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Scattering with longitudinally coherent matter beams

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I present a derivation of the many qualitative changes to basic scattering theory that result when a (partially) coherent matter beam inelastically interacts with a quantum target. The weak beam limit, where only *one* object in the beam interacts with the quantum target, is developed. Some of the basic changes to scattering theory are as follows. (1) The transition probability can increase as the square of the number of particles in the beam. (2) The transition probability is not proportional to the convolution of the total inelastic cross section with the momentum distribution of the beam. (3) The transition probability to different final states of the target does not depend on the population in the initial states but depends on the *amplitudes* for the initial states. (4) The *total* transition probability depends on the differential cross section integrated over all final angles *and* on the differential cross section only in the forward scattering direction. (5) The transition probability can be nonzero even when the beam misses the target. (6) In the perturbative limit, the transition probability can be related to classical, large scale properties of the beam (such as the average density).

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I. INTRODUCTION

Scattering theory is well understood when the beam of incident particles is incoherent [1]. The basic trends that control the scattering process have been known since the introduction of quantum theory. Often, information from a scattering event is all that is available to aid our understanding of a quantum system. Therefore, it is important to understand what properties of the beam of incident particles control transition probabilities in a quantum target. When the beam is incoherent, there are a number of well known properties of the beam that control the transition probability (e.g., energy, current density, overlap with the target, etc.). Until recently [2,3], the coherence properties of the matter beam has not been thought to affect the transition probabilities. The purpose of this paper is to extend the studies begun in Refs. [2,3] which showed that the coherence properties of the beam can dominate all other parameters that control the transition probability. For the purposes of this paper, a beam is considered to be incoherent if the off-diagonal density matrix elements in momentum space are zero and the beam has some coherence if off-diagonal density matrix elements are nonzero.

This paper is meant to address the lack of general theory for scattering by longitudinally coherent matter beams. Recently, there has been the development of two types of longitudinally coherent matter beams. In Refs. [4–7] the practical development of atom lasers was discussed; these matter beams have interesting coherence properties since the output is from a Bose-Einsten condensate. In Refs. [8,9], a pulsed electron gun was predicted and demonstrated; a pulsed electron gun can deliver a few keV electron beam in a pulsed mode with a period between pulses in the range 10–100 ps. It is highly likely that one or both of these sources will be used in a scattering arrangement. To give an idea of the type of system addressed in this paper, Fig. 1 shows a schematic drawing of the interaction of three electron pulses interacting with an atom.

The purpose of this paper is to show that when a longitudinally coherent beam interacts with a quantum target all of the generic properties of scattering theory can be violated, sometimes very strongly. Some aspects of scattering with longitudinally coherent beams has been presented in two previous publications [2,3]. In this paper, I will derive the previous results in more detail. I will also present new results for several situations involving coherent beams and targets. I will also present calculations for several different situations to illustrate the possibilities for scattering with coherent beams.

Before addressing the issues of scattering theory with longitudinally coherent beams, I enumerate some of the well known and simple parameters that control transition probabilities when incoherent beams interact with a quantum target. All of the observations are for the weak beam and weak target limit. A weak beam is one where all of the transition probabilities are small so that double scattering events on a single quantum target can be ignored; thus, the possibility of one incident particle causing a transition from state a to state b then a second incident particle causing a transition from state b to state c will be assumed to be negligibly small. A weak target is one where the properties of the beam do not substantially change as the beam traverses the target; thus, the depletion of the beam by scattering or energy loss by the beam while traversing the target will be assumed to be negligibly small. Below is a list of well known properties of scattering by an incoherent beam.

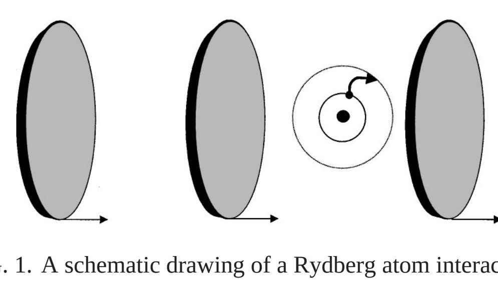

FIG. 1. A schematic drawing of a Rydberg atom interacting with an electron beam bunched in the longitudinal direction.

(1) When all other parameters are kept fixed, the transition probability increases linearly with the number of particles in the beam. If the number of particles in the beam is doubled, then the transition probability doubles.

(2) Transition probabilities are proportional to the total inelastic scattering cross section convolved with the momentum distribution of the beam. The transition probability changes with the expectation value of the momentum and the width of the momentum distribution.

(3) The population in a final state depends on the initial distribution of population in the states of the quantum target. If the target is initially in two states with different energies, the transition probability does not depend on whether the target is in a coherent superposition of states (such as a wave packet) or whether the states are incoherently populated. Equivalently, the final population only depends on the diagonal elements of the density matrix for the target.

(4) The total transition probability is proportional to the integral of the differential cross section over all scattering angles. The differential cross section can only be obtained by measuring the momentum vector of the scattered particle after the transition.

(5) The transition probability is proportional to the time integral of the current density of the beam at the quantum target. Thus, an experimental determination of the cross section involves the estimation of the overlap of the beam with the quantum target. If the beam misses the target, then the transition probability is zero.

(6) The transition probability arises from the interaction of the quantum target with an individual particle in the beam. The large-scale, average structure of the beam plays no role in the scattering except the property of point (5).

In the following sections, I will show that all of these properties can be strongly violated when using longitudinally coherent beams. There are two restriction that will be imposed for this paper, in addition to the weak beam and weak target assumptions discussed above. The first is that the target is assumed to be at a low enough temperature so that the Doppler width of lines is a small fraction of the line spacing. The second is that the incident particles cannot be excited during the scattering. The method described below can be simply extended to remove these restrictions, but these extensions are beyond the scope of this paper. Finally, the mass of the projectile will be assumed to be much less than the target mass to avoid the complications of the formulas due to large target recoil; again, the inclusion of large target recoil is straightforward but does not appear to add anything of interest. Atomic units are used throughout this paper unless explicitly stated otherwise.

II. ULTRAWEAK BEAMS

First, I will treat the case of ultra-weak beams. In this case, there is effectively only one particle in the beam. The limit to the beam strength is discussed in Ref. [2] and in Sec. III. Both of the possible situations, a target in one initial state and a target in a coherent superposition of states, will be treated.

A. One initial state

The simplest scattering case is when one incident particle interacts with one quantum target. We can use either a time dependent or time independent treatment of the scattering to obtain the relevant scattering parameters. It is perhaps clearer to start from the time independent picture and derive a time dependent scattering wave function from this.

The target wave functions will be written as Φ_a with energies E_a. The wave function when the projectile is at large distances from the target can be written as

$$\Psi_{\mathbf{k},a}=\frac{1}{(2\pi)^{3/2}}\left[e^{i\mathbf{k}\cdot\mathbf{r}}\Phi_a+\sum_b \Phi_b\frac{e^{ik_{ba}r}}{r}f_{b\leftarrow a}(k_{ba}\hat{\mathbf{r}}\leftarrow\mathbf{k})\right], \tag{1}$$

where $\mathbf{k}$ is the incident particle's momentum and $k_{ba}=\sqrt{2M(E_a-E_b)+k^2}$ is the magnitude of the momentum after the transition $b\leftarrow a$. All of the scattering information is contained in the scattering amplitudes $f_{b\leftarrow a}$. The transition with $a\leftarrow a$ gives elastic scattering. The differential cross section can be directly obtained from this scattering wave function as

$$\frac{d\sigma_{b\leftarrow a}}{d\Omega}(\hat{\mathbf{r}},k)=\frac{k_{ba}}{k}|f_{b\leftarrow a}(k_{ba}\hat{\mathbf{r}}\leftarrow k\hat{\mathbf{z}})|^2, \tag{2}$$

where I have taken the incident momentum to be in the z direction, i.e., $\mathbf{k}=k\hat{\mathbf{z}}$. It is very important to note how the scattering amplitudes change if the position of the target is moved. The relationship between the scattering amplitude when the scatterer is centered at the point $\mathbf{r}_0$ and the amplitude when the scatterer is centered at 0 is

$$f_{b\leftarrow a}(\mathbf{k}'\leftarrow\mathbf{k})|_{\mathbf{r}_0}=f^{(0)}_{b\leftarrow a}(\mathbf{k}'\leftarrow\mathbf{k})e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_0}. \tag{3}$$

This phase factor plays no role in observables (like cross section) for one particle scattering from a target that is in an energy eigenstate.

