Semiclassical calculation of the diffusion constant for the Λ system momentum

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We present a one-dimensional, semiclassical calculation of the momentum diffusion constant for a stationary Λ atom. We show that if the difference detuning between the driving fields is zero, the diffusion vanishes, and we interpret this behavior in terms of the atom-field eigenstates. We present explicit solutions to the equations of motion in the special case where one of the driving fields vanishes and compare them to the case of a two-level atom at a field node. Finally, we examine the correspondence between the semiclassical and quantum-mechanical analyses at zero difference detuning and we show a correspondence between the semiclassical and quantum-mechanical dark states when the driving fields are superpositions of plane waves with the same magnitude of wave vector.

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I. INTRODUCTION

The cooling and the trapping of Λ three-level atoms in Raman resonant fields (see Fig. 1) have been of great interest for some time. The Λ system is shown in Fig. 1 and consists of two long-lived ground states $|a\rangle$ and $|b\rangle$ and an excited state $|e\rangle$. We assume that this system is excited by two laser fields E_1 and E_2 , where E_1 interacts only with the transition $|a\rangle \rightarrow |e\rangle$ and \mathbf{E}_2 interacts only with the transition from the ground state $|b\rangle \rightarrow |e\rangle$. It has been shown that if E_1 and E_2 are counterpropagating traveling waves with no difference detuning Δ , then there is no momentum diffusion in the steady state [1]; consequently, there is no limit on the narrowness of the momentum distributions. Unfortunately, though there is compression in momentum space, there is no semiclassical cooling or compression in position space. In contrast, it has been shown that if the two driving fields are standing waves, then there can be significant compression in position space, as well as semiclassical cooling and

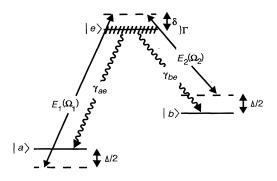


FIG. 1. A system.

velocity-selective coherent population trapping [2,3]. A trapping configuration that uses these forces has been proposed [4]. The ultimate temperature and density that can be achieved in a standing-wave Raman trap may be limited by the diffusive processes which accompany the cooling and trapping [5].

In this paper, we present a semiclassical calculation of the momentum diffusion coefficient D_p for a stationary atom in one dimension [6]. This calculation shows that if the difference detuning $\Delta=0$, then the diffusion coefficient D_p will be zero. This semiclassical result is independent of all other field parameters, including the functional form of the fields. It is consistent with the well-known result that $D_p = 0$ if the two excitation fields are counterpropagating traveling waves [7]. It is also consistent with the fully quantum-mechanical proof of the existence of a state with zero diffusion in the case where the two excitation fields are standing waves and the difference detuning $\Delta=0$ [2]. This calculation is, however, more general since it also allows the momentum diffusion coefficient to be evaluated for cases where $\Delta \neq 0$. Finally, we examine the correspondence between the semiclassical and quantum-mechanical analyses at zero difference detuning and we show that there is a correspondence between quantum-mechanical and semiclassical dark states when the driving fields are superpositions of plane waves with the same magnitude of wave vector.

II. DESCRIPTION OF SEMICLASSICAL CALCULATION

A. Hamiltonian and equations of motion

In the semiclassical description, the Hamiltonian H for the Λ system is given by

$$H = H_A - \mathbf{d} \cdot \mathbf{E}(z, t) . \tag{1}$$

Here $H_A = -\hbar\omega_{ae}|a\rangle\langle a| - \hbar\omega_{be}|b\rangle\langle b|$ is the bare atomic Hamiltonian and d is the electric-dipole operator. We restrict ourselves to one spatial dimension z and take $\mathbf{E}(z,t)$ to have a positive-frequency component

$$\mathbf{E}^{(+)}(z,t) = \frac{1}{2} [\hat{\epsilon}_1 E_1(z) e^{-i\omega_1 t} + \hat{\epsilon}_2 E_2(z) e^{-i\omega_2 t}] . \tag{2}$$

We assume that the polarizations $\hat{\epsilon}_{1,2}$ are chosen such that $E_{1,2}(z)$ interact separately with the $|a,b\rangle \rightarrow |e\rangle$ transitions. Eliminating antiresonant terms and transforming to the rotating frame, we have

$$H_A = \hbar(\delta_1|a\rangle\langle a| + \delta_2|b\rangle\langle b|), \qquad (3)$$

$$-\mathbf{d} \cdot \mathbf{E}(z) = -\frac{\hbar}{2} [\Omega_1 | e \rangle \langle a | + \Omega_2 | e \rangle \langle b | + \text{H.c}] . \quad (4)$$

