

# Scattering Theory with Pulsed Matter Beams

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## Abstract

*We discuss a theory for the interaction of a quantum target with a pulsed matter beam. We find that coherent transitions in the target due to the pulsed nature of the beam can qualitatively change scattering probabilities from those of a continuous beam. In this paper, we concentrate on the perturbative limit and show the connection to classical intuition.*

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**Key words:** wave-packets, scattering theory, Rydberg atoms, perturbation theory, semiclassical approximation

Ugo Fano made numerous key contributions to the understanding of correlated motion in atoms and molecules (for example, see Refs. 1, 2). In these studies, he focused on the key physical features of the system that controlled the interaction between different degrees of freedom. An interesting feature of his approach is his ability to cast the final answer in terms of parameters that are independent of the particular system and a small number of physical parameters that are system dependent. Often, these parameters could be measured and used to characterize the dynamics of a wide variety of atoms, molecules, and more complicated quantum systems.

Generally, he is also driven to use quantum theory to derive results that had previously arisen in classical form. An example of this is his papers on the index of refraction of solids.<sup>(3)</sup> In these papers, the Lorentz-Lorenz expression for the index of refraction was derived using general quantum expressions for properties of the solid and second quantization for the photon field.

Over time his interest in density matrices led to an interesting and influential review paper on the subject<sup>(4)</sup> in which he discussed states with less than maximum information; he was interested in specifying the density matrix directly in terms of the information that is available on a system.<sup>1</sup> Density matrices are useful because they can be used to describe systems that are only partially coherent. The coherence of a quantum system is embodied in off-diagonal terms of the density matrix. Expressing a final result in terms of density matrices can be useful in discovering the dependence of coherence.

For this paper, we touch on all of these aspects in order to address the problem of the interaction of a quantum target with a modulated matter beam. We have presented a brief development of this topic<sup>(5)</sup> with a much more detailed and exhaustive treatment to be given later. There are several reasons for studying such a system. As discussed below, there is a paradox involved in applying the usual ideas from scattering theory to this problem; we resolve the paradox by showing that many familiar features of scattering theory do

not apply. In this paper, we concentrate on the perturbative limit in order to clearly show the physical mechanisms controlling the scattering by a pulsed beam. We cast the final result into a form that shows the connection to classical expressions. And we show how the final result can be compactly expressed in terms of the density matrix for particles in the beam.

A simplified cartoon of the system we investigate is shown in Fig. 1. We imagine a quantum target interacting with a matter beam. A type of coherence is imprinted onto the matter beam so that the beam has a pulsed structure in the longitudinal direction. For the purpose of our discussion, we do not need the particles in the beam to be completely coherent although a large level of coherence can be obtained using pulsed "atom lasers"<sup>(6-9)</sup> or the "pulsed electron gun."<sup>(10,11)</sup> We only require enough coherence so that the beam is pulsed; the specific coherent requirements will be discussed below. The beam can cause transitions in the target that will be probed after the beam has passed the quantum scatterer. The question we address is: what, if any, affect will the coherence have on any inelastic scattering probability?

Normal scattering theory has many well-known properties when the beam is weak and the target is weak. By a weak beam, we mean that the beam is too weak for double scattering to be important; thus, we do not need to worry about the beam causing a transition from state A to state B and then later causing a second transition from state B to state C. By a weak target, we mean that the properties of the beam do not change to an appreciable extent while interacting with the scatterers; thus, we do not need to worry about a large fraction of the beam being scattered by the target. In these limits, it is well known that the probability for inelastic scattering only depends on the probability of having an incident particle with momentum  $\mathbf{p}$ .<sup>(12,13)</sup> This means that the inelastic scattering probability does not depend on any coherence property of the beam. It is also well known that the scattering probability is proportional to the number of objects in the beam if all other parameters (energy, spatial