We can use the time independent wave function to answer questions about how coherence properties of a ''one particle'' beam affect transition probabilities. The coherence properties of the beam can be expressed through the density matrix for the particles of the beam. To develop a treatment of the scattering including total or partial coherence, I will start from a wave packet picture and use a completely coherent wave function obtained by superposing the time independent wave function of Eq. (1):

$$\Psi_a(t)=\int \Psi_{\mathbf{k},a}e^{-i(E_a+k^2/2M)t}A(\mathbf{k})d^3\mathbf{k}, \tag{4}$$

where the amplitudes must satisfy $\int|A(\mathbf{k})|^2d^3\mathbf{k}=1$ to obtain unit normalization. In general, the amplitude A is complex. For example, if the $A_0(\mathbf{k})$ makes a wave packet, then the amplitude $A(\mathbf{k})=A_0(\mathbf{k})[1+\exp(-i\mathbf{k}\cdot\mathbf{R})]/\sqrt{2}$ gives a double wave packet state with the second packet shifted in space by an amount $\mathbf{R}$. The strategy for obtaining transition probabilities will be to first develop the transition probability using the fully coherent wave function; then at a later stage average the final results over the different realizations of the beam.

The wave packet that results from Eq. (4) can be written in the form of an unscattered part and a scattered part. This time dependent wave function may be symbolized as

$$\Psi_a(t)=\Phi_a e^{-iE_a t}\psi^{\rm inc}(\mathbf{r},t)+\sum_b \Phi_b e^{-iE_b t}\psi^{\rm sca}_{b\leftarrow a}(\mathbf{r},t), \tag{5}$$

where the incident wave packet may be obtained from $\psi^{\rm inc}(\mathbf{r},t)=(2\pi)^{-3/2}\int A(\mathbf{k})\exp[i(\mathbf{k}\cdot\mathbf{r}-k^2t/2M)]d^3\mathbf{k}$. When the target is at $\mathbf{r}_0$, the scattered wave has the form

$$\psi^{\rm sca}_{b\leftarrow a}(\mathbf{r},t)=\frac{1}{(2\pi)^{3/2}}\int\frac{e^{ik_{ba}r}}{r}f^{(0)}_{b\leftarrow a}(k_{ba}\hat{\mathbf{r}}\leftarrow\mathbf{k})A(\mathbf{k})\times\exp\left[-i\frac{k_{ba}^2}{2M}t+i(\mathbf{k}-k_{ba}\hat{\mathbf{r}})\cdot\mathbf{r}_0\right]d^3\mathbf{k} \tag{6}$$

in the limit $t\to\infty$.

The transition probability can be obtained from the time dependent wave function. The probability for the transition is simply $P_{b\leftarrow a}=\langle\psi^{\rm sca}_{b\leftarrow a}|\psi^{\rm sca}_{b\leftarrow a}\rangle$ as $t\to\infty$. The expression for the scattered wave function from Eq. (6) can be used to obtain a closed form expression for the transition probability. The result is a triple integral:

$$P_{b\leftarrow a}=\frac{1}{(2\pi)^3}\int d^3\mathbf{r}d^3\mathbf{k}d^3\mathbf{k}'A^*(\mathbf{k}')A(\mathbf{k})\times f^{(0)*}_{b\leftarrow a}(k'_{ba}\hat{\mathbf{r}}\leftarrow\mathbf{k}')f^{(0)*}_{b\leftarrow a}(k_{ba}\hat{\mathbf{r}}\leftarrow\mathbf{k})\frac{1}{r^2}\times e^{i[(k_{ba}-k'_{ba})r+(\mathbf{k}-\mathbf{k}'+k'_{ba}\hat{\mathbf{r}}-k_{ba}\hat{\mathbf{r}})\cdot\mathbf{r}_0+(k_{ba}^2-k'^2_{ba})t/2]}. \tag{7}$$

Performing the integration over r gives a factor of $2\pi\delta(k_{ba}-k'_{ba})$ and averaging the x,y components of $\mathbf{r}_0$ over a range L_x,L_y gives a factor of $(2\pi)^2\delta(k_x-k'_x)\delta(k_y-k'_y)/L_xL_y$. The product of these two terms is $(2\pi)^3\delta(\mathbf{k}-\mathbf{k}')/(L_xL_y[dk_{ba}/dk_z])$ where I have used the usual relation $\delta[f(x)]=\delta(x)/|f'(x)|$ if $f(x)$ has its only zero at $x=0$. The relation for the derivative $dk_{ba}/dk_z=k_z/k_{ba}$ can be accurately approximated by k/k_{ba} since by definition the beam is traveling in the z direction; any transverse velocities are much smaller than the average velocity in the z direction and the corrections to k/k_{ba} are proportional to $(k_x^2+k_y^2)/k^2$. The scattering probability can be simplified to

$$P_{b\leftarrow a}=\frac{1}{L_xL_y}\int d^2\hat{\mathbf{r}}d^3\mathbf{k}\frac{k_{ba}}{k}|f^{(0)}_{b\leftarrow a}(k_{ba}\hat{\mathbf{r}}\leftarrow\mathbf{k})A(\mathbf{k})|^2=\frac{1}{L_xL_y}\int d^3\mathbf{k}\sigma_{b\leftarrow a}(k)|A(\mathbf{k})|^2, \tag{8}$$

where $\sigma_{b\leftarrow a}$ is the inelastic cross section which only depends on the magnitude of $\mathbf{k}$. This formula has a simple physical interpretation: the scattering probability is the average value of the inelastic cross section $\langle\sigma_{b\leftarrow a}\rangle$, times the time integrated current density (which is 1 particle over an area L_xL_y). Note that the transition probability only depends on $|A(\mathbf{k})|^2$ which is the probability density for the incident particle to have wave number $\mathbf{k}$. The density matrix for the incident particle in wave number space is defined to be $\rho(\mathbf{k},\mathbf{k}')=\langle A(\mathbf{k})A^*(\mathbf{k}')\rangle$ where $\langle\cdots\rangle$ means to average over the different realizations of this one particle beam scattering off one quantum target; using this definition, the transition probability only depends on diagonal elements of the density matrix. Thus, the transition probability does not depend on any momentum coherence properties of the beam; coherence properties of the beam are manifest in off-diagonal elements of the density matrix. Another way of seeing this idea is that the coherence of a wave packet is embodied in a well specified phase relationship of the different wave numbers $\mathbf{k}$ of the incident particle; if the final result only depends on $|A(\mathbf{k})|^2$ then this phase relationship is irrelevant.

This derivation immediately shows the points (2), (4), and (6) discussed in the Introduction. If there are N particles in the beam, then it is usually assumed that the transitions from each of the particles add incoherently so that the total transition probability is N times the result of 1 particle; this is the origin of the point (1) of the Introduction. If the target is initially in two nondegenerate states a and a' then the probability to excite the atom to state b is the probability to be in state a times $P_{b\leftarrow a}$ plus the probability to be in state a' times $P_{b\leftarrow a'}$; it does not matter that the target could be in a coherent superposition of the states a and a' because the transition can happen at any time and the relative phase factor between the two states, $\exp[i(E_a-E_{a'})t]$, will average to zero. This gives point (3) of the Introduction.

Point (5) of the Introduction is intuitively obvious but somewhat subtle to show analytically. To motivate this result, I assume that the transverse modulation of the beam is small on a distance scale of $1/k$. Instead of performing the average over $\mathbf{r}_0$ fix it at the transverse position $(x_0,y_0,0)$ of the target. The integral over r can be performed in Eq. (7) to give a factor of $2\pi\delta(k_{ba}-k'_{ba})$ which can again be approximated by $2\pi\delta(k_z-k'_z)k_{ba}/k$ since the transverse momenta are much smaller than the longitudinal momenta. The integration over k_x,k_y, and $k'_xk'_y$ can be performed if we use a wave function defined partly in position space and partly in momentum space: $\psi(x,y,k_z)\equiv\int A(\mathbf{k})\exp[i(k_xx+k_yy)]dk_xdk_y/2\pi$. This function can be interpreted as the amplitude to find the particle at the transverse position x,y with a momentum k_z. In terms of this function, the transition probability is

$$P_{b\leftarrow a}=\int dk_z\sigma_{b\leftarrow a}(k_z)|\psi(x_0,y_0,k_z)|^2 \tag{9}$$

which agrees with point (5) of the Introduction.

This section has shown the origin for all of the usual general features of scattering theory. In the following sections, I will show how to extend treatment of scattering to encompass beams with momentum coherence. The results will violate all of the general features of conventional scattering theory.