We have defined the detuning $\delta_{1,2}$ and the Rabi frequencies $\Omega_{1,2}$ by

$$\delta_{1,2} = \omega_{1,2} - \omega_{(a,b)e}$$
, (5)

$$\Omega_{1,2} = \frac{\langle e | \mathbf{d} \cdot \hat{\epsilon}_{1,2} | a, b \rangle E_{1,2}}{\hbar} . \tag{6}$$

We further define the common mode detuning δ and the differential detuning Δ by

$$\delta = \frac{1}{2}(\delta_1 + \delta_2) , \qquad (7)$$

$$\Delta = \delta_1 - \delta_2 , \qquad (8)$$

so that we can symmetrize H_A by displacing the zero of energy by $-\hbar\delta$. Making this transformation, we have for H

$$\begin{split} H &= \frac{\hbar \Delta}{2} (|a\rangle\langle a| - |b\rangle\langle b|) - \hbar \delta |e\rangle\langle e| \\ &- \frac{\hbar}{2} [\Omega_1 |e\rangle\langle a| + \Omega_1^* |a\rangle\langle e| \\ &+ \Omega_2 |e\rangle\langle b| + \Omega_2^* |b\rangle\langle e|] \;. \end{split} \tag{9}$$

Assuming that the population of $|e\rangle$ decays at a rate Γ , with rates $\gamma_{(a,b)e}$ to $|a,b\rangle$, we get the equations of motion of the density-matrix elements by projection over the following master equation for the density matrix ρ :

$$\frac{d\rho}{dt} = \frac{1}{i\hbar} [H,\rho] - \frac{\Gamma}{2} \{ |e\rangle\langle e|,\rho \}
+ (\gamma_{ae}|a\rangle\langle a| + \gamma_{be}|b\rangle\langle b|)\rho_{ee} .$$
(10)

We will use the equations of motions for the density-matrix elements when computing D_p .

B. Diffusion constant

The diffusion constant D_p measures the rate of heating of the atomic momentum distribution and is defined as [6].

$$2D_{p} = \frac{d}{dt} (\langle \mathbf{p} \cdot \mathbf{p} \rangle - \langle \mathbf{p} \rangle \cdot \langle \mathbf{p} \rangle) . \tag{11}$$

To calculate these time derivatives, we use the Heisen-

berg equation of motion $d\mathbf{p}(t)/dt = (1/i\hbar)[\mathbf{p}(t), H]$. The internal operators of the atom commute with the momentum operator when taken at the same time, as do the creation and annihilation operators of the vacuum field \mathbf{E}_{vac} . Since for O(z), any operator function of z, we have $[p_z, O(z)] = -i\hbar\partial O(z)/\partial z$, and since \mathbf{E}_{vac} has zero average gradient [8],

$$\frac{d\langle \mathbf{p}(t)\rangle}{dt} \equiv \langle \mathbf{f}(t)\rangle = \langle \nabla \Omega_1 | e \rangle \langle a | + \nabla \Omega_2 | e \rangle \langle b | + \text{H.c.} \rangle ,$$
(12)

$$\frac{d\langle \mathbf{p} \cdot \mathbf{p} \rangle}{dt} = \langle \mathbf{p} \cdot \mathbf{f}(t) \rangle + \langle \mathbf{f}(t) \cdot \mathbf{p} \rangle = 2 \operatorname{Re} \langle \mathbf{f}(t) \cdot \mathbf{p}(t) \rangle . \tag{13}$$

With this substitution, the diffusion constant becomes

$$D_{p} = \operatorname{Re} \int_{0}^{\infty} dt \left[\langle \mathbf{f}(0) \cdot \mathbf{f}(t) \rangle - \langle \mathbf{f}(0) \rangle \cdot \langle \mathbf{f}(t) \rangle \right]. \tag{14}$$

