p_i is the relative momentum before the collision, and p_f is the relative momentum after the collision.

$$|\Psi\rangle=|\Psi_g\rangle+|\Psi_e\rangle\ , \tag{3}$$

where

$$|\Psi_g\rangle=\int dp\,|p\rangle C_p(t)\exp\left[-i\varepsilon(p)\frac{t}{\hbar}\right]\ , \tag{4}$$

$$|\Psi_e\rangle=\int d\varepsilon\,|\varepsilon\rangle C_\varepsilon(t)\exp\left[-i(\varepsilon+\hbar\omega_0)\frac{t}{\hbar}\right]\ . \tag{5}$$

We have assumed that we are only looking at an excitation of continuum states so there are no bound states. The form of Eqs. (4) and (5) is written for a one-dimensional analysis but could be extended to three dimensions. We would, however, have to consider explicitly the role of the relative angular momentum of the pair. This relative angular momentum alters the effective potential experienced in the relative motion of the pair. This in turn will effect the velocity on the excited potential and the survival of excited atoms to small separations. For clarity in explaining our method we shall look in detail at the $l=0$ case. Our method is, however, applicable to the general case.

Continuing with the derivation, the equations of motion for the excited-state modes can be written

$$\begin{aligned} i\dot{C}_\varepsilon(t)=&-i\frac{\Gamma_e}{2}C_\varepsilon(t)\\ &+i\int dp\,\Omega e^{-i\omega_1 t}\langle\varepsilon|p\rangle C_p(t)\\ &\times\exp\left[i[\varepsilon+\hbar\omega_0-\varepsilon(p)]\frac{t}{\hbar}\right]\ . \end{aligned} \tag{6}$$

At this stage we have explicitly added in the damping rate from the excited state Γ_e, assumed independent of R and t. This is a good assumption, for example, for the 0_u^+ excited state, which is the dominant potential for the RE mechanism in cesium. The Rabi frequency Ω is proportional to the amplitude of the laser field and the dipole moment of the transition. We assume, as mentioned above, that Ω is sufficiently small for saturation not to be a problem.

In the steady-state limit, assuming that $C_\varepsilon(0)=0$ and that $C_p(t)\approx\delta(p-p_i)$, the solution of Eq. (6) is easily found to be

$$C_\varepsilon(t)=\langle\varepsilon|p_i\rangle\hbar\Omega\frac{\exp\left[i[\varepsilon-\hbar\Delta-\varepsilon(p_i)]\frac{t}{H}\right]}{\varepsilon-\hbar\Delta-\varepsilon(p_i)+\frac{i}{2}\hbar\Gamma_e} . \tag{7}$$

The detuning Δ is specified as $\Delta=\omega_1-\omega_0$. If we substitute Eq. (7) into Eq. (5) then we may construct the excited-state density matrix

$$\begin{aligned}\rho_{ee}&=|\Psi_e\rangle\langle\Psi_e|\\&=\hbar^2|\Omega|^2\int d\varepsilon_1\int d\varepsilon_2\frac{|\varepsilon_2\rangle\langle\varepsilon_1|\langle p_i|\varepsilon_1\rangle\langle\varepsilon_2|p_i\rangle}{\left[\varepsilon_1-\hbar\Delta-\varepsilon(p_i)-\frac{i}{2}\hbar\Gamma_e\right]\left[\varepsilon_2-\hbar\Delta-\varepsilon(p_i)+\frac{i}{2}\hbar\Gamma_e\right]}\end{aligned} \tag{8}$$

We now use WKB theory to evaluate the double overlap integral $\langle p_i|\varepsilon_1\rangle\langle\varepsilon_2|p_i\rangle$. We shall assume that it is only necessary to use the part of the WKB wave function that contributes in the stationary phase limit. With this assumption the overlap takes the form

$$\langle p_i|\varepsilon_1\rangle\langle\varepsilon_2|p_i\rangle=\int\frac{dR_a}{[2\pi v_i v(R_a)]^{1/2}}\exp\left[-\frac{i}{\hbar}\int_{R_t}^{R_a}[p_{\varepsilon_1}(R)-p_i]dR\right]\int\frac{dR_b}{[2\pi v_i v(R_b)]^{1/2}}\exp\left[\frac{i}{\hbar}\int_{R_t}^{R_b}[p_{\varepsilon_2}(R)-p_i]dR\right] , \tag{9}$$