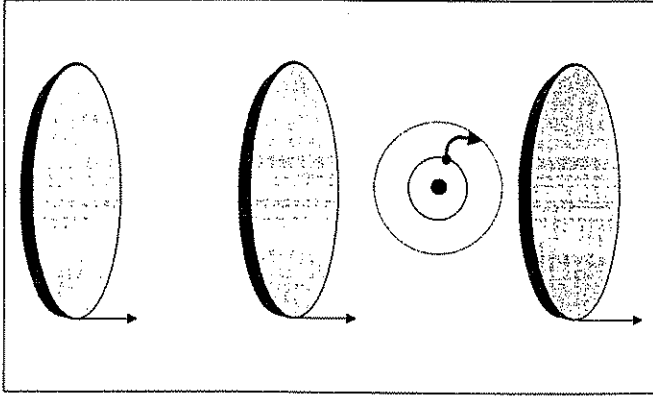


Figure 1. A schematic drawing of a Rydberg atom interacting with a beam bunched in the longitudinal direction.

width, momentum distribution, etc.) are kept fixed. Finally, the total transition probability between two specific states depends on the inelastic cross section integrated over all angles.

Ordinary properties of scattering theory cannot be reconciled with our intuition of how a pulsed beam will interact with a quantum target. To be specific, let us take the case of a pulsed electron beam interacting with a highly excited alkali atom. If we imagine the electrons as a charge distribution, then at a fixed point in space we would expect to have a classical electric field that oscillates in the beam direction with a period given by the distance between the pulses of electrons divided by the speed of electrons. It should be possible to use this oscillating electric field to drive a resonant transition in the atom when the period of the electric field matches the beat period  $\hbar/(E_1 - E_2)$  of a transition in the atom. This aspect of our intuition violates the expectation that inelastic transitions do not depend on coherence properties of the beam. This also violates the expectation from scattering theory that transition probabilities are proportional to the number of particles in the beam. To see this, remember that a transition *amplitude* caused by an oscillating electric field is proportional to the field strength, which is proportional to the number of particles in a beam; thus, our intuition says that the pulsed beam should give a transition probability proportional to the square of the number of particles in the beam. Finally, this coherent scattering must be a sort of scattering from a collective property of the beam and thus no single electron will be strongly scattered. Therefore, our intuition says that the coherent scattering between two specific states will depend on the inelastic scattering amplitude in the forward direction, which violates the usual scattering theory,<sup>2</sup> where the transition probability between two states integrates the inelastic cross section over all directions the electron can scatter into.

Although classical intuition for scattering by a pulsed beam violates quantum-scattering theory in several places, it should not be dismissed. In this case, classical intuition is a reliable guide to a correct description of the phenomena. We show below that the usual derivation of inelastic scattering leaves out a term in the transition probability. It is this missing term that gives all of the effects that our intuition claims should be present.

The derivation treats the scattering as if the incident particles are completely coherent and can be treated as a normalizable wave-packet of finite extent; this allows us to use a wave-function description of the dynamics instead of a density matrix formalism. At a later stage, we will introduce the incoherence into the beam and relate our results to the momentum space density matrix of the beam. To be specific, we will take the electron beam to be traveling in the  $z$ -direction. For one incident electron and one scatterer, the normalized wave-function of the collision complex is

$$\Psi(t) = \Phi_a e^{-iE_a t} \psi_a^{\text{inc}}(\mathbf{r}, t) + \sum_b \Phi_b e^{-iE_b t} \psi_{b \leftarrow a}^{\text{sca}}(\mathbf{r}, t), \quad (1)$$

where  $E_a$  is the energy and  $\Phi_a$  is the wave-function for state  $a$  of the target and  $\psi_a^{\text{inc}}(\mathbf{r}, t)$  is the incident electron's wave-function, which does not include any effects from the target, and  $\psi_{b \leftarrow a}^{\text{sca}}(\mathbf{r}, t)$  is the scattered part of the wave-function leaving the target in state  $b$ ; the part of the scattered wave with  $a \leftarrow a$  gives the elastic scattering. The normalization is chosen so that  $\langle \psi_a^{\text{inc}}(\mathbf{r}, t) | \psi_a^{\text{inc}}(\mathbf{r}, t) \rangle = 1$ .