The time zero is chosen for convenience and we have rewritten $\mathbf{p}(t) = \int dt' \mathbf{f}(t')$. In this analysis, we only consider the diffusion in the steady state, so we can assume that the atom is in the steady state at time zero. We then may replace $\langle \mathbf{f}(0) \rangle \cdot \langle \mathbf{f}(t) \rangle$ with $\langle \mathbf{f}(0) \rangle \cdot \langle \mathbf{f}(0) \rangle$ so that finally [6],

$$D_{p} = \operatorname{Re} \int_{0}^{\infty} dt \left[\langle \mathbf{f}(0) \cdot \mathbf{f}(t) \rangle - \langle \mathbf{f}(0) \rangle \cdot \langle \mathbf{f}(0) \rangle \right]. \tag{15}$$

Using (12) for the force and defining the projection operators

$$\begin{split} P_{ij} &= |i\rangle\langle j|, \\ S &= \{\nabla\Omega_1 P_{ea}, \nabla\Omega_1^* P_{ae}, \nabla\Omega_2 P_{be}, \nabla\Omega_2^* P_{eb}\} \end{split}$$

we may rewrite the diffusion constant as

The final terms are due to the commutator between (free) fields and represent the momentum recoil due to spontaneous emission. We can add them in by noting that the decay from the upper state due to spontaneous emission occurs at a rate $\gamma_{ea}(\gamma_{eb})$, the momentum uncertainty per spontaneous decay is simply $\hbar^2 k_1^2 (\hbar^2 k_2^2)$, and the number of decays is governed by the excited state population, which is $\rho_{ee} = \langle P_{ae}^{\dagger} P_{ae}(0) \rangle$.

We see from (16) that D_p depends on the two-time correlation functions of the atomic operators. In order to calculate these correlations, we use the quantum regression theorem [9]. This theorem relates the equation of motion of a two-time correlation function such as $\langle P_{ae}(0)P_{ae}(t)\rangle$ to that of a single operator equation of motion such as $\langle P_{ae}(0)P_{ae}(t)\rangle$ is formally equivalent to $\langle P_{ae}(t)\rangle$ = $\mathrm{tr}[\rho P_{ae}(t)] = \rho_{ea}$ with ρ replaced by $\rho P_{ae}(0)$ [10]. For example, if we solve the equation of motion of $\langle P_{ae}(t)\rangle$ for an arbitrary set of initial conditions and write

$$\langle P_{ae}(t) \rangle = u_0(t) + u_1(t) \langle P_{ae}(0) \rangle + u_2(t) \langle P_{ae}(0) \rangle + u_3(t) \langle P_{be}(0) \rangle + u_4(t) \langle P_{eb}(0) \rangle + u_5(t) \langle P_{aa}(0) \rangle + u_6(t)(t) \langle P_{ee}(0) \rangle + u_7(t) \langle P_{bb} \rangle + u_8(t) \langle P_{ba}(0) \rangle + u_9(t) \langle P_{ab}(0) \rangle ,$$

$$(17)$$

then

$$\langle P_{ae}(0)P_{ae}(t)\rangle = (u_0 + u_6)\langle P_{ae}(0)\rangle + u_2\langle P_{aa}(0)\rangle + u_4\langle P_{ab}(0)\rangle . \quad (18)$$

Proceeding in this way and using Laplace transforms to calculate quantities such as $\int_0^\infty dt \ u_i(t)$, we arrive at an expression for D_p . This expression is quite complicated in general, so a plot better indicates the physical features of the diffusion.

III. NUMERICAL RESULTS

In Fig. 2, we plot D_p against differential detuning Δ for the following sets of parameters: $\Omega_1 = \Omega_2 = 5.0$ (dotted line) and $\Omega_1 = 1.0$, $\Omega_2 = 7.0$ (dashed line). All frequencies are given in units of $\gamma_{ea} = \gamma_{eb} = 1.0$ and momenta are expressed in units of $\hbar k$, where k is the field momentum. (We choose the frequencies of the driving fields to be equal for convenience.) Notice that the effective Rabi frequency $\Omega = \sqrt{\Omega_1^2 + \Omega_2^2}$ is the same for both plots. Two features of the plot are striking. First, the diffusion constant D_p exhibits the Raman dip characteristic of the excited-state population, and second, D_p actually vanishes when $\Delta = 0$, which is precisely when the excited-state population vanishes. In fact, the result that $\Delta = 0$ gives $D_p = 0$ holds for general monochromatic driving fields.