where R_t is the classical turning point, v_i is the ground-state velocity, and $v(R)$ is the excited-state velocity. To calculate these integrals we treat their product as a double integral. We then expect the largest contribution to this overlap to come from the region in phase space about the line $R_a=R_b$. This is only strictly valid when $\varepsilon_1=\varepsilon_2$, but is should be a good approximation for small damping. We therefore make a change of variables to reflect this,

$$\eta_1=R_b-R_a,\quad R_1=R_a\ \ (\text{or } R_b) . \tag{10}$$

Using these new variables the overlap may be written as

$$\int\frac{dR_1}{2\pi v_i}\exp\left[-\frac{i}{\hbar}\int_{R_t}^{R_1}[p_{\varepsilon_1}(R)-p_{\varepsilon_2}(R)]dR\right]\int d\eta_1\frac{\exp\left[\frac{i}{\hbar}\int_{R_1}^{R_1+\eta_1}[p_{\varepsilon_2}(R)-p_i]dR\right]}{[v(R_1)v(R_1+\eta_1)]^{1/2}} . \tag{11}$$

If we expand $p_{\varepsilon_2}(R)$ about $p_{\varepsilon_2}(R_1)$ using a Taylor expansion

$$p_{\varepsilon_2}(R)=p_{\varepsilon_2}(R_1)+\frac{d}{dR_1}p_{\varepsilon_2}(R_1)(R-R_1)+\cdots=p_{\varepsilon_2}(R_1)-\frac{1}{v(R_1)}\left.\frac{dV_e}{dR}\right|_{R=R_1}(R-R_1)+\cdots , \tag{12}$$

then the exponential inside the η_1 integral takes the form

$$\exp\left[\frac{i}{\hbar}\int_{R_1}^{R_1+\eta_1}[p_{\varepsilon_2}(R)-p_i]dR\right]=\exp\left[\frac{i}{\hbar}\left[[p_{\varepsilon_2}(R_1)-p_i]\eta_1-\frac{1}{2v(R_1)}\left.\frac{dV_e}{dR}\right|_{R=R_1}\eta_1^2+\cdots\right]\right] . \tag{13}$$

In our later analysis we shall assume that the main contribution to the density matrix occurs when η_1 is small, so that we can truncate the expansion in Eq. (13). For the moment, however, we may define without approximation a function $F_{\varepsilon_2}(R_1,p_i)$ such that

$$\langle p_i|\varepsilon_1\rangle\langle\varepsilon_2|p_i\rangle=\int\frac{dR_1}{2\pi v_i}\exp\left[-\frac{i}{\hbar}\int_{R_t}^{R_1}[p_{\varepsilon_1}(R)-p_{\varepsilon_2}(R)]dR\right]F_{\varepsilon_2}(R_1,p_i) . \tag{14}$$

Now, if we have defined $R_1=R_b$ in Eq. (10) then we would still have obtained Eq. (14), except with $F_{\varepsilon_1}(R_1,p_i)$. Therefore, in general, we have

$$F_\varepsilon(R_1,p_i)=\int_{-\infty}^{\infty}d\eta_1\frac{\exp\left[\frac{i}{\hbar}\left[[p_\varepsilon(R_1)-p_i]\eta_1-(\pm)\frac{1}{2v(R_1)}\frac{dV_e}{dR}\Big|_{R=R_1}\eta_1^2+\cdots\right]\right]}{\{v(R_1)v[R_1(\pm)\eta_1]\}^{1/2}} , \tag{15}$$

where $(+)$ refers to ε_2, $(-)$ to ε_1. The choice of ε_1 and ε_2 as ε is made to ensure the convergence of the integrals in Eq.

(14) as they tend towards their limits. Hence the excited-state distribution has the form

$$\rho_{ee}=\frac{\hbar^2|\Omega|^2}{2\pi}\int d\varepsilon_1\int d\varepsilon_2\frac{|\varepsilon_2\rangle\langle\varepsilon_1|\int dR_1\exp\left[-\frac{i}{\hbar}\int_{R_t}^{R_1}[p_{\varepsilon_1}(R)-p_{\varepsilon_2}(R)]dR\right]F_\varepsilon(R_1,p_i)}{v_i\left[\varepsilon_1-\hbar\Delta-\varepsilon(p_i)-\frac{i}{2}\hbar\Gamma_e\right]\left[\varepsilon_2-\hbar\Delta-\varepsilon(p_i)+\frac{i}{2}\hbar\Gamma_e\right]}\ . \tag{16}$$