Once we obtain the scattered wave, the probability for the incident particle to cause a transition in the target to state  $b$  is  $P_{b \leftarrow a} = \langle \psi_{b \leftarrow a}^{\text{sca}} | \psi_{b \leftarrow a}^{\text{sca}} \rangle$ . To connect this result to the usual scattering cross sections we can use the energy-dependent scattering wave-function at large  $r$ :

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

where  $k_b = (2(E_a - E_b) + k^2)^{1/2}$  from energy conservation. Moreover, the differential cross section can be obtained from the scattering amplitude in the form

$$\frac{d\sigma}{d\Omega}(\hat{\mathbf{r}}, k) = \frac{k_b}{k} |f_{b \leftarrow a}(k_b \hat{\mathbf{r}} \leftarrow k\hat{\mathbf{z}})|^2. \quad (3)$$

The incident direction is chosen to be in the  $z$ -direction for the definition of the differential cross section.<sup>3</sup>

Many of the usual features of scattering theory can be derived from the definition of the transition probability. We first make a wave-packet using the wave-function from (2):

$$\Psi(t) = \int \Psi_{\mathbf{k},a} \exp[-i(E_a + k^2/2)t] A(\mathbf{k}) d^3\mathbf{k}, \quad (4)$$

where to obtain unit normalization the amplitudes must satisfy  $\int |A(\mathbf{k})|^2 d^3\mathbf{k} = 1$ . In general, the amplitude  $A$  is complex. For example, if we have an  $A_0(\mathbf{k})$  that makes a wave-packet, then the amplitude  $A(\mathbf{k}) = A_0(\mathbf{k})[1 + \exp(-i\mathbf{k} \cdot \mathbf{R})]/2^{1/2}$  gives a two wave-packet state with the second packet shifted in space by an amount  $\mathbf{R}$ . We assume that the  $A$  are strongly peaked around the vector  $\mathbf{k}_0 = (0, 0, k_0)$ . The scattering probability for a target at  $\mathbf{r}_0$  can be obtained as a triple integral

$$P_{b \leftarrow a} = \frac{1}{(2\pi)^3} \int d^3\mathbf{r} d^3\mathbf{k} d^3\mathbf{k}' \times A^*(\mathbf{k}') f_{b \leftarrow a}^{(0)*}(k'_b \hat{\mathbf{r}} \leftarrow \mathbf{k}') f_{b \leftarrow a}^{(0)}(k_b \hat{\mathbf{r}} \leftarrow \mathbf{k}) A(\mathbf{k}) \times \frac{1}{r^2} \exp\{i[(k_b - k'_b)r + (\mathbf{k} - \mathbf{k}' + k'_b \hat{\mathbf{r}} - k_b \hat{\mathbf{r}}) \cdot \mathbf{r}_0]\}, \quad (5)$$

where  $k'_b = (2(E_a - E_b) + k'^2)^{1/2}$ . Performing the integration over  $r$  gives a factor of  $2\pi\delta(k_b - k'_b)$ , and averaging the  $x, y$  components of  $\mathbf{r}_0$  over a range  $L_x, L_y$  gives a factor of  $(2\pi)^2 \delta(k_x - k'_x) \delta(k_y - k'_y) / L_x L_y$ . The product of these two terms is  $(2\pi)^3 \delta(\mathbf{k} - \mathbf{k}') / (L_x L_y [dk_b/dk])$ , where we have used the usual relation  $\delta(f(x)) = \delta(x)/|f'(x)|$  if  $f(x)$  has its only zero at  $x = 0$ . If we now use the relation  $dk_b/dk = k/k_b$  then the scattering probability can be simplified to

$$P_{b \leftarrow a} = \frac{1}{L_x L_y} \int d^2\hat{\mathbf{r}} d^3\mathbf{k} \frac{k_b}{k} |f_{b \leftarrow a}^{(0)}(k_b \hat{\mathbf{r}} \leftarrow \mathbf{k}) A(\mathbf{k})|^2 = \frac{1}{L_x L_y} \int d^3\mathbf{k} \sigma_{b \leftarrow a}(k) |A(\mathbf{k})|^2, \quad (6)$$