B. Several initial states, coherent beam

The case where the target is prepared in several initial states and the beam exhibits some longitudinal coherence provides an interesting change from point (3) in the Introduction. As one physical example, have a radial Rydberg wave packet on the target atom interact with a short pulse electron beam; the transition probability will depend on whether the Rydberg wave packet is at large r or at small r when the electron pulse passes the atom. To derive this change from point (3), I will again use a wave packet derivation and at a later point I will average over the different realizations for the target to account for any incoherences. We will use the complex coefficients of the initial states to represent a general state of the target $\Phi(0)=\Sigma_a \Phi_a A_a$. This gives a full wave function of the form

$$\Psi(t)=\sum_a \Psi_a(t)A_a, \tag{10}$$

where the wave function from Eq. (5) has been used. Since the incident wave only depends on the $A(\mathbf{k})$ and does not depend on the initial state, the scattered wave for the case of several initial states is simply $\psi_b^{\mathrm{sca}}=\Sigma_a \psi_{b\leftarrow a}^{\mathrm{sca}} A_a$.

Just as in the case where there is only one target state, I can use the norm of the scattered wave to give the probability for exciting state b: $P_b=\langle \psi_b^{\mathrm{sca}}|\psi_b^{\mathrm{sca}}\rangle$. Again, this probability may be expressed as a triple integral, but with the difference that there will be sums over the initial states as well. As $t\to\infty$, the closed form expression for the probability is

$$P_b=\frac{1}{(2\pi)^3}\sum_{aa'} A_a A_{a'}^* \int d^3\mathbf{r} d^3\mathbf{k} d^3\mathbf{k}' A^*(\mathbf{k}')A(\mathbf{k}) \times f_{b\leftarrow a'}^{(0)*}(k'_{ba'}\hat{\mathbf{r}}\leftarrow\mathbf{k}')f_{b\leftarrow a}^{(0)*}(k_{ba}\hat{\mathbf{r}}\leftarrow\mathbf{k})\frac{1}{r^2} \times e^{i[(k_{ba}-k'_{ba'})r+(\mathbf{k}-\mathbf{k}'+k'_{ba'}\hat{\mathbf{r}}-k_{ba}\hat{\mathbf{r}})\cdot\mathbf{r}_0+(k_{ba}^2-k'^2_{ba'})t/2]}, \tag{11}$$

where $A(\mathbf{k})$ does not have a subscript a to indicate that the incident wave is independent of the initial states. As in the previous section several of the integrations can be performed exactly. The integral over r gives a factor of $2\pi\delta(k_{ba}-k'_{ba'})$ and averaging over the x,y components of $\mathbf{r}_0$ over a range L_xL_y gives a factor of $(2\pi)^2\delta(k_x-k'_x)\delta(k_y-k'_y)/L_xL_y$. The product of these two terms is $(2\pi)^3\delta(\mathbf{k}+\hat{\mathbf{z}}\Delta k_{aa'}-\mathbf{k}')/(L_xL_yk'_z/k_{ba})$ where manipulations similar to those from the previous section have been performed. Note that the z component of the momenta have been shifted by an amount $\Delta k_{aa'}=\sqrt{2M(E_a-E_{a'})+k_z^2}-k_z$ that arises from energy conservation; after the collision leaving the target in state b, the size of the momentum k_{ba} must equal that from $k_{ba'}$. Substituting the delta functions and performing the integration over $d^3\mathbf{k}'$ gives the transition probability

$$P_b=\frac{1}{L_xL_y}\sum_{aa'} A_a A_{a'}^* \int d^2\hat{r} d^3\mathbf{k} A^*(\mathbf{k}+\Delta k_{aa'}\hat{\mathbf{z}})A(\mathbf{k}) \times\frac{k_{ba}}{k_{a'a}} f_{b\leftarrow a'}^{(0)*}(k_{ba}\hat{\mathbf{r}}\leftarrow\mathbf{k}+\Delta k_{aa'}\hat{\mathbf{z}})f_{b\leftarrow a}^{(0)*}(k_{ba}\hat{\mathbf{r}}\leftarrow\mathbf{k}), \tag{12}$$

where I have again used the relation $k^2 \gg k_x^2+k_y^2$ to approximate $\sqrt{2M(E_a-E_{a'})+k_z^2}=k_{aa'}$. Equation (12) is essentially exact and is the main result of this section.

The result for a ''one particle'' beam scattering from a target in a superposition of states is fairly complicated so that it is worthwhile exploring different aspects to gain familiarity with the physics that it embodies. First, examine the case where the target is only in a statistical superposition so that the density matrix for the target $\rho_{aa'}=\langle A_a A_{a'}^*\rangle$, is diagonal. If $\rho_{aa'}=\delta_{aa'}\rho_{aa}$ (where ρ_{aa} is the probability to be in state a), then the probability to excite state b is simply the weighted average of the individual excitation probabilities from Eq. (8): $P_b=\Sigma_a P_{b\leftarrow a}\rho_{aa}$. This result says that no coherence effects arise in the ultra weak beam limit unless the target itself is in a coherent superposition of states. This agrees with the analysis of Ref. [10]; here they found that longitudinal coherence properties of a beam have no effect unless the target has some sort of time dependence. A completely incoherent target does not change with time. However, if the density matrix is not diagonal, then the target is in a wave packet state and the properties of the target do evolve with time; thus the conditions are satisfied and there is possible interesting effects from longitudinal coherence properties of the beam.

For the rest of this section, the density matrix of the target is assumed to be nondiagonal. Next, examine the case where the width of the amplitude in momentum $A(\mathbf{k})$ is much smaller than $\Delta k_{aa'}$. In this case the product $A^*(\mathbf{k}+\Delta k_{aa'}\hat{\mathbf{z}})A(\mathbf{k})$ is always effectively zero unless $a=a'$ $(\Delta k_{aa}=0)$. Since all of the cross terms go to zero, again the result is a weighted average of the individual excitation probabilities from Eq. (8): $P_b=\Sigma_a P_{b\leftarrow a}\rho_{aa}$. The physical reason for this is that the resolution of the beam is high enough to energy analyze the scattered wave and unambiguously identify each piece that corresponds to the different initial states.

Next, examine the case where the coherence properties of the beam are such that the off-diagonal elements of the beam's density matrix do not extend to momentum differences of $\Delta k_{aa'}$; i.e., $\rho(\mathbf{k},\mathbf{k}+\Delta k_{aa'}\hat{\mathbf{z}})=0$ unless $a=a'$. Since all of the cross terms go to zero, again the result is a weighted average of the individual excitation probabilities from Eq. (8): $P_b=\Sigma_a P_{b\leftarrow a}\rho_{aa}$. The physical reason for this result is different from that of the previous paragraph because it is not necessary for the beam to have high-energy resolution. The reason for a reduction to a statistical result is that the incoherence in the beam implies that the incident particle cause transitions at random times that are long compared to the beat period $h/|E_a - E_{a'}|$. Thus there is a random phase that causes the cross terms to average to zero. This agrees with the point (3) of the Introduction.

Now, let us turn to the case where the density matrix for the target and for the beam will allow nonstatistical transition probabilities. There is one last requirement for the interesting coherence effects to be manifest in the total transition probability. Namely, the product of scattering amplitudes (the $f^{(0)*}f^{(0)}$ product) must be comparable to the differential cross section of the individual transitions. This is not guaranteed. For example, if the 46*s* and 46*p* Rydberg states of Rubidium are used as the initial states, then the differential cross section for transition to the 46*d* is quite different; the differential cross section from the 46*p* state is strongly peaked in the forward direction while from the 46*s* state there is a minimum in the forward direction. Thus, the effect from coherent initial states will probably be most easily observed when initial states of very similar character are used.

Perhaps the most interesting situation is where there is a longitudinal coherence in the beam due to a simple time dependent modulation (for example, a series of pulses). For the rest of the discussion, I will assume that the transverse structure is uninteresting and that the momentum distribution in the transverse direction is very strongly peaked around 0. In this case, the transition probability can be compactly written as

$$P_b = \frac{1}{L_x L_y} \sum_{aa'} \rho_{aa'} \int dk_z \xi_{aa'}(k_z) \rho_z(k_z, k_z + \Delta k_{aa'}), \tag{13}$$

where

$$\xi_{aa'}(k_z) = \int d^2\hat{r} \frac{k_{ba}}{k_{aa'}} f^{(0)}_{b\leftarrow a}(k_{ba}\hat{\mathbf{r}} \leftarrow k_z \hat{\mathbf{z}}) \times f^{(0)*}_{b\leftarrow a'}(k_{ba}\hat{\mathbf{r}} \leftarrow [k_z + \Delta k_{aa'}]\hat{\mathbf{z}}) \tag{14}$$

reduces to the total cross section for $a=a'$ and ρ_z is the integral of the density matrix over the k_x, k_y components. Equation (13) shows that the probability for transition into state *b* depends on off-diagonal elements of the density matrix of the beam if the target is prepared in a coherent superposition of states.