A. Qualitative discussion of numerical results

1. Vanishing of D_n for $\Delta = 0$

A simple way to understand the result of vanishing diffusion when $\Delta=0$ is the following. The diffusion constant represents the rate of change of an expectation value in a particular state. If that state is an eigenstate of

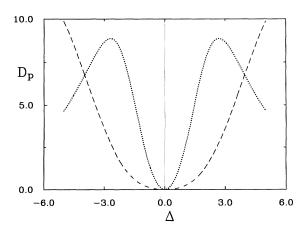


FIG. 2. Plots of diffusion for $\Omega_1 = \Omega_2 = 5.0\Gamma$ (dotted line) and $\Omega_1 = 1.0\Gamma$, $\Omega_2 = 7.0\Gamma$ (dashed line).

the full Hamiltonian, then no expectation values can change. When $\Delta=0$, one can see from the Hamiltonian (9) that the state $|-\rangle$ is an eigenstate of H with eigenvalue zero, where

$$|-\rangle = \frac{1}{\sqrt{\Omega_1^2 + \Omega_2^2}} (\Omega_2 |a\rangle - \Omega_1 |b\rangle , \qquad (19)$$

$$H|-\rangle = 0. (20)$$

Since $|-\rangle$ is decoupled from the laser excitation, we know that when $\Delta = 0$, the state $|-\rangle$ is an eigenstate of the atom plus laser photons system. Yet what makes $|-\rangle$ unique in terms of diffusion is that it is an eigenstate of the atom plus laser photons plus vacuum field (spontaneous photons) system. Since the dark state is never excited into $|e\rangle$, it is never connected with spontaneous photons and remains stationary. This should be contrasted with a two-level dressed state, in which the dressed state is an eigenstate of the atom plus laser system, but each dressed state contains a component of the excited state. This component couples the dressed state to the vacuum field so that spontaneous emissions occur and one dressed state decays into another, preventing them from qualifying as eigenstates of the extended atomlaser-vacuum system. We should note that the vanishing of the diffusion constant here is not a strictly valid result since the idea of a semiclassical diffusion constant is based on adiabatic elimination of fast internal variables and when the condition $\Delta = 0$ is fulfilled, the internal time scale of the atom is no longer fast. However, we can still use the result as a consistency check for our calculation.

2. Effect of unequal Rabi frequencies

The case of unbalanced Rabi frequencies clearly exhibits a broader region around its minima than the case of balanced Rabi frequencies. This is understandable if we the process in the dark state $\{|-\rangle, |+\rangle \equiv (1/\Omega)(\Omega_1|a\rangle + \Omega_2|b\rangle), |e\rangle\}.$ show that $|-\rangle$ is coupled to $|+\rangle$ at a rate $\Delta \sin 2\theta$, where $\tan(\theta) = \Omega_1/\Omega_2$ [11]. The $|+\rangle$ state then strongly couples to the excited state at a rate Ω , while $|-\rangle$ is never directly coupled to the excited state. If Ω_1 is much larger than Ω_2 , $\sin(2\theta)$ tends toward zero, so that the coupling between $|-\rangle$ and $|+\rangle$ is very small even for a range of nonzero Δ . Thus, as the fields become unbalanced, the coupling to the excited state, and thus the diffusion, becomes less sensitive to changes in the differential detuning, giving rise to a broadened area around the minima. We note in passing that if we plotted the diffusion constant as a function of $\Delta \sin 2\theta$, the widths of the two plots should be the same.

3. Analytic solution at a field node

Finally, we discuss the special case of a three-level atom at a field node. This case is of particular interest since in a two-level atom at a standing-wave field node, even though the excited-state population is zero, the diffusion is nonzero. This has been interpreted by stating that even though the field value is zero, the atom's fluctuating dipole moment interacts with the nonzero field gradient, giving rise to a random diffusive force [6]. This is not the case in the three-level system, as we will now show expicitly.

When one of the driving fields (Ω_1) vanishes, the optical Bloch equations predict that the population will all be pumped into $|a\rangle$. In this limit, the Λ system would appear like a two-level system at a field node, so intuitively we expect that D_p would be given by an expression similar to that of a two-level system at a field node. However, our calculation indicates that D_p always vanishes when $\Delta=0$. One way to understand this result physically is to look back to the optical Bloch equations.