This equation will describe the energy distribution as the atom accelerates towards the other atom on the excited state. We now want to calculate the rate of scattering into final momentum states after the excited atom has spontaneously emitted a photon. This is given by

$$\begin{aligned}T&=|\langle p_f|\Psi_e\rangle|^2\\&=\langle p_f|\rho_{ee}|p_f\rangle\\&=\frac{\hbar^2|\Omega|^2}{2\pi}\int d\varepsilon_1\int d\varepsilon_2\frac{\langle p_f|\varepsilon_2\rangle\langle\varepsilon_1|p_f\rangle\int dR_1\exp\left[-\frac{i}{\hbar}\int_{R_t}^{R_1}[p_{\varepsilon_1}(R)-p_{\varepsilon_2}(R)]dR\right]F_\varepsilon(R_1,p_i)}{v_i\left[\varepsilon_1-\hbar\Delta-\varepsilon(p_i)-\frac{i}{2}\hbar\Gamma_e\right]\left[\varepsilon_2-\hbar\Delta-\varepsilon(p_i)+\frac{i}{2}\hbar\Gamma_e\right]}\ .\end{aligned} \tag{17}$$

The second overlap integral $\langle p_f|\varepsilon_2\rangle\langle\varepsilon_1|p_f\rangle$ may be determined in exactly the same fashion as above to give

$$\langle p_f|\varepsilon_2\rangle\langle\varepsilon_1|p_f\rangle=\int\frac{dR_2}{2\pi v_f}\exp\left[\frac{i}{\hbar}\int_{R_t}^{R_2}[p_{\varepsilon_1}(R)-p_{\varepsilon_2}(R)]dR\right]F_\varepsilon^*(R_2,p_f)\ . \tag{18}$$

The complex-conjugate sign (asterisk) indicates that we have a minus sign in the F integral given by Eq. (15). Hence

$$T=\frac{\hbar^2|\Omega|^2}{4\pi^2}\int d\varepsilon_1\int d\varepsilon_2\frac{\int dR_1\int dR_2S(R_2,R_1)F_\varepsilon(R_1,p_i)F_\varepsilon^*(R_2,p_f)}{v_iv_f\left[\varepsilon_1-\hbar\Delta-\varepsilon(p_i)-\frac{i}{2}\hbar\Gamma_e\right]\left[\varepsilon_2-\hbar\Delta-\varepsilon(p_i)+\frac{i}{2}\hbar\Gamma_e\right]}\ , \tag{19}$$

where we have defined

$$S(R_2,R_1)=\exp\left[\frac{i}{\hbar}\int_{R_1}^{R_2}[p_{\varepsilon_1}(R)-p_{\varepsilon_2}(R)]dR\right]\ . \tag{20}$$

At this stage we perform the ε_1 and ε_2 integrations by defining complex contours and by using the residue theorem. For ε_1 we choose a semicircular contour in the upper-half plane and for ε_2 we choose the same contour in the lower-half plane. In both cases we have a simple pole so that

$$T=\frac{\hbar^2|\Omega|^2}{v_iv_f}\int dR_1\int dR_2S(R_2,R_1)F_{\hbar\Delta+\varepsilon(p_i)\pm(i/2)\hbar\Gamma_e}(R_1,p_i)F^*_{\hbar\Delta+\varepsilon(p_i)\pm(i/2)\hbar\Gamma_e}(R_2,p_f)\ . \tag{21}$$

The ± notation refers to the choice for ε as explained after Eq. (15).

Equation (21) is a general expression involving four integrations that describe the rate of transition into final momentum states p_f. The only approximations we have made are connected with the use of the WKB wave functions. Since it would be very difficult to obtain a solution for this equation we shall now make an approximation by truncating the Taylor series expansion in Eq. (13). This is justified by assuming that the main contributions to the overlap in Eq. (9) occur when η_1 is small. In the absence of damping it is possible to show that the result of this approximation is equivalent to the quasistatic profile that is obtained by making a stationary phase approximation. Provided the damping is small [defined precisely in Eq. (23) below] we would expect the result with damping to be a convolution of a line width with the quasistatic (stationary phase) result. However, this is difficult to demonstrate rigorously, and we do not discount the presence of other contributions to the overlap.