Although Eq. (13) is exact and can be readily evaluated in specific circumstances, the visualizable physical processes that contribute to the transition probability are not obvious. To make clear the physical content, I will address a common situation in an approximate manner. For many cases, the ξ functions hardly have any dependence on k_z over the width of the momentum distribution. When the ξ functions hardly change with k_z, they can be pulled outside of the integral in Eq. (13) by setting $\xi_{aa'}(k_z) = \xi_{aa'}(\overline{k_z})$ with $\overline{k_z}$ being the average momentum. The density matrix in momentum space can be related to the density matrix in space through a double Fourier transform

$$\rho_z(k_z, k_z') = \frac{1}{2\pi} \int dz dz' \rho_z(z, z') e^{i(k_z' z' - k_z z)}. \tag{15}$$

This fact can be used to obtain an expression for the transition probability in terms of the the Fourier transform of the density of the beam in the *z* direction:

$$P_b = \frac{1}{L_x L_y} \sum_{aa'} \rho_{aa'} \xi_{aa'}(\overline{k_z}) \int \rho_z(z,z) e^{i\Delta k_{aa'} z} dz, \tag{16}$$

where $\rho_z(z,z)$ is the density of the beam in the *z* direction at $t=0$. The transition arising from the aa' term is proportional to the Fourier transform of the density with a wave number $\Delta k_{aa'}$. The case where $a=a'$ gives the integral of the density which is 1. The cross terms with $a \neq a'$ are only nonzero to the extent that the beam has a modulation in space with a wavelength $2\pi/\Delta k_{aa'}$.

The result in Eq. (16) directly leads to an interpretation of the origin of the coherent transition when the target is prepared in a superposition of states. The target has many different frequencies, $E_a - E_{a'}$, of motion that result from the superposition of initial states. The spatial modulation of the beam with a wavelength λ translates through the velocity v of the beam into a time modulation at the target given by $\lambda/v = M\lambda/k_z$. Thus the beam needs a spatial modulation $\lambda = 2\pi k_z/(M|E_a - E_{a'}|)$. Using the approximation $\Delta k_{aa'} \simeq M(E_a - E_{a'})/k_z$ when $k_z \gg \Delta k_{aa'}$, the same condition as in Eq. (16) is obtained.

As an example, consider the case where the beam is specifically modulated so that the Fourier transform of the density is strongly peaked at $\lambda = 0, \pm 2\pi v/\omega$. The transition probability will equal that for incoherent initial states if ω does not match any of the frequencies, $E_a - E_{a'}$ of the target. Thus, the expectation is that the transition probability can be made to vary sharply with the wave length modulation of the beam. This should be testable by experiment.

Finally, there is another interpretation of the result. In order to have modulation of the beam density, the beam must have energy components that are modulated such that there are several peaks in energy with a spacing ΔE. If the ΔE spacing of the beam matches an energy difference in the target, then part of the wave with energy E can scatter from state *a* and finish with energy $E + E_a - E_b$ while the part of the wave with energy $E + \Delta E$ can scatter from state a' and finish with energy $E + \Delta E + E_{a'} - E_b$. If $\Delta E = E_a - E_{a'}$ the two process are indistinguishable and can interfere. Thus the cross terms in Eq. (13) can be thought of as arising from the interference of indistinquishible paths.

In Sec. IV, I will investigate several interesting possibilities for observing the coherence terms. I will also mention some of the basic physical ideas that can be observed experimentally.

III. WEAK BEAMS

Now I will address the case of weak beams where it is necessary to account for many particles in the beam although I am still only considering the case of one particle causing the transition. The division between ultraweak and weak beams will be clearly specified below.

It is not obvious that the analysis of the scattering probability qualitatively changes if there are *N* particles in the beam of transverse area L_xL_y. The transition probability from state a to b is usually assumed to be $N\langle\sigma_{b\leftarrow a}\rangle/L_xL_y \equiv\zeta\langle\sigma_{b\leftarrow a}\rangle$; i.e., the transition probability equals the inelastic cross section averaged over the momentum distribution in the incident beam times the time integral of the particle current density. This result arises from the assumption that each incident particle contributes incoherently to the transition. But is this assumption correct? It is relatively easy to extend the derivation to N particles in the beam and test this assumption.

A. One initial state

To check the assumption that scattering probability is the incoherent sum of the probabilities from each particle in the beam, we write out a wave function for an N particle beam [2] where the only assumption is that there is only one scattering event; this wave function is

$$\Psi_a^{(N)}(t)=\Phi_a e^{-iE_at}\prod_{j=1}^{N}\psi_a^{\mathrm{inc},j}(\mathbf{r}_j,t)+\sum_b \Phi_b e^{-iE_bt}\times\sum_{j'}\left\{\psi_{b\leftarrow a}^{\mathrm{sca},j'}(\mathbf{r}_{j'},t)\prod_{j\neq j'}\psi_a^{\mathrm{inc},j}(\mathbf{r}_j,t)\right\}. \quad (17)$$

The j superscript on the incident and scattered wave functions is meant to indicate that the wave packet for each incident particle is not necessarily related to any of the other packets. In Eq. (17), we made the assumption that the initial state of the incident beam is such that the wave function for the incident particles is a product of one particle functions. This situation can occur when the incident wave is the output from an atom laser since the atoms are bosons. This situation also holds when all lengths of a packet are smaller than the average distance between adjacent projectiles because the incident particles are distinguishable.

The transition probability can be obtained from the norm of the many particle scattered wave. Coherent and incoherent probabilities for exciting the target to state b are given by

$$P_{b\leftarrow a}^{(N)}=\sum_j\langle\psi_{b\leftarrow a}^{\mathrm{sca},j}|\psi_{b\leftarrow a}^{\mathrm{sca},j}\rangle+\sum_{j\neq j'}\langle\psi_a^{\mathrm{inc},j}|\psi_{b\leftarrow a}^{\mathrm{sca},j}\rangle\times\langle\psi_{b\leftarrow a}^{\mathrm{sca},j'}|\psi_a^{\mathrm{inc},j'}\rangle, \quad (18)$$

where unit normalization of the incident packets has been used. The first term of Eq. (18) is the incoherent sum of probabilities from each individual projectile and the second term arises from the coherent effect of the projectiles on the target. It is important to remember that the coherent term is zero unless the incident wave packet has an energy width that is larger than the energy change in the target; if the energy width of the packet is too small there is no overlap between the incident and scattered waves because they do not contain the same energy components. Because the coherent term is an overlap of the initial and scattered wave, it will be easier to observe the effect for transitions where the inelastic cross section is peaked in the forward direction. As discussed below, the second term of Eq. (18) is proportional to off-diagonal elements of the density matrix.

Properties of the scattered packet prevent a strong overlap with the incident packet because the incident packet has a momentum distribution strongly peaked in the z direction whereas the scattered wave has a larger angular distribution of momentum. This means that $\langle\psi_{b\leftarrow a}^{\mathrm{sca},j}|\psi_{b\leftarrow a}^{\mathrm{sca},j}\rangle \gg|\langle\psi_a^{\mathrm{inc},j}|\psi_{b\leftarrow a}^{\mathrm{sca},j}\rangle|^2$. It is illustrative to use this fact to approximate Eq. (18) in the form

$$P_{b\leftarrow a}^{(N)}\simeq\sum_{j=1}^{N}\langle\psi_{b\leftarrow a}^{\mathrm{sca},j}|\psi_{b\leftarrow a}^{\mathrm{sca},j}\rangle+\left|\sum_{j=1}^{N}\langle\psi_a^{\mathrm{inc},j}|\psi_{b\leftarrow a}^{\mathrm{sca},j}\rangle\right|^2 \quad (19)$$

which can serve as the basis for discussing the physical processes important for scattering with a pulsed incident beam.