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 cross section  $\langle \sigma_{b \leftarrow a} \rangle$  times the time-integrated current density (which is 1 particle over an area  $L_x L_y$ ). 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 in wave-number space is  $\rho(\mathbf{k}, \mathbf{k}') = \langle A(\mathbf{k}) A^*(\mathbf{k}') \rangle$ , where  $\langle \dots \rangle$  means to average over the different realizations of this one particle beam scattering off one quantum target; using this definition, we find that the transition probability only depends on diagonal elements of the density matrix. Because of this the transition probability does not depend on any 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 electron; if the final result

only depends on  $|A(\mathbf{k})|^2$ , then this phase relationship is irrelevant.

It is not obvious that the analysis changes if there are  $N$  particles in the beam of transverse area  $L_x L_y$ ; the time integral of the current density is  $\zeta = N/L_x L_y$ . The transition probability from state  $a$  to state  $b$  is usually assumed to be  $N \langle \sigma_{b \leftarrow a} \rangle / L_x L_y = \zeta \langle \sigma_{b \leftarrow a} \rangle$ , 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. To check the assumption that the 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 where the only assumption is that there is only one scattering event; this wave-function is

$$\Psi(t) = \Phi_a e^{-iE_a t} \prod_{j=1}^N \psi_a^{\text{inc},j}(\mathbf{r}_j, t) + \sum_b \Phi_b e^{-iE_b t} \sum_{j'} \left\{ \psi_{b \leftarrow a}^{\text{sca},j'}(\mathbf{r}_{j'}, t) \prod_{j \neq j'} \psi_a^{\text{inc},j}(\mathbf{r}_j, t) \right\}. \quad (7)$$

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 (7), 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 objects because the incident particles are distinguishable.

Coherent and incoherent probabilities for exciting the target to state  $b$  are given by

$$P_{b \leftarrow a}^{(N)} = \sum_j \langle \psi_{b \leftarrow a}^{\text{sca},j} | \psi_{b \leftarrow a}^{\text{sca},j} \rangle + \sum_{j \neq j'} \langle \psi_a^{\text{inc},j} | \psi_{b \leftarrow a}^{\text{sca},j} \rangle \langle \psi_{b \leftarrow a}^{\text{sca},j'} | \psi_a^{\text{inc},j'} \rangle, \quad (8)$$

where unit normalization of the incident packets has been used. The first term of (8) 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 waves, 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 (8) 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

$$\langle \psi_{b \leftarrow a}^{\text{sca},j} | \psi_{b \leftarrow a}^{\text{sca},j} \rangle \gg |\langle \psi_a^{\text{inc},j} | \psi_{b \leftarrow a}^{\text{sca},j} \rangle|^2.$$

It is illustrative to use this fact to approximate (8) in the form

$$P_{b \leftarrow a}^{(N)} \approx \sum_{j=1}^N \langle \psi_{b \leftarrow a}^{\text{sca},j} | \psi_{b \leftarrow a}^{\text{sca},j} \rangle + \left| \sum_{j=1}^N \langle \psi_a^{\text{inc},j} | \psi_{b \leftarrow a}^{\text{sca},j} \rangle \right|^2, \quad (9)$$

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 waves, be comparable to 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 (9) 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 (9) *exactly* equals the transition from state  $a$  to state  $b$  calculated using first-order time-dependent perturbation theory and the time-dependent coupling potential generated by the incident wave-packets  $|\psi_a^{\text{inc},j}|^2$ . 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.