Letting ρ be the atomic density matrix and setting δ_1 , the detuning on the $|a\rangle \rightarrow |e\rangle$ transition, equal to zero for convenience, we find that the equations of motion of ρ_{ae} and ρ_{ab} become decoupled from the other density-matrix elements. In particular, if Γ is the total decay rate of the state $|e\rangle$,

$$\frac{d\rho_{ae}}{dt} = -\frac{\Gamma}{2}\rho_{ae} + \frac{1}{2}i\Omega_2\rho_{ab} , \qquad (21)$$

$$\frac{d\rho_{ab}}{dt} = \frac{1}{2}i\Omega_2^*\rho_{ab} . \tag{22}$$

We notice that this equation of motion for ρ_{ae} is not the same as the equation of motion for the coherence σ_{ge} in an undriven two-level system, which is given by

$$\frac{d\sigma_{ge}}{dt} = -\frac{\Gamma}{2}\sigma_{ge} , \qquad (23)$$

where Γ is the decay rate. In the three-level system there is the extra term ρ_{ab} which corresponds to the coherences between the two ground states. This extra term represents the coherent excitation of the two ground states and marks a fundamental difference between the two- and three-level systems.

We find, using the quantum regression analysis, that D_p depends only on ρ_{ae} . If we write the time-dependent solution of ρ_{ae} (for an arbitrary set of initial conditions) as $\rho_{ae} = a_0(t) + a_{ae}(t)\rho_{ae}(0) + a_{ab}\rho_{ab}(0) + a_{eb}\rho_{eb}(0) + \cdots$, and so on for the nine density-matrix elements, we find that

$$D_p = \int_0^\infty a_{ae}^* \rho_{aa}(0) dt . \tag{24}$$

Combining (21) and (22) above, we notice that the equation of motion for a_{ae} is formally equivalent to that of a damped harmonic oscillator with damping rate $\Gamma/2$ and natural frequency Ω_2 . The solution is

$$a_{ae} = \frac{-\lambda_{-} - \frac{1}{2}\Gamma}{\lambda_{+} - \lambda_{-}} e^{\lambda_{+}t} + \frac{\lambda_{+} + \frac{1}{2}\Gamma_{2}}{\lambda_{+} - \lambda_{-}} e^{\lambda_{-}t}, \qquad (25)$$

where

$$\lambda_{+} = -\Gamma \pm -(\Gamma^{2} - 4\Omega_{2}^{2})^{1/2} . \tag{26}$$

Integrating this solution shows that D_p vanishes; it is important to notice that D_p does not vanish because the kernel of the integral is identically zero, but rather because of a sign change in the force correlation over time.

In the limit that $\Omega_2 \ll \Gamma$, there is a simple physical interpretation of this cancellation. In this limit, $\lambda_+ \simeq -\Omega_2^2/2\Gamma^2$ and $\lambda_- \simeq -\Gamma/2$; λ_+ is the rate at which the amplitude of the $|+\rangle$ state decays into the $|-\rangle$, while λ_+ is the natural decay rate of $|e\rangle$ into $|-\rangle$. The amplitudes corresponding to these decays are exactly out of phase: because Ω_1 vanishes, the $|+\rangle$ state is simply $|b\rangle$ and the population flopping between $|e\rangle$ and $|b\rangle$ occurs at the Rabi flopping rate. The amplitude extrema of these two states occur exactly 180° out of phase, so that the time development of $e \rangle$ and $|b \rangle$ is out of phase. The decays of their amplitudes therefore have opposite signs; the rapidly decaying term (λ_{-}) corresponds to a direct decay from $|e\rangle$ to $|a\rangle$, while the slowly decaying term (λ_+) corresponds to a decay from $|b\rangle$, mediated by the driving field Ω_2 and out of phase with the direct decay. The oppositely phased amplitudes lead to a vanishing D_n .

IV. CORRESPONDENCE BETWEEN SEMICLASSICAL AND QUANTUM-MECHANICAL RESULTS

One of the difficulties with the semiclassical result that $D_p = 0$ when $\Delta = 0$ is that the semiclassical theory is based on an adiabatic elimination of fast internal variables and that when $\Delta \rightarrow 0$, the internal time scale of a stationary atom can become very long. In this section, we address the question of the correspondence between the semiclassical and quantum-mechanical results that the diffusion is zero at $\Delta = 0$.