How can the coherent transition probability, which depends on the small overlap of the initial and scattered wave, be comparable or larger than the incoherent transition probability? The answer is that although an individual contribution to the incoherent term is larger than one for the coherent term, there are N times more contributions to the coherent term. Therefore, the coherent contribution to the probability can be dominant for large numbers of projectiles N. We interpret the second term in Eq. (19) as arising from the coherent field from all of the projectiles acting on the target. This interpretation arises from the form of this term in which the amplitudes from each individual particle are superposed and the probability is the absolute value squared. Another reason for this interpretation is that in the first order Born approximation the second term in Eq. (19) *exactly* equals the transition from state a to b calculated using first order time dependent perturbation theory and the time dependent coupling potential generated by the incident wave packets $|\psi_a^{\mathrm{inc},j}|^2$. We can also think of the coherent term as arising because part of the scattered wave of each particle overlaps the incident wave; in this case, it is impossible to know which particle caused the transition and therefore the amplitudes must be added coherently.

Now, I want to obtain a complete expression for the transition probability to the final state b in terms of scattering amplitudes and physical parameters of the beam. The first term in Eq. (19) is simply the incoherent sum of the individual transitions from each particle of the beam. This gives the usual expression for the transition probability. The second term has to be approached somewhat more cautiously. In the limit that $t\to\infty$, each of the individual overlaps can be expressed as a triple integral in the form

$$\langle\psi^{\mathrm{inc},j}|\psi_{b\leftarrow a}^{\mathrm{sca},j}\rangle=\frac{1}{(2\pi)^3}\int d^3\mathbf{r}d^3\mathbf{k}d^3\mathbf{k}'A_j^*(\mathbf{k}')A_j(\mathbf{k})\times f_{b\leftarrow a}^{(0)}(k_{ba}\hat{\mathbf{r}}\leftarrow\mathbf{k})\frac{1}{r}\times e^{i(k_{ba}r-\mathbf{k}'\cdot\mathbf{r}+[\mathbf{k}-k_{ba}\hat{\mathbf{r}}]\cdot\mathbf{r}_0)}. \quad (20)$$

As in the previous sections, many of the integrations can be performed analytically. The plane wave $\exp(-i\mathbf{k}'\cdot\mathbf{r})$ can be expanded into partial waves. This allows the integration over

$d^3\mathbf{r}$ to be performed which gives a factor of $i(2\pi)^2\delta(k'-k_{ba})/k'$ with the replacement of $\hat{\mathbf{r}}$ by $\hat{\mathbf{k}}'$. Next, averaging the x,y position of the target over a large are L_xL_y gives a factor of $(2\pi)^2\delta(k_x-k_x')\delta(k_y-k_y')/(L_xL_y)$. This reduces the overlap to a single integral of the form

$$\langle\psi^{\text{inc},j}|\psi^{\text{sca},j}_{b\leftarrow a}\rangle=\frac{2i\pi}{L_xL_y}\int d^3\mathbf{k}A_j^*(\mathbf{k}+\Delta k_{ab}\hat{z})A_j(\mathbf{k})\times f^{(0)}_{b\leftarrow a}(\mathbf{k}+\Delta k_{ab}\hat{z}\leftarrow\mathbf{k})/(k_z+\Delta k_{ab}). \tag{21}$$

The sum over j of all of the overlaps replaces the products of the A amplitudes with N times the one particle density matrix. Thus, the amplitude that arises in Eq. (19) is

$$\sum_{j=1}^{N}\langle\psi^{\text{inc},j}|\psi^{\text{sca},j}_{b\leftarrow a}\rangle=\frac{2i\pi N}{L_xL_y}\int d^3\mathbf{k}\rho(\mathbf{k},\mathbf{k}+\Delta k_{ab}\hat{z})\times f^{(0)}_{b\leftarrow a}(\mathbf{k}+\Delta k_{ab}\hat{z}\leftarrow\mathbf{k})/(k_z+\Delta k_{ab}). \tag{22}$$

This expression clearly shows that the coherent result from the multiple electron scattering depends on the off-diagonal density matrix elements of the momentum components of the beam. If the beam is completely incoherent, then the density matrix in Eq. (22) is zero and the only contribution to the transition probability is from the incoherent scattering from individual particles of the beam. There are a number of interesting features about the combination of Eqs. (19) and (22) that should be noted. First, the coherent amplitude is proportional to N which means the probability is proportional to N^2. Compare to point (1) of the Introduction. Second, the amplitude in Eq. (22) depends on off diagonal density matrix elements which means the transition probability is not simply a convolution over the momentum distribution of the beam. Compare to point (2) of the Introduction. Third, the amplitude in Eq. (22) is proportional to the scattering amplitude only in the forward direction. Compare to point (4) of the Introduction. Some of the other points of the Introduction will be discussed in the following two sections.

While the expression in Eq. (22) is perfectly accurate and can be used to calculate the transition probabilities, it is not very easy to get a physical feeling for the mechanisms that control this amplitude. To this end, an approximate expression will be derived for a common type of scattering. If the change in momentum, Δk_{ab}, is much less than the incident momentum and the initial spread in momentum is much smaller than the momentum, then very often the scattering amplitude does not vary rapidly with the initial momentum. If this is true then the scattering amplitude and the inverse momentum factor in Eq. (22) can be pulled out of the integral and an average value of the momentum substituted. Now, as in Sec. II B, the only term left inside the momentum integral is the density matrix which can be related to the Fourier transform of the one-particle, beam density in the z direction. This gives a final expression

$$\sum_{j=1}^{N}\langle\psi^{\text{inc},j}|\psi^{\text{sca},j}_{b\leftarrow a}\rangle=\frac{2i\pi N}{L_xL_y\overline{k_z}}f^{(0)}_{b\leftarrow a}(\overline{k_{ba}}\hat{\mathbf{z}}\leftarrow\overline{k_z}\hat{\mathbf{z}})\times\int dz\rho_z(z,z)e^{i\Delta k_{ab}z} \tag{23}$$

with $\overline{k_z}$ being the average momentum and $\overline{k_{ba}}$ being the final momentum.

The transition probabilities from both the incoherent and the coherent scattering terms can be combined to give

$$P^{(N)}_{b\leftarrow a}=\zeta\sigma_{b\leftarrow a}+2\pi\zeta^2\left|\int\rho_z(z,z)e^{i\Delta k_{ab}z}dz\right|^2\left(\frac{d\sigma_{b\leftarrow a}}{qdq}\right)\Bigg|_{q=q_0}, \tag{24}$$

where $\zeta=N/L_xL_y$ is the time integral of the beam-current density and $q_0=|\Delta k_{ab}|$ is the minimum size of the momentum transfer. The minimum size of the momentum transfer occurs when the scattered particle travels in the same direction as the incident particle, $\theta=0$; $q_0\simeq M|E_a-E_b|/k$ when the incident energy is large compared to the energy given to the target. The differential cross section $d\sigma/qdq=\int d\phi(d\sigma/d\Omega)/kk_{ba}$ with the k,k_{ba} the initial and final wave numbers. The transitions where the inelastic, differential cross section is strongly peaked in the forward direction will show the effects of beam modulation most strongly. For the interaction of a fast charged particle with a neutral atom, it is the dipole allowed transitions that are peaked in the forward direction; the other multipole transitions (monopole, quadrupole, etc.) have a minimum in the forward scattering direction.

The result in Eq. (24) can be interpreted to give a physical picture of the scattering. The first term is simply the expected result from incoherent scattering: the transition probability is the inelastic cross section times the time integrated current density. The second term is similar to the result from Sec. II B since the coherence comes from having a density modulation in the beam with a wavelength given by $2\pi/\Delta k_{ab}$; however, the origin of this term is quite different. In Sec. II B the coherent scattering fit within the recent ideas of scattering theory in the sense that the target had a time dependent modulation that could interact with time dependent modulations of the beam. In this section, the target is assumed to be in an energy eigenstate and thus it is expected that a modulated beam will not have an effect on the transition. The coherent scattering term in Eq. (24) arises because the scattered wave from each of the j electrons can overlap the unscattered wave; thus it is not possible to identify which electron caused the transition. This implies the scattering *amplitudes* from each of the electrons should be added.

The results in this section violate expectations from standard scattering theory in several places. First, it violates property (1) from the Introduction: the transition probability has a part proportional to the number of the incident particles in the beam *and* a term proportional square of the number of incident particles. There is a violation of property (2) since the transition probability depends on longitudinal coherence properties of the beam: the coherent transition amplitude depends on off-diagonal density matrix elements. There is a violation of property (4) since the *total* transition probability depends on the inelastic cross section *and* on the differential inelastic cross section in the forward scattering direction; this gives the opportunity for measuring the forward scattering differential cross section without measuring momentum components of the scattered particle. Finally, these results also violate property (6) since the transition probability depends on the large-scale (macroscopic) structure of the beam in the longitudinal direction: the transition depends on a Fourier transform of the longitudinal density of the beam.