Years of use have accustomed us to the behavior of scattering processes with incoherent matter beams. In a previous paper,<sup>(5)</sup> we have discussed an expression for the coherent scattering in terms of usual scattering parameters. Here, we will discuss the first-order perturbation theory limit. This limit is illustrative because it allows closed-form

expressions in terms of parameters that should be important according to our intuition; specifically, we will show that the coherent transition probability in (9) is exactly the same as the transition probability from the collective classical field generated by the particles of the beam. To lowest order in the coupling between states  $a$  and  $b$ , the scattered wave can be written as the solution of

$$\left( i \frac{\partial}{\partial t} - H_0 \right) \psi_{b \leftarrow a}^{\text{sca},j}(\mathbf{r}, t) = V_{ba}(\mathbf{r}) \psi_{b \leftarrow a}^{\text{inc},j}(\mathbf{r}, t) e^{i(E_b - E_a)t}, \quad (10)$$

where  $H_0 = \mathbf{p}^2/2$  is the kinetic energy operator and the position-dependent matrix element  $V_{ba}(\mathbf{r}) = \langle \Phi_b | V | \Phi_a \rangle$ . This equation has the solution

$$\psi_{b \leftarrow a}^{\text{sca},j}(\mathbf{r}, t) = -i \int_{-\infty}^t e^{-iH_0(t-t')} V_{ba}(\mathbf{r}) \psi_a^{\text{inc},j}(\mathbf{r}, t') e^{i(E_b - E_a)t'} dt'. \quad (11)$$

For the example of a transition between one-electron states of an atom,  $V_{ba}(\mathbf{r}) = \int d^3\mathbf{r}' \Phi_b^*(\mathbf{r}') \Phi_a(\mathbf{r}') / |\mathbf{r} - \mathbf{r}'|$ . We can now perform the projection of the incident wave on the scattered wave to obtain

$$\begin{aligned} & \langle \psi_a^{\text{inc},j} | \psi_{b \leftarrow a}^{\text{sca},j} \rangle \\ &= -i \int_{-\infty}^t \int d^3\mathbf{r} \psi_a^{\text{inc},j*}(\mathbf{r}, t) e^{-iH_0(t-t')} V_{ba}(\mathbf{r}) \psi_a^{\text{inc},j}(\mathbf{r}, t') e^{i(E_b - E_a)t'} dt' \\ &= -i \int_{-\infty}^t \int d^3\mathbf{r} [e^{-iH_0(t-t')} \psi_a^{\text{inc},j}(\mathbf{r}, t)]^* V_{ba}(\mathbf{r}) \psi_a^{\text{inc},j}(\mathbf{r}, t') e^{i(E_b - E_a)t'} dt' \quad (12) \\ &= -i \int_{-\infty}^t \int d^3\mathbf{r} \psi_a^{\text{inc},j*}(\mathbf{r}, t') V_{ba}(\mathbf{r}) \psi_a^{\text{inc},j}(\mathbf{r}, t') e^{i(E_b - E_a)t'} dt' \\ &= -i \int_{-\infty}^t \bar{V}_{ba}^{(j)}(t') e^{i(E_b - E_a)t'} dt', \end{aligned}$$

where

$$\bar{V}_{ba}^{(j)}(t) = \int V_{ba}(\mathbf{r}) \rho^{(j)}(\mathbf{r}, t) d^3\mathbf{r}$$

is the time-dependent interaction between the states  $a$  and  $b$  that arises from the time-dependent density from particle  $j$ . If we sum the contributions from all of the particles in the beam, we obtain the coherent-scattering amplitude

$$A_{b \leftarrow a}(t) \equiv \sum_j \langle \psi_a^{\text{inc},j} | \psi_{b \leftarrow a}^{\text{sca},j} \rangle = -i \int_{-\infty}^t \bar{V}_{ba}(t') e^{i(E_b - E_a)t'} dt', \quad (13)$$

where

$$\bar{V}_{ba}(t) = \int V_{ba}(\mathbf{r}) \rho(\mathbf{r}, t) d^3\mathbf{r}$$

is the time-dependent interaction between the states  $a$  and  $b$  that arises 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 when the classical field oscillates with the same frequency as the beat frequency of the states. From this analysis, we can identify dipole-allowed transitions as those being most amenable to coherent excitation; furthermore, it is only transitions that 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.