Continuing with this approximation, we must now calculate each of the components in Eq. (21). First, $S(R_2,R_1)$ is expanded as

$$S(R_2,R_1)=\exp\left[\frac{i}{\hbar}\int_{R_1}^{R_2}\left\{\left[2\mu\left[\varepsilon(p_i)+\hbar\Delta+\frac{i}{2}\hbar\Gamma_e-V_e(R)\right]\right]^{1/2}-\left[2\mu\left[\varepsilon(p_i)+\hbar\Delta-\frac{i}{2}\hbar\Gamma_e-V_e(R)\right]\right]^{1/2}\right\}dR\right]\ . \tag{22}$$

The constant μ is the reduced mass for the two-atom system. If we assume that the complex energy is a small perturbation on the real energy where $\varepsilon_1=\varepsilon_2$, that is

$$\tfrac{1}{2}\hbar\Gamma_e \leq \tfrac{1}{5}[\varepsilon(p_i)+\hbar\Delta-V_e(R)] \ , \tag{23}$$

then, using a binomial expansion, we find that

$$S(R_2,R_1)=\exp\left[-\int_{R_1}^{R_2}\frac{\Gamma_e}{v(R)}dR\right] . \tag{24}$$

The velocity on the excited state $v(R)$ is given by

$$v(R)=\frac{\{2\mu[\varepsilon(p_i)+\hbar\Delta-V_e(R)]\}^{1/2}}{\mu} . \tag{25}$$

We now clearly see that Eq. (24) represents the survival of the incoming atom on the excited state. The approximation in Eq. (23) limits our derivation to atom temperatures around the Doppler limit and well above the recoil limit.

To determine the form of $F_{\varepsilon(p_i)+\hbar\Delta\pm(i/2)\hbar\Gamma_e}$ we shall assume initially that only the linear term in Eq. (15) is important. If we again assume Eq. (23) and also that to first order

$$[v(R_1)v(R_1\pm\eta_1)]^{1/2}=v(R_1) \ , \tag{26}$$

then we find the result

$$F_{\hbar\Delta+\varepsilon(p_i)\pm(i/2)\hbar\Gamma_e}(R_1,p_i)=\int\frac{d\eta_1}{v(R_1)}\exp\left[\frac{i}{\hbar}(\{2\mu[\varepsilon(p_i)+\hbar\Delta-V_e(R_1)]\}^{1/2}-[2\mu\varepsilon(p_i)]^{1/2})\eta_1-(\pm)\frac{\Gamma_e\eta_1}{2v(R_1)}\right] . \tag{27}$$

The $(\pm)$ sign is now chosen (corresponding to choosing ε_2 or ε_1 for ε) so that Eq. (27) converges as $\eta_1\rightarrow\pm\infty$, which is equivalent to writing

$$F_{\hbar\Delta+\varepsilon(p_i)\pm(i/2)\hbar\Gamma_e}(R_1,p_i)=\int\frac{d\eta_1}{v(R_1)}\exp\left[\frac{i}{\hbar}(\{2\mu[\varepsilon(p_i)+\hbar\Delta-V_e(R_1)]\}^{1/2}-[2\mu\varepsilon(p_i)]^{1/2})\eta_1-\frac{\Gamma_e|\eta_1|}{2v(R_1)}\right] . \tag{28}$$

This integral produces a Lorentzian, which may be written

$$F_{\hbar\Delta+\varepsilon(p_i)\pm(i/2)\hbar\Gamma_e}(R_1,p_i)=\frac{4\Gamma_e}{\Gamma_e^2+\left[\frac{2v(R_1)}{\hbar}(\{2\mu[\varepsilon(p_i)+\hbar\Delta-V_e(R_1)]\}^{1/2}-[2\mu\varepsilon(p_i)]^{1/2})\right]^2} . \tag{29}$$

This equation may be interpreted as the width in energy of excitation about the resonance point for the photon being absorbed. Similarly, for the region where the spontaneous emission occurs we find

$$F^*_{\hbar\Delta+\varepsilon(p_i)\pm(i/2)\hbar\Gamma_e}(R_2,p_f)=\int\frac{d\eta_2}{v(R_2)}\exp\left[\frac{i}{\hbar}(\{2\mu[\varepsilon(p_i)+\hbar\Delta-V_e(R_2)]\}^{1/2}-[2\mu\varepsilon(p_f)]^{1/2})\eta_2-\frac{\Gamma_e|\eta_2|}{2v(R_2)}\right] . \tag{30}$$

Now, because of the acceleration of the atom in the excited state due to the potential $V_e(R)$, we can drop the decay term in Eq. (30). This means the integral will reduce to a delta function

$$F^*_{\hbar\Delta+\varepsilon(p_i)\pm(i/2)\hbar\Gamma_e}(R_2,p_f)=\frac{2\pi}{v(R_1)}\delta(\{2\mu[\varepsilon(p_i)+\hbar\Delta-V_e(R_2)]\}^{1/2}-[2\mu\varepsilon(p_f)]^{1/2}) . \tag{31}$$

Of course, strictly speaking this corresponds to a Lorentzian function with very small width.