B. Perturbative limit

It is instructive to examine the perturbative limit [3] of the coherent scattering in order to obtain an intuitive understanding of the reason for the coherent scattering. This limit allows a direct connection between the quantum formulation of coherent scattering and classical intuition of the interaction of a quantum target with an extended, macroscopic object.

The derivation will be based on the time dependent equation for the scattered wave to lowest order in the interaction between the jth incident particle and the target. To lowest order in the interaction potential, the scattered wave can be written as the solution of

$$\left(i\frac{\partial}{\partial t} - H_0 \right) \psi^{\mathrm{sca},j}_{b\leftarrow a}(\mathbf{r},t) = V_{ba}(\mathbf{r})\psi^{\mathrm{inc},j}_{a}(\mathbf{r},t)e^{i(E_b-E_a)t}, \tag{25}$$

where $H_0 = \mathbf{p}^2/2M$ is the kinetic energy operator and the position dependent matrix element $V_{ba}(\mathbf{r}) = \langle \Phi_b | V | \Phi_a \rangle$. For the example of a transition between one-electron states of an atom, $V_{ba}(\mathbf{r}) = \int d^3\mathbf{r}' \Phi_b^*(\mathbf{r}')\Phi_a(\mathbf{r}')/|\mathbf{r}-\mathbf{r}'|$. This equation has the solution

$$\psi^{\mathrm{sca},j}_{b\leftarrow a}(\mathbf{r},t) = -i\int_{-\infty}^{t} e^{-iH_0(t-t')}V_{ba}(\mathbf{r}) \times \psi^{\mathrm{inc},j}_{a}(\mathbf{r},t')e^{i(E_b-E_a)t'}dt'. \tag{26}$$

We can now perform the projection of the incident wave on the scattered wave to obtain

$$\begin{aligned}\langle \psi^{\mathrm{inc},j}_{a} | \psi^{\mathrm{sca},j}_{b\leftarrow a}\rangle &= -i\int_{-\infty}^{t}\int d^3\mathrm{r}[e^{-iH_0(t'-t)}\psi^{\mathrm{inc},j}_{a}(\mathbf{r},t)]^* \\ &\quad \times V_{ba}(\mathbf{r})\psi^{\mathrm{inc},j}_{a}(\mathbf{r},t')e^{i(E_b-E_a)t'}dt' \\ &= -i\int_{-\infty}^{t}\tilde{V}^{(j)}_{ba}(t')e^{i(E_b-E_a)t'}dt',\end{aligned} \tag{27}$$

where $\tilde{V}^{(j)}_{ba}(t) = \int V_{ba}(\mathbf{r})\rho^{(j)}(\mathbf{r},t)d^3\mathbf{r}$ is the time dependent interaction between the states a and b that arise from the time dependent density from particle j. If we sum the contribution from all of the particles in the beam, we obtain the coherent scattering amplitude

$$\sum_j \langle \psi^{\mathrm{inc},j}_{a} | \psi^{\mathrm{sca},j}_{b\leftarrow a}\rangle = -i\int_{-\infty}^{t}\tilde{V}_{ba}(t')e^{i(E_b-E_a)t'}dt', \tag{28}$$

where $\tilde{V}_{ba}(t) = \int V_{ba}(\mathbf{r})\rho(\mathbf{r},t)d^3\mathbf{r}$ is the time dependent interaction between the states a and b that arise from the time dependent density of all of the particles in the beam. This is exactly the term that should be expected from classical intuition: the density of particles generates a time dependent potential $\tilde{V}(\mathbf{r},t) = \int d^3\mathbf{r}'\rho(\mathbf{r}',t)/|\mathbf{r}-\mathbf{r}'|$ that couples states a and b and it is this time dependent coupling that generates transitions. When the density of particles has a modulation in space, the transition probability can be greatly enhanced if the classical field oscillates with the same frequency as the transition frequency of the states. These results violate property (6) of the Introduction since the transition probability depends on the large scale structure of the beam in the longitudinal direction.

From this analysis, we can identify dipole allowed transitions as those being most amenable to coherent excitation by charged particles; furthermore, it is only transitions which preserve the magnetic quantum number, m, in the beam direction that will be enhanced since this is the direction in which the ''classical electric field'' from the beam is oscillating. This is the same trend we found from the expression Eq. (24); for electron-atom scattering, the coherent transition most strongly affects the excitation into dipole allowed states.

C. Transverse and longitudinal coherence

The perturbative expression for the coherent transition amplitude can be used to show that a beam that misses the target can still cause transitions. In essence, a coherent beam has a time and position dependent density which generates a time dependent potential at the target $\tilde{V}(\mathbf{r},t) = \int d^3\mathbf{r}'\rho(\mathbf{r}',t)/|\mathbf{r}-\mathbf{r}'|$. This time dependent potential can cause a transition between states a and b if the potential has Fourier components $E_a - E_b$. This result contains the usual scattering result; in the limit of an incoherent beam, the short time average of the beam density does not vary with time. Thus, the potential, $\tilde{V}$, does not have Fourier components $E_a - E_b$ and there are no transitions unless the beam overlaps the target.

These results violate property (5) of the Introduction: ''no transitions unless the beam and target overlap.'' This effect is similar to the theoretical method for treating ion atom scattering [11] in the sense that one does not treat the electrons and nucleus of the ion as independent objects.

IV. DISCUSSION

It is clear that scattering with a longitudinally coherent beam has several interesting consequences. In this section, I will present calculations for several situations where the longitudinal coherence of a beam will have an observable effect. These will provide illustration for some of the ideas discussed in the previous section.

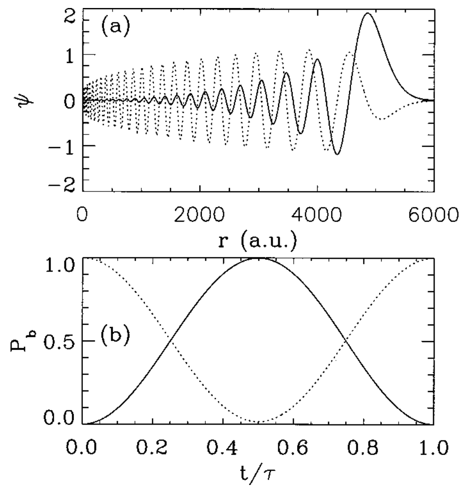

FIG. 2. (a) The dotted line is the Rb wave packet at $t=0$: $(53s+54s)2^{-1/2}$. The solid line is the wave packet at $t=\tau/2$: $(53s-54s)2^{-1/2}$. (b) The normalized scattering probability $P_b=P(t)/\max(P)$ for a one pulse electron beam causing the transition to the $53p$ state (solid line) and to the $62p$ state (dotted line); t/τ is the time of arrival of the electron pulse in units of the wave packet period. Note the transition to the $53p$ state is 180° out of phase with the expectation that the transition is reduced when the electron is at large r.

A. Ultraweak beams, coherent target

In this case, the beam is so weak that the many particle effects of the next section are not present. This case can be thought of as a quantum target that is in a wave packet state interacting with a one particle beam that is also in a wave packet. This situation raises interesting possibilities. For example, a wave packet constructed of Rydberg states on the atom gives a probability distribution for the Rydberg electron that radially oscillates with a period that can be experimentally controlled through excitation to specific states; if the time when a charged particle passes the atom can be controlled, then the dependence of the transition on the radial distance of the Rydberg electron can be experimentally determined.

To take a specific example, I will consider the scattering of a 1 keV electron from a Rb atom in a radial wave packet consisting of the $53s$ (state 1) and $54s$ (state 2) states. This gives a wave packet with a probability distribution that radially oscillates with a period of roughly 19.4 ps. For simplicity, I take the two states to be equally populated and with a phase relationship so that at $t=0$ the Rydberg electron has the smallest $\langle r\rangle$ [dotted line of Fig. 2(a)] and at $t=9.7$ ps the largest $\langle r\rangle$ [solid line of Fig. 2(a)]. If the radial wave functions are both chosen to be positive at $r=0$, then the density matrix is $\rho_{aa'}=1/2$.