Physically, the vanishing of D_p semiclassically arises from the existence of the dark state, which is an eigenstate of H. We now want to see whether this semiclassical dark state will carry over to the quantum-mechanical dark state $|D\rangle$, where $|D\rangle$ contains both internal and translational (center-of-mass) degrees of freedom. Semiclassically, one can always construct a dark state at each point z, using the prescription (19). We want to see under what conditions one can also construct a quantum-mechanical dark state which does not experience momentum diffusion. As before, we restrict ourselves to one spatial dimension z.

In order to construct the quantum-mechanical dark state, we consider the full Hamiltonian H, including the kinetic terms:

$$H = \frac{\hat{p}_z^2}{2M} + H_A - \mathbf{d} \cdot \mathbf{E}(\hat{\mathbf{z}}) ; \qquad (27)$$

 H_A and $-\mathbf{d} \cdot \mathbf{E}(\mathbf{\hat{z}})$ are the same as those given in Eqs. (4) and (9), except that we treat the position $\mathbf{\hat{z}}$ as an operator. The two criteria for constructing a dark state $|D\rangle$ are that first, $|D\rangle$ must not "see" the laser interaction, so it must have eigenvalue zero with respect to the dipole interaction term, and second, $|D\rangle$ must be a stationary state, so it must be an eigenstate of H:

$$-\mathbf{d} \cdot \mathbf{E}(\widehat{\mathbf{z}}) | D \rangle = 0 , \qquad (28)$$

$$H|D\rangle = \lambda_D|D\rangle . \tag{29}$$

We take $|D\rangle$ as a superposition of the two ground states, where each of the ground states has some associated translational state $|\psi_i\rangle$:

$$|D\rangle = |\psi_a\rangle \otimes |a\rangle + |\psi_b\rangle \otimes |b\rangle . \tag{30}$$

Letting $\psi_i(z) = \langle z | \psi_i \rangle$, condition (28) for a dark state gives

$$\psi_a(z)\Omega_1(z) = -\psi_b(z)\Omega_2(z) , \qquad (31)$$

so that

$$\psi_{a,b}(z) = \pm f(z)\Omega_{2,1}(z)$$
, (32)

where f(z) is some function of z that we may choose. Condition (29) then implies that

$$\left[-\frac{\hslash^2}{2M} \frac{\partial^2}{\partial z^2} - \lambda_D \right] [\psi_{a,b}(z)] = 0 , \qquad (33)$$

$$\left[-\frac{\hbar^2}{2M} \frac{\partial^2}{\partial z^2} - \lambda_D \right] [f(z)\Omega_{2,1}(z)] = 0.$$
 (34)

Condition (34) is the general criterion for the quantum-mechanical dark state and it can place restrictions on the allowed fields $\Omega_{1,2}(z)$. We now specialize our analysis to the case in which the ground states $|a\rangle$ and $|b\rangle$ are degenerate; this situation arises, for example, when the Λ system is derived from a degenerate $J_g=1 \rightarrow J_e=1$ transition driven with σ_+ and σ_- circularly polarized light. When $|a\rangle$ and $|b\rangle$ are degenerate, the condition $\Delta=0$ requires that the monochromatic fields $\Omega_1(z)$ and $\Omega_2(z)$ have the same magnitude of wave vector \mathbf{k} , so they can be written as

$$\Omega_{1,2}(z) = A_{1,2}^{+} e^{ikz} + A_{1,2}^{-} e^{-ikz}, \qquad (35)$$

where the A^{\pm} are some complex amplitudes. In this case, we may choose f(z) to be a constant, because $\Omega_{1,2}(z)$ automatically obey the condition (23). It is interesting to note that in this case, the semiclassical dark state corresponds, up to normalization constants, to the position representation of the quantum-mechanical dark state $|D\rangle$. This means that in the cases of standing- or traveling-wave excitation on a Λ system with degenerate ground states, one has a correspondence between the semiclassical and quantum-mechanical dark states.

V. SUMMARY

In summary, we have presented a calculation of the semiclassical diffusion constant for the three-level Λ system. We find that the diffusion constant vanishes in the steady state for the three-level Λ system, provided $\Delta=0$ and for $\Delta\neq 0$, the shape of the diffusion constant follows the qualitative behavior of the Raman dip, including a broadening of the dip for unbalanced Rabi frequencies. We have also studied the correspondence between the semiclassical and quantum-mechanical dark states. Since the steady state of the Λ system typically is reached on a very long time scale, in the future it would be worthwhile to investigate the behavior of the diffusion in the transient regime.

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