The delta function in Eq. (31) can then be used to perform the R_2 integration in Eq. (21). Making a change of variables from p [in Eq. (31)] to R_2 we have an extra factor

$$\left[\frac{d}{dR_2}p(R_2)\right]^{-1}=v(R_2)\left[\frac{d}{dR_2}V_e(R_2)\right]^{-1} . \tag{32}$$

The value of R_2 is therefore constrained to satisfy

$$V_e(R_2)=\hbar\Delta-[\varepsilon(p_f)-\varepsilon(p_i)] . \tag{33}$$

Finally, putting together all the pieces, we have

$$T=\frac{2\pi\hbar^2|\Omega|^2}{v_i v_f}\int dR_1\left[\frac{dV_e}{dR_2}\right]^{-1}\exp\left[-\int_{R_1}^{R_2}\frac{\Gamma_e}{v(R)}dR\right]\frac{4\Gamma_e\delta(V_e(R_2)-\hbar\Delta+\varepsilon(p_f)-\varepsilon(p_i))}{\Gamma_e^2+\left[\frac{2v(R_1)}{\hbar}(\{2\mu[\varepsilon(p_i)+\hbar\Delta-V_e(R_1)\}^{1/2}-[2\mu\varepsilon(p_i)]^{1/2})\right]^2}\ . \tag{34}$$

This is the most general form of our WKB solution. At this stage we should make a few comments. First of all, the delta-function condition on R_2 in Eq. (34) is consistent with energy conservation. However, it does not satisfy the Franck-Condon principle for all points of excitation because the velocity on the excited-state potential is given by Eq. (25), rather than the Franck-Condon value

$$v_{\mathrm{FC}}(R)=\frac{\{2\mu[\varepsilon(p_i)+V_e(R_1)-V_e(R)]\}^{1/2}}{\mu}\ , \tag{35}$$

which maintains $v_{\mathrm{FC}}(R_1)=v_i$. We see that $v_{\mathrm{FC}}(R)$ is only equal to $v(R)$ if $V_e(R_1)=\hbar\Delta$, i.e., we are at resonance for the transition. The question whether to use $v_{\mathrm{FC}}(R)$ or $v(R)$ remains an ambiguity in the classical method of Julienne and Vigué [5]. However, it is clear from our WKB method that energy conservation is the more fundamental principle in the theories of Gallagher and Pritchard [4] and Julienne and Vigué and that $v(R)$ defined in Eq. (25) is the more natural choice to describe the excited-state velocity of the incoming atom.

Nevertheless, it is possible to show that, for a range of excitation points, the Franck-Condon principle and the principle of energy conservation can be simultaneously satisfied. If we limit the range of R_1 to be around resonance so that

$$|\hbar\Delta-V_e(R_1)|\le\tfrac{1}{5}\varepsilon(p_i)\ , \tag{36}$$

then we may expand the survival term $S(R_2,R_1)$ in Eq. (22) as

$$S(R_2,R_1)=\exp\left[\frac{i}{\hbar}\int_{R_1}^{R_2}\left[\frac{\hbar\Delta-V_e(R_1)+\frac{i}{2}\hbar\Gamma_e}{v_{\mathrm{FC}}(R)}-\frac{\hbar\Delta-V_e(R_1)-\frac{i}{2}\hbar\Gamma_e}{v_{\mathrm{FC}}(R)}\right]dR\right]\ , \tag{37}$$

which simplifies to an equation corresponding to Eq. (24)

$$S(R_2,R_1)=\exp\left[-\int_{R_1}^{R_2}\frac{\Gamma_e}{v_{\mathrm{FC}}(R)}dR\right]\ . \tag{38}$$

Similarly, if the approximation in Eq. (36) is valid then we may expand Eq. (29) using the binomial theorem, to obtain the line-shape function

$$F_\varepsilon(R_1,p_i)=\frac{4\Gamma_e}{\Gamma_e^2+4\left[\frac{\hbar\Delta-V_e(R_1)}{\hbar}\right]^2}\ . \tag{39}$$

Hence, for the range of R_1 where the approximation are valid we obtain

$$T=\mathrm{const}\times\int dR_1\exp\left[-\int_{R_1}^{R_2}\frac{\Gamma_e}{v_{\mathrm{FC}}(R)}dR\right]\times\frac{1}{1+4\left[\frac{\hbar\Delta-V_e(R_1)}{\hbar\Gamma_e}\right]^2}\ . \tag{40}$$

This is exactly the form of the Julienne and Vigué expression obtained using classical methods. Because this expression is still consistent with Eq. (33), we see that in this limit it is possible to satisfy the Franck-Condon principle and have energy conservation. It is now completely arbitrary as to whether $v_{\mathrm{FC}}(R)$ or $v(R)$ is used to track the excited-state velocity, because they both may be used to define the survival when Eq. (36) is valid.