I chose to examine the transition to 2 different final states: the $53p$ and the $62p$ states. The scattering amplitudes can be numerically evaluated using a first order Born approximation. The amplitudes can be numerically integrated in Eq. (14) to obtain the following values for the transition $\xi_{aa'}$ matrix to the $53p$ state ($\xi_{11}=56.3$ Tb, $\xi_{12}=\xi_{21}^*=-55.6$ Tb, $\xi_{22}=55.0$ Tb) and to the $62p$ state ($\xi_{11}=2.67$ Gb, $\xi_{12}=\xi_{21}^*=3.26$ Gb, $\xi_{22}=4.01$ Gb). There are a couple properties of this matrix that should be noted. First, all elements are real at this level approximation for the case when both initial states have the same angular momentum. For the transitions chosen, $2|\xi_{21}|\simeq\xi_{11}+\xi_{22}$ which means that beam coherence will drastically change the transition probability.

In the first case, I suppose the incident electron is in a wave packet that is a single pulse and will be modeled by a Gaussian $\rho_z(z,z)=[\Delta z\sqrt{\pi}]^{-1}\exp[-(z-z_0)^2/\Delta z^2]$, where Δz is a spatial width of the beam and z_0 is the position of the incident pulse at $t=0$. The Fourier transform of the longitudinal density needed in Eq. (16) can be obtained analytically as $\exp[i\Delta k_{aa'}z_0-\Delta z^2\Delta k_{aa'}^2/4]$. Before evaluating the expression for the transition probability, note that the cross terms which give the coherent scattering rapidly decrease if $\Delta z>1/\Delta k_{21}$; this condition can be recast as a condition on the time width of the incident electron: $\Delta t=\Delta z/k$ where k is the momentum of the incident electron. Since the incident electron's energy is much greater than the energy spacing of the states making the wave packet, the difference in wave number $\Delta k_{21}\simeq(E_2-E_1)/k$. Thus the condition for observing effects from the coherent target is that the time width of the incident electron pulse times the beat frequency $|E_2-E_1|$ be smaller than 1. This makes sense on physical grounds since there should not be any coherence effects if there are several radial oscillations of the Rydberg wave packet while the incident electron passes the atom.

I introduce one last parameter to get a final formula that shows the relevant physics as clearly as possible. This is the time that the incident electron packet passes the atom: $t=z_0/k$. At the high incident energies and small energy differences of the target states, the factor $\Delta k_{aa'}z_0\simeq(E_a-E_{a'})t$. When the time width of the beam is much shorter than the period of the wave packet, the excitation cross section to the $53p$ and $62p$ states can be written as $\sigma(t)=\sigma_{\rm sum}+\sigma_{\rm osc}\cos[(E_a-E_{a'})t]$ where $\sigma_{\rm sum}=111.3$ Tb and $\sigma_{\rm osc}=-111.2$ Tb for the $53p$ final state and 6.73 and 6.52 Gb, respectively, for the $62p$ final state. In Fig. 2(b), I plot $\sigma(t)/(\sigma_{\rm sum}+|\sigma_{\rm osc}|)$ for the two cases. It is clear that the combined coherence of the target and beam can produce interesting effects if the incident electron pulse is short.

There is a simple lesson that can be learned from Fig. 2. It should be experimentally possible to measure in which region of space the electron makes a transition. For many final states, a transition from a high Rydberg state occurs much more strongly when the Rydberg electron is close to the nucleus than when the electron is at the outer turning point ($62p$ final state in Fig. 2). This property has been surmised from calculations on the radial dependence of the transition matrix elements. However, the transition to the $53p$ state (which is between the $53s$ and $54s$ states) is enhanced when the electron is far from the nucleus which disagrees with expectations. This simple case should be explored in order to show that it is possible to experimentally observe the changing properties of scattering amplitudes with position.

There are many possible schemes that could be used to observe the effect in Fig. 2. I will briefly discuss two possibilities. The most important point is that the time between the peaks in Fig. 2 correspond to a travel distance of $\sim$380 μm for a 1 keV electron beam. If an electron pulse travels through a gas of Rydberg atoms all in the same wave packet state, then the excitation cross section will oscillate in the beam direction with a wavelength of $\sim$380 μm. The excited atoms can be detected in a position dependent manner by ramping an electric field perpendicular to the beam direction so that the electrons stripped from the Rydberg atoms are imaged onto a CCD camera. Resolution of roughly 100 μm can be obtained with this arrangement; this is over a factor of 2 better than needed to detect the signal in Fig. 2. Another possible experimental arrangement is to only excite Rydberg atoms in a small region of space and detect all of the excited atoms by ramping an electric field; the time of the collision relative to the wave packet can be controlled by delaying the time of the creation of the wave packet. With optical light it should be possible to focus the light to a spot smaller than $\sim$100 μm which is all that would be needed to see the effect of the pulsed electron beam.

The case considered in this section is only meant to illustrate a general possibility. There are more interesting situations that occur in molecular physics that might be worth investigating. For example, the transition between two electronic states depends on the positions of the nuclei. A vibrational wave packet on the molecule can interact with a pulsed electron beam; by varying the time of the interaction, the strength of the transition can be mapped as a function of position of the nuclei since the nuclear positions move in a wave packet. Two simple, physical cases can be used as illustration. (1) A vibrational wave packet on H_2 ground state potential curve. Measure the dissociation cross section as a function of the time of interaction with a pulsed electron beam. This will give an *experimental* determination of the dependence of the ${}^1\Sigma_g \rightarrow {}^1\Sigma_u$ transition on the internuclear separation. (2) A vibrational wave packet on the NO ground state potential curve. Measure the dissociation cross section into specific atomic states as a function of the time of interaction with a pulsed electron beam. This will give an *experimental* determination of electronic state specific cross sections as a function of internuclear separation. In polyatomic molecules, there is also the possibility for measuring the time dependence of the flow of vibrational energy by interaction with a pulsed electron beam.

B. Weak beam, single initial state

Now, I will consider examples where the beam is weak (sequential transitions such as $a \rightarrow b$ then $b \rightarrow c$ are neglected) but strong enough so that the coherence of the beam can affect the total transition probabilities. This case can be thought of as the quantum target interacting with the fluctuations (individual particles) in a beam *and* with the large scale ''macroscopic'' properties of the beam.

1. Longitudinal coherence

In Ref. [2], we considered how a sequence of pulses can change the apparent cross section for a particular state. In this section, I will consider a similar case but show how the coherence can change the relative cross section to different states. Thus it is possible to control the excitation probability to the specific final states by varying the time between electron pulses. To take a specific example, I will consider the scattering of a 1 keV electron beam with a Rb atom in the 53s state. The transition cross section to eight different states will be investigated: 49p through 56p. The electron beam at $t=0$ will consist of a cosine modulated exponential

$$\rho_z(z,z) = \frac{1}{\Delta z \sqrt{\pi}} \exp\left[-\frac{z^2}{\Delta z^2}\right]\left[1+\cos\left(\frac{2\pi z}{\lambda}\right)\right], \quad (29)$$

where Δz is a spatial width of the beam and the spatial modulation of the beam $\lambda \ll \Delta z$.

The transition probability arises from two qualitatively different mechanisms. There is an incoherent term that arises from the scattering of an electron so that it does not overlap the initial beam direction; this gives a probability equal to the inelastic cross section times the time integral of the electron current density. This term is present in all scattering experiments. There is a coherent scattering term that arises from an electron in the beam causing a transition but the scattered electron still overlaps with the incident wave after the transition. Since it is impossible to tell which electron causes the transition, the amplitudes for each electron in the beam must be added. This term may be qualitatively related to a semiclassical approximation where the modulated electron density of the beam generates a modulated electric field at the atom; the time varying electric field causes transitions on the atom. Since it is the amplitudes that are added, the transition probability from the coherent scattering is proportional to the square of the time integral of the current density.

The transition probability can be obtained from Eq. (24). There are four factors that contribute: ζ, the time integrated current density, $\sigma_{b\leftarrow a}$, the inelastic cross section, $d\sigma/qdq$, the differential cross section in the forward scattering direction, and the Fourier transform of the $t=0$ beam density. A useful quantity is the effective cross section for a transition which is the transition probability divided by the time integrated current density. The effective cross section can be written in the form

$$\sigma_{\text{eff}} = \sigma \cdot (1+\zeta |F|^2/\zeta_{\text{min}}), \quad (30)$$

where σ is the usual inelastic cross section, ζ_{min} is the minimun time integrated current for which the coherent transition probability can equal the incoherent transition probability and F is the Fourier transform of the $t=0$ density in Eq. (24). In the limit, $\zeta \ll \zeta_{\text{min}}$ this definition reduces to the usual definition of cross section.