Scattering theory has a long history, so it is natural to ask how this result fits within the more usual theories and why the coherent-scattering term hasn't appeared in experiments performed to date. Transitions from (13) are neglected in usual scattering theory and in experiments performed to date because the beams have not contained time-dependent densities of the correct frequencies. In most experiments and in the usual scattering theory,  $\rho(\mathbf{r}, t)$  is essentially time independent on the time-scales of the target,  $\tau = h/|E_a - E_b|$ . Typically, the average density is a smooth function of time; the Fourier transform of  $\tilde{V}_{ba}(t)$  in (13) is strongly peaked in frequency with a width much less than  $|E_a - E_b|$ . In this case,

$$\sum_j \langle \psi_a^{\text{inc},j} | \psi_{b \leftarrow a}^{\text{sca},j} \rangle \approx 0$$

and thus the transition probability reduces to the usual expression in terms of the inelastic cross section and the time-integrated current density. We note that it should be possible to measure the result of the coherent scattering by deliberately modulating the particle beam and by using highly excited states of atoms (where the energy differences are small) in order to slow down the atomic dynamics. To be specific, we believe that an electron beam that is modulated on a  $\sim 10$  ps time-scale<sup>(10,11)</sup> can be accelerated to keV energies and made to interact with Rydberg states of alkali atoms; there are transition periods of highly excited atoms of this time-scale and thus a possible signal is to change the transition probability by changing the period of modulation of the electron beam.

It might not be clear that any coherence of the beam is necessary to get a transition since the final results only depend on the time-dependent density of particles in space. The important point is that a modulation of the beam in space *automatically* implies a level of coherence between momentum components of the beam. We can rewrite the

transition amplitude using

$$\begin{aligned} A_{b \leftarrow a}(\infty) &= -i \int_{-\infty}^{\infty} dt \int d^3\mathbf{r} \rho(\mathbf{r}, t) V_{ba}(\mathbf{r}) e^{i(E_b - E_a)t} \\ &= -2\pi i \int d^3\mathbf{k} d^3\mathbf{k}' \rho(\mathbf{k}, \mathbf{k}') U_{ba}(\mathbf{k}' - \mathbf{k}) \\ &\quad \times \delta\left(E_b - E_a + \frac{k'^2}{2} - \frac{k^2}{2}\right), \end{aligned} \quad (14)$$

where  $U_{ba}(\mathbf{q}) = (2\pi)^{-3} \int d^3\mathbf{r} V_{ba}(\mathbf{r}) \exp(-i\mathbf{q} \cdot \mathbf{r})$  is the Fourier transform of the interaction potential. If there is no coherence between the different momentum components, then the density matrix is  $\rho(\mathbf{k}, \mathbf{k}') = 0$  unless  $\mathbf{k} = \mathbf{k}'$ , and the transition amplitude is zero because it is proportional to  $\delta(E_b - E_a)$  with  $E_b \neq E_a$ .

Clearly, there are many interesting aspects that arise when using modulated matter beams. There is one last interesting feature that can be obtained from this form of the transition amplitude. If the beam only has longitudinal coherence and there is no transverse coherence, then the density matrix is proportional to delta functions of  $k_x - k'_x$  and  $k_y - k'_y$ , which give

$$A_{b \leftarrow a}(\infty) \propto \int d^3\mathbf{k} \frac{\rho(\mathbf{k}, \mathbf{k} + \Delta k \hat{z}) U(\hat{z} \Delta k)}{k_z + \Delta k}, \quad (15)$$

where  $\Delta k = (2(E_a - E_b) + k^2)^{1/2} - k$  is the minimum change in momentum. This equation clearly shows that the final scattering amplitude depends on the off-diagonal density matrix elements in the longitudinal direction. But perhaps more importantly, it shows that the transition amplitude is proportional to the scattering amplitude (which is proportional to  $U[\mathbf{q}]$ ) only in the forward direction. This means that the *total* transition probability will depend on the total cross section from the incoherent scattering and on the differential scattering cross section in the forward direction from the coherent scattering.