As a final comment, if we had maintained the quadratic term in Eq. (15) and/or taken the next order of the expansion in Eq. (26), then we would obtain a general solution for $F_\varepsilon(R_1,p_i)$ of the form

$$F_\varepsilon(R_1,p_i)=\int d\eta_1[i(a\eta_1-b\eta_1^2)-c|\eta_1|]\ . \tag{41}$$

This integral corresponds to adding both a Gaussian and Lorentzian width broadening the delta function. We would expect the Gaussian component to be a small perturbation on the line shape given in Eq. (30) because $V_e(R)$ is slowly varying (i.e., reasonably flat) at the point of excitation.

III. TRAP-LOSS PROCESS FOR CESIUM

In this section, we shall use the results of our WKB derivation to check the theory of Julienne and Vigué [5] and Gallagher and Pritchard [4]. For the case of trap loss in atomic sodium, we do not expect Eq. (34) to give significantly different results from those stated by Julienne and Vigué, because most of the contribution comes from around the resonance point, where approximation Eq. (36) is valid. As we have already shown, in this range the two methods are equivalent.

However, in the investigation of trap loss in cesium, Julienne and Vigué have suggested that most of the survival originates in the far wing of the absorption line shape. In this regime, where Eq. (36) is no longer valid, we cannot justify the use of equation Eq. (40), using either $v_{\mathrm{FC}}(R)$ or $v(R)$. We would therefore like to discover if there is a significant difference between using Eq. (34) and Eq. (40).

To make our analysis we shall use exactly the same experimental parameters as Julienne and Vigué [5]. For the cesium 0_u^+ state, the excited-state linewidth is $\Gamma_e=\frac{4}{3}\gamma=4.30107\times10^7\ \mathrm{s}^{-1}$, and we shall assume that the laser field is tuned one atomic linewidth to the red of the atomic resonance, i.e., $\Delta=-\gamma$. At this detuning, the excited-state potential causes the ground-excited transition to come into resonance at $R_r=2928a_0$ ($\approx \lambda$) so that

$$\frac{C}{R_r^3}=\hbar|\Delta|=\hbar\gamma\rightarrow C=\hbar\gamma(2928a_0)^3\ . \tag{42}$$

The initial temperature of the incoming atom on the ground state is $T_i=1$ mK, with $p_i=\sqrt{2\mu k_B T_i}$. Julienne and Vigué suppose that the trap depth is of the order 1 K, which corresponds to a final temperature of $T_f=2$ K for the incoming atom, if there is to be sufficient energy for each atom to escape from the trap.

Finally, it is not necessary to specify the Rabi frequency Ω as it forms a constant in Eq. (34). However, if we assume that $|\Omega|\leq\Gamma_e$, then we are certainly in a nonsaturated regime where or theory is justified.

We are now ready to numerically integrate an expression of the form

$$T=\mathrm{const}\times\int dR_1 T(R_1)\ , \tag{43}$$

where

$$T(R_1)=S(R_2,R_1)F(R_1)\ . \tag{44}$$

The various choices for S and F are given by the choice of theory used. We shall label choice 1 as our theory presented in Sec. II which gives Eq. (24) for S and Eq. (29) for F. The classical theory of Julienne and Vigué, while maintaining the Franck-Condon principle we shall designate as choice 2, involves Eq. (38) for S and Eq. (39) for F. Finally, choice 3 is defined as where the lineshape is given by Eq. (39) as in the classical theory, but the survival is determined using energy-conserving principles, Eq. (24).

The integral over R_1 in Eq. (43) can be limited to $R_{\mathrm{lower}}=200a_0$ and $R_{\mathrm{upper}}=4000a_0$, because $T(R_1)$ is effectively zero outside this range. The value of dR_1 is chosen sufficiently small that a simple trapezoidal rule may be used for the integration. For $T_f=2$ K the delta-function condition in Eq. (34) specifies that $R_2=146a_0$.