In Fig. 3, I show the transition probability divided by the time integrated current density for the transition from the 53s state of Rb to eight different np final states; the transition probability divided by ζ is an effective cross section for the transition. In Table I, I give the relevant parameters for the eight transitions. The time width of the electron beam is chosen to be $\sim$35 ps and the wavelength modulation was chosen to enhance the transition to the 55p state. Without the modulation, the transitions to the 52p and 53p states completely dominate all other transitions. It would be relatively

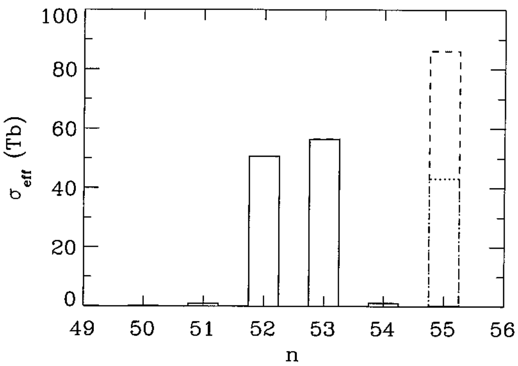

FIG. 3. The effective cross section for electron impact excitation from the 53s state into np states for $n=49-56$ for electrons with 1 keV incident energy. The solid line is the usual cross section which holds when the time integrated electron current $\zeta\to 0$. The dotted and dashed lines are for an electron beam specifically chosen to enhance transition to the 55p state. The dotted line has a time integrated electron current of $\zeta=2\ \mu\mathrm{m}^{-2}$ and the dashed line has $\zeta=4\ \mu\mathrm{m}^{-2}$. This shows that extremely weak transitions can be enhanced in electron scattering when the coherence properties of the beam are controlled.

simple to make a beam that emphasized the 53p transition over the 52p transition (and vice versa); for example, a time integrated current density of $\zeta=700\ \mathrm{mm}^{-2}$ could give an effective cross section into the 53p state over 10 times larger than into the 52p state if the modulation of the beam was chosen properly. Figure 3 shows a much more difficult arrangement. In this situation, I have shown that it is possible to make the transition to the 55p state larger than any other although it is negligibly small without a coherent beam. This shows that it is possible to manipulate the probabilities for excitation into different final states by controlling the modulation of an electron beam.

There are two experimental arrangements that could detect the coherent scattering. Perhaps the simplest arrangement, is to measure the transition probability versus the current density for a short pulse electron beam. For dipole allowed transitions, the probability will increase similar to a quadratic function of the integrated current density if the time width of the pulse is shorter than the transition period. Another arrangement can have a small number of equally spaced short pulses interacting with the atom. For dipole allowed transitions, the probability will depend on the time between the pulses if there is enough electrons and the pulses are shorter than the transition period.

TABLE I. Parameters for transition from the 53s state of Rb to nearby np states caused by a 1 keV electron beam. $\tau=2\pi/(E_{53s}-E_{np})$ is the transition period, σ is the usual definition of the inelastic cross section, and $\zeta_{\min}$ is the minimum time integrated current density that can give equal amounts of coherent and incoherent scattering.

n	τ (ps)	σ (Tb)	$\zeta_{\min}$ (mm^{-2})
49p	−4.815	0.0516	6220
50p	−6.96	0.167	2900
51p	−11.95	0.994	935
52p	−36.7	50.6	88
53p	38.6	56.3	80
54p	13.2	1.09	800
55p	8.12	0.193	2250
56p	5.96	0.0636	4360

2. Transverse and longitudinal coherence

Beams that contain transverse and longitudinal coherence can qualitatively change expectations of scattering by causing transitions even when the beam does not overlap the target. These nonstandard transitions can occur due to the coherent interaction of the incident particles with the target. At the perturbative level, the coherent transitions can be related to the interaction of the quantum target with the ''classical fields'' generated by the beam. For example, an electron pulse that has a small extent in the transverse and longitudinal directions generates a classical electric field proportional to the charge of the pulse and inversely proportional to the squared distance from the pulse. If the electron pulse moves past a quantum target with a kinetic energy of 1 keV, then the time varying electric field can cause transitions in the target.

I will take a very simplified case as an illustration. In this case, a single pulse of electrons with a kinetic energy of 1 keV will interact with a Rb atom in the 53s state. The pulse has a spherical charge distribution given by $\rho=N(\Delta\sqrt{\pi})^{-3}\exp\{-[(x-b)^2+y^2+(z-vt)^2]/\Delta^2\}$, where N is the number of electrons, b is the impact parameter for the charge distribution, and v is the velocity. The integrated current density at the target (at $x=y=z=0$) is $\zeta=N(\Delta\sqrt{\pi})^{-2}\exp(-b^2/\Delta^2)$. The electric field at the target is $\mathbf{F}(t)=(b,0,vt)Q(t)/r^3(t)$, where $r^2(t)=b^2+v^2t^2$ is the distance from the target to the center of the charge cloud and

$$Q(t)=4(\Delta^2\sqrt{\pi})^{-1}\int_0^{r(t)}\tilde{r}^2e^{-\tilde{r}^2/\Delta^2}d\tilde{r} \tag{31}$$

is the charge contained within a sphere of radius r centered on the charge cloud.

In Fig. 4, a specific case is chosen to show the transition from Rb 53s state to 53p state with experimentally reasonable parameters. The radius of the charge cloud is chosen to be $\Delta=100\ \mu$m with an energy of 1 keV. The number of electrons was chosen to be 14 so the incoherent (solid line) and coherent (dashed line) transition probabilities are roughly equal for zero impact parameter. The coherent transition probability decreases proportional to $\exp(-2b|E_1-E_2|/v)$ for large impact parameter, b, whereas the incoherent transition probability decreases as a Gaussian. Since the coherent transition probability is proportional to the square of the number of particles, it should be possible to measure a transtion when the beams do not overlap simply by increasing the number of electrons in the beam. For example, if the number of electrons is increased to 1400 the coherent transition probability at 400 μm is 5.6×10^{-5} whereas the incoherent transition probability is 2.8×10^{-11}.

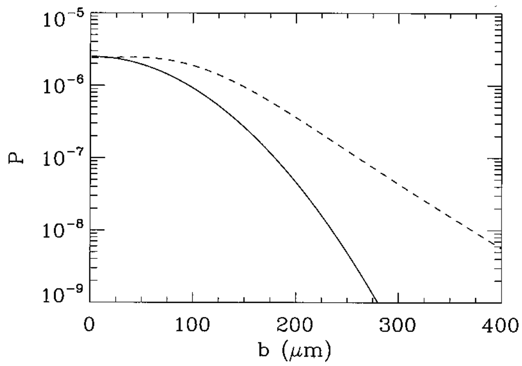

FIG. 4. The transition probability from the Rb 53*s* state to the 53*p* state for a Gaussian spatial distribution of electrons in the beam; the beam density is proportional to $\exp\{-[(x-b)^2+y^2+(z-vt)^2]/\Delta^2\}$. The solid line is for the incoherent transition probability: the cross section times the overlap of the beam with the target. The dashed line is the coherent transition from the collective field of the beam. For this case, the width of the beam is $\Delta=100$ μm, the kinetic energy is 1 keV, and there are 14 electrons in the electron pulse. The solid line is proportional to the number of electrons while the dashed line is proportional to the square of the number of electrons in the pulse.

The only difficulty in performing an experiment to show this effect arises from mutual repulsion of the electrons in the incident beam. Transverse spreading can be suppressed by using a moderately strong magnetic field in the beam direction. The longitudinal spreading cannot be suppressed. The only cure is to shorten the time between the creation of the pulse and the time of interaction with the target. As an order of magnitude estimate, the outward force on an electron at the edge of the cloud is N/Δ^2; as a criterion, we can say that the cloud should expand by less than 10% which leads to a restriction on the time to be $\Delta t \sim \sqrt{\Delta^3/10N}$. For 1000 particles in a 100 μm pulse this translates to a time of 0.6 ns. This is a travelling distance of 1.2 cm for a 1 keV electron beam which seems to be experimentally reasonable.

V. CONCLUSIONS

I have described a theoretical formulation of a longitudinally coherent beam interacting with a quantum target. I have found that it is possible to violate all of the well-known qualitative properties of scattering theory if the beam has longitudinal coherence. The properties (1)–(6) discussed in the Introduction can be completely wrong in many situations. I have also calculated transition probabilities in several situations to show that it is possible to observe these effects. It seems likely that there are many other interesting phenomena that become possible when using a longitudinally coherent beam; these phenomena include obtaining a level of experimental control over scattering, measuring how scattering depends on internal properties such as the spatial configuration of objects in the target, measuring differential cross sections without measuring the scattered particle, ... Since there are several prospective beam sources with longitudinal coherence, it is worthwhile to further investigate this type of system.

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