In conclusion, we would like to suggest another physical reason for the coherent-scattering term. When a beam of particles interacts with a quantum scatterer, there are two mechanisms for causing a transition. In the usual case, the incident particle scatters from the target and changes energy and momentum. After the scattering, it is possible to tell which incident particle has caused the transition; thus, the transition probability is the incoherent sum over all of the distinguishable possible causes of the transition. In the coherent case we discussed, the projectile continues in the forward direction after the scattering but with changed momentum because of the energy transferred to the target; however, if the projectile has a coherent energy spread that is greater than the energy transfer, then it is not possible to know which projectile caused the transition because it still

overlaps the unscattered wave-packet. Since it is not possible to tell which particle caused the transition, the amplitudes for all of the possibilities need to be added coherently and then squared to obtain the transition probability. This analysis suggests that dipole-allowed transitions for the interaction of a fast electron with a quantum target will be good candidates to observe effects from pulsed beams; the inelastic, differential cross section is only peaked in the forward-scattering direction for dipole-allowed transitions.

Scattering theory with modulated matter beams has been discussed in this paper, with the focus on the change in the transition probability that results from having a pulsed beam of particles interacting with a quantum target. We find that if the scattered wave overlaps the initial wave, then there is the possibility for the transition *amplitudes* of the different incident particles to add coherently. In our analysis, we have used several aspects of Fano's work; density matrices, the correlation that develops between a beam electron and a target through electron-electron interactions, and the expression of the final result in terms of classically intuitive parameters were all used in our discussion. We find that the coherent part of the transition amplitude violates many of the usual assumptions in scattering theory. (1) The total transition probability is proportional to the square of the number of particles in the beam. (2) The total transition is proportional to the differential cross section only in the

forward-scattering direction. (3) The transition probability depends on coherence properties of the beam; in other words, the transition probability depends on off-diagonal elements of the density matrix in momentum space. (4) The transition probability can be related to classical, large-scale properties of the beam (for example, average charge density). The study of scattering using coherent beams is just beginning and we expect many other interesting properties to emerge in future studies.

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### Résumé

*Nous discutons d'une théorie traitant l'interaction d'une cible quantique avec un faisceau de particules pulsées. Nous trouvons que des transitions cohérentes induites par les pulsations du faisceau influent sur les probabilités de transition, qui diffèrent alors qualitativement des probabilités induites par un faisceau continu. Dans cet article, nous concentrons notre étude sur la limite perturbatrice et sur les liens avec l'intuition classique.*

### Endnotes

- <sup>1</sup> A pure state can be specified by the coefficients  $C_j$  of the basis states that construct it:  $|\Psi\rangle = \sum_j C_j |\psi_j\rangle$ . In the simplest representation, a density matrix can be considered to be the expectation value of the operator  $|\Psi\rangle\langle\Psi|$ , which has the simple form  $\rho_{ij} = C_i C_j^*$  for a pure state.
- <sup>2</sup> This behavior should be contrasted with the optical theorem, where the total cross section (summed over all possible final states and integrated over all angles) may be obtained from the imaginary part of the elastic-scattering amplitude in the forward direction.
- <sup>3</sup> 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

$$f_{b \leftarrow a}(\mathbf{k}' \leftarrow \mathbf{k})|_{\mathbf{r}_0} = f_{b \leftarrow a}^{(0)}(\mathbf{k}' \leftarrow \mathbf{k})e^{i(\mathbf{k}' - \mathbf{k}) \cdot \mathbf{r}_0}. \quad (16)$$

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