The results for the various choices are displayed in Figs. 2–4, where to make comparisons easier we plot choice 1 versus choice 2 in Fig. 2, choice 1 versus choice 3 in Fig. 3, and choice 2 versus choice 3 in Fig. 4. In order that $S(R_1)$, $F(R_1)$, and $T(R_1)$ may be compared on the same plot we have multiplied $T(R_1)$ by an extra factor of 100. Figure 4 is similar to that depicted in Fig. 6 of Julienne and Vigué [5], except that our treatment does not consider the decrease in the survival at small R due to angular momentum effects. With the same constant factor used in Eq. (43) for each choice, the integrated rate T has the values

$$\begin{aligned}T_{\mathrm{choice}\ 1}&=0.7097\ ,\\ T_{\mathrm{choice}\ 2}&=0.5526\ ,\\ T_{\mathrm{choice}\ 3}&=0.9752\ .\end{aligned} \tag{45}$$

Now, Julienne and Vigué also find a ratio of approximately 60% between choice 2 and choice 3. When they used these values in an expression for the collision rate coefficient, the energy-conserving result was found to be too high to agree with the experimental results, which gave some justification for the choice that satisfies the Franck-Condon principle. However, our new energy-conserving choice (choice 1) gives a value for T which is approximately 25% smaller than with choice 3, so that

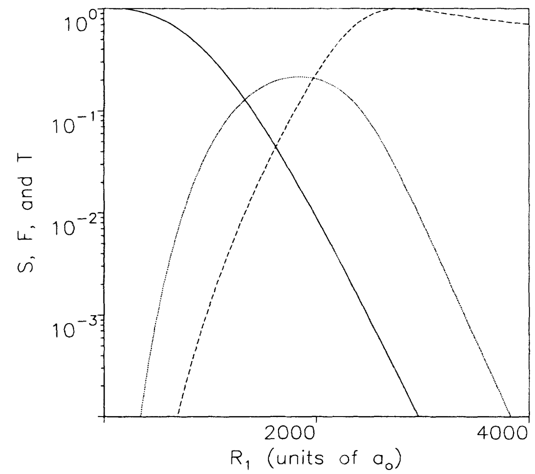

FIG. 2. Graph of survival $S(R_1)$, line shape $F(R_1)$, and rate $T(R_1)$ (small dashes) vs R_1 (interatomic separation at excitation) for choice 1 (semiclassical result with energy conservation, solid lines) and choice 2 (JV result with Franck-Condon principle, small dashes). Parameters: $dR_1=2a_0$, $T_i=1$ mK, $T_f=2$ K, $\gamma=-\Delta=3.2258\times10^7\ \mathrm{s}^{-1}$.

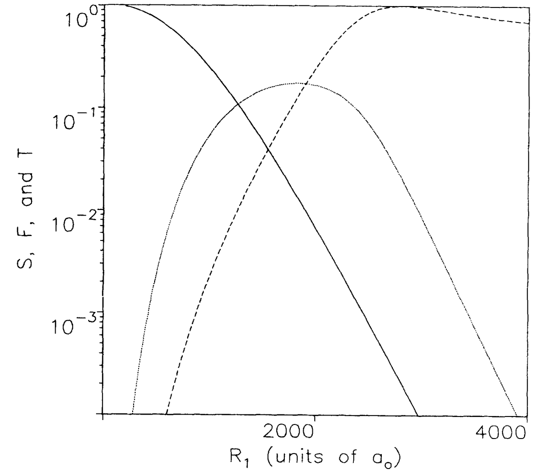

FIG. 3. Graph of survival $S(R_1)$, line shape $F(R_1)$ and rate $T(R_1)$ vs R_1 (interatomic separation at excitation) for choice 1 (semiclassical result with energy conservation, solid lines) and choice 3 (JV result with energy conservation, small dashes). Parameters: $dR_1=2a_0$, $T_i=1$ mK, $T_f=2$ K, $\gamma=-\Delta=3.2258\times10^7\ \mathrm{s}^{-1}$.

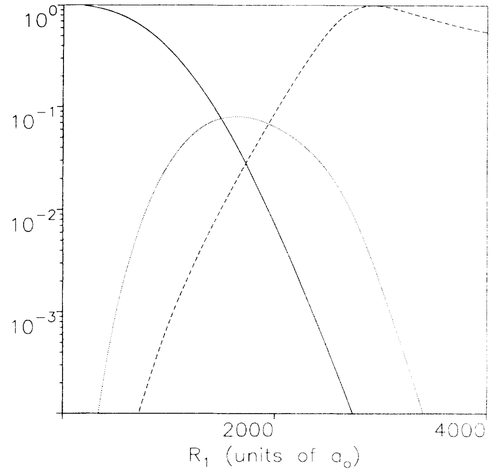

FIG. 4. Graph of survival $S(R_1)$, line shape $F(R_1)$, and rate $T(R_1)$ vs R_1 (interatomic separation at excitation) for choice 2 (JV result with Franck-Condon principle, solid lines) and choice 3 (JV result with energy conservation, small dashes). Parameters: $dR_1=2a_0$, $T_i=1$ mK, $T_f=2$ K, $\gamma=-\Delta=3.2258\times10^7$ s^{-1}.

the fit with experiment is much better. The reason for this reduction can be seen by looking at Fig. 3. The survival function is the same in both cases, but the lineshape $F(R_1)$ tails off more quickly on the inner far wing for choice 1. Since this is where a considerable proportion of $T(R_1)$ occurs, a significant reduction in overall T can be achieved.

Comparing choices 1 and 2 in Fig. 2, the survival in the inner wing for the energy-conserving choice is larger, as the incoming atom is given a greater initial velocity on the excited state for small R_1. However, this is again balanced by the smaller value for the lineshape at these values of R.

IV. CONCLUSION

In this paper we have produced a semiclassical WKB theory for the excited-state potential absorption and spontaneous emission process which forms part of the loss mechanism for atoms in an optical trap. Our intention was to provide a firmer justification for the classical models of trap loss developed by Gallagher and Pritchard [4] and Julienne and Vigué [5]. We have explicitly performed our calculation for the radiative escape mechanism, Eq. (1). However, because the fine-structure mechanism also involves an absorption profile and a survival to small separations (where now a fine-structure change occurs), our results also apply for Eq. (2).

In our analysis we have only treated part of the total problem considered by Julienne and Vigué and have ignored angular momentum effects and the physics of the short-range collisions. Therefore the theory we have presented is not intended to replace the existing trap-loss theory. Instead we consider we have achieved two main results. First, the semiclassical analysis clearly demonstrates that the principle of energy conservation is more fundamental than the Franck-Condon principle. This means that the velocity on the excited state is determined in order to satisfy overall energy conservation rather than conserve velocity during a photon transition. Second, the best results for trap-loss coefficients will be obtained by using Eq. (29) for the absorption line shape and Eq. (24) to describe the survival on the excited state. If the principle excitation occurs around resonance we have shown that the result is identical to that obtained using the Julienne and Vigué theory. However, for cesium traps, the main contribution to the trap loss arises from excitation in the inner far wing of the absorption line shape, and the results are significantly different.

To determine the reason for the reduction in the line shape it is useful to write F, from Eq. (29), as

$$F_\varepsilon(R_1,p_i)=\frac{4\Gamma_e}{\Gamma_e^2+4\left[\frac{2v(R_1)}{v(R_1)+v_i}\left[\frac{\hbar\Delta-V_e(R_1)}{\hbar}\right]\right]^2} . \tag{46}$$

Comparing this expression with Eq. (39), we see that our new form of the line shape is the Julienne and Vigué result with the addition of a factor

$$\chi=\frac{2v(R_1)}{v(R_1)+v_i} . \tag{47}$$

At the Franck-Condon point $v(R_1)=v_i$, so that $\chi=1$. However, for off-resonant absorption in the inner wing of the line shape, $v(R_1)>v_i$ and so the line shape is reduced by a factor χ^2. The upper limit of χ is 2 so that the maximum reduction in the line shape is a factor of 4. We can interpret this reduction as resulting from oscillations in the overlap between ground and excited states if the velocity on each level is significantly different.

It is also significant that χ is similar to the "correction" factor used by Band and Julienne [6] in their optical-Bloch-equation method. We have generalized our method to include angular momentum and compared the results of the averaged survival and excitation results with their calculations. We find a close comparison with the results in Ref. [6], and our method also appears to give half the reduction obtained using the new form of their equations [8]. We will continue to investigate this relationship.

In developing our semiclassical WKB theory we have had to make several assumptions. First, it was necessary to assume that the atoms were not saturated by the effect of the laser field. This would affect the way the population in the excited state is created as the atom moves through the resonance for the transition. In addition, our method is based on a WKB wave function and the principle of stationary phase. It is possible, therefore, that there are extra contributions to the integral away from the point of stationary phase. Any extra terms should be revealed by solving numerically the integrals contained in the full expression Eq. (21). This method should also provide a low-intensity justification of the assumptions made in the optical-Bloch-equation calculation.

To act as a final check on the results of this paper we are developing a quantum-mechanical treatment of the

RE trap-loss mechanism (Holland, Smith, and Burnett [9]). This approach will go one step further than the optical-Bloch technique of Band and Julienne [6] and explicitly solve the Schrödinger equation describing the evolution of the ground- and excited-state wave functions. The effect of the spontaneous emission is the included using the quantum Monte Carlo method of Dalibard, Castin, and Mølmer [10].

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