van Hove’s theory of scattering of probe particles by a macroscopic target is generalized so as to relate the differential cross section for atomic ejection via stimulated Raman transitions to one-particle momentum-time correlations and momentum distributions of 1D trapped gases. This method is well suited to probing the longitudinal momentum distributions of 1D gases in situ, and examples are given for bosonic and fermionic atoms.

If an ultracold atomic gas is probed by high-energy particle scattering so that the struck boson recoils with an energy large compared with typical interactions in the target system then measurement of the differential scattering cross section leads to determination of the dynamic structure factor [1–3]. There are some situations not amenable to such a treatment. For example, it follows from the Fermi-Bose mapping theorem [4] that the dynamic structure factor [1–3] of hard core bosons (Tonks gas [5, 6]) in a tightly confined atom waveguide [7–9] is identical with that of the corresponding ideal Fermi gas, although their momentum distributions are quite different. Here we introduce another approach based on a generalization [10, 11] of the classical van Hove theory [12] of scattering of probe particles by a macroscopic target. We apply this very general approach to stimulated Raman transitions between two different hyperfine levels of a 1D trapped gas, for example, a Bose-Einstein condensate (BEC). Raman transitions have been demonstrated as a mechanism for outcoupling of coherent atom beams from a BEC [13–15], and Bloch et al. [16] have employed radio-wave output coupling to measure the spatial coherence of trapped atomic gases.

Here we propose using Raman outcoupling to determine single-atom momentum-time correlations and momentum distributions of 1D trapped gases. The relevant reactive scattering process in the case of a sodium BEC experiment is [17] photon + $^1$S$_0$ BEC $\rightarrow$ photon$'$ + boson + $^3$S$_1$ BEC$'$ where photon denotes a photon absorbed from an incident laser beam, photon$'$ denotes a photon emitted into a second overlapping laser beam via a stimulated Raman transition, boson$'$ denotes an ejected atom in the untrapped $m = 0$ magnetic sublevel, which originally belonged to an $N$-atom BEC of atoms in the $m = -1$ sublevel, and BEC$'$ denotes an $(N - 1)$-atom excited state of the residual BEC. The same scheme applies to the experiments on Bragg spectroscopy of sodium BECs [17, 18] but there the internal state of the scattered atom boson remains in the trapped state $m = -1$. It is this distinction that allows our scheme to yield the momentum distribution directly by examination of the ejected atoms in contrast to Bragg spectroscopy which yields the dynamic structure factor.

Another recent proposal [19] for measuring the one-particle density matrix via the reactive scattering process impurity + BEC $\rightarrow$ impurity + boson + BEC$'$ simultaneously assumes a high energy incident impurity (Born approximation) and an S-wave pseudopotential impurity-boson interaction justified only for low energy collisions, and requires measurement of a differential cross section involving two outgoing particles. Some recent work [20] on the use of photoionization measurements for determination of correlation functions of the Bose field used a different scheme (tightly focused laser beam, measurement of photoelectron energy but not angular distribution) with emphasis on temporal rather then spatial correlations.

**Derivation**: A crucial point [11] is that in order to probe one-particle correlations one should use a reactive scattering process which effectively removes one particle from the target system; this leads to the hole propagator and a related one-particle momentum-time correlation function. For the case of the above-described Raman process, we use the following simple choice of asymptotic initial and final states: $|i\rangle = |\text{laser}\rangle |B_i\rangle = U |B_i\rangle$ and $|f\rangle = a_{k,m=0}^\dagger |\text{laser}\rangle |B_f\rangle = a_{k,m=0}^\dagger U |B_f\rangle$. The laser state vector is a single-mode coherent state with respect to each of the two Raman beams, one with wave vector $k_1$ and polarization index $\lambda_1$ and the other with wave vector $k_2$ and polarization index $\lambda_2$. Its most convenient representation for our purposes is $|\text{laser}\rangle = \hat{U} |0\rangle$ where the unitary operator $\hat{U} = e^{i\hat{F}}$ with $\hat{F} = c_1 b_{k_1,\lambda_1}^\dagger + c_2 b_{k_2,\lambda_2}^\dagger + \text{h.c.}$. The mean photon occupation numbers are $n_j = |c_j|^2$ and the occupation number dispersions are $\sqrt{n_j}$, negligible compared to $n_j \gg 1$. For concreteness in notation we consider the case of a sodium BEC target but stress that the treatment is not restricted to bosonic atoms or equilibrium states. Then $|B_i\rangle$ is the $N$-boson
state vector describing $N$ magnetically trapped bosons in their electronic ground state and magnetic sublevel $m = -1$, including all effects of their mutual interactions. \( \hat{a}_{k,m=0}^\dagger \) creates an atom with wave vector $k$ in the untrapped $m = 0$ magnetic sublevel, and $|B_f\rangle$ is an $(N - 1)$-boson final state of the residual BEC after the $m = 0$ atom has been ejected. The geometry of this process is shown in Figure 1 where we show a cigar shaped BEC of length $L$ along the longitudinal direction $x$. We assume that the BEC is tightly confined in the transverse plane $r_T = (y,z)$ using an atom waveguide. At resonance the energy difference $\hbar c(k_1 - k_2)$ between the photon absorbed by the atom (number 1) and that emitted (number 2) is equal to the energy splitting $\Delta$ between a trapped atom with $m = -1$ and that of the untrapped atom with $m = 0$ ($\Delta$ includes both the Zeemen splitting and difference in confinement energy between the two states). The net momentum $\hbar (k_1 - k_2)$ transferred to the atom will be in the forward direction $z$ as shown provided that the indicated angles of the two beams satisfy $\sin \theta_2 / \sin \theta_1 = k_1 / k_2 \approx 1$. The requirement is then $\theta_2 = \theta_1 + \epsilon$ with $\epsilon \approx [(k_1 - k_2) / k_2] \tan \theta_1 \ll 1$. In the design of experiments the polarizations $\lambda_1$ and $\lambda_2$ of the two laser beams must be chosen appropriately, and a suitable detuning must be used to inhibit spontaneous transitions \[1\]. Inclusion of these details changes the differential cross section only by a multiplicative factor and will not be considered here.

FIG. 1. Geometry of the Raman outcoupling

The appropriate Hamiltonian is $\hat{H} = \hat{H}_B + \hat{H}_{0ph} + \hat{H}_{0a} + \hat{V}$ where $\hat{H}_B$ is the second quantized many-body Hamiltonian of the trapped $m = -1$ BEC atoms including their mutual interactions and $\hat{V}$ is the interaction of the $N$-atom system with the quantized electromagnetic field. The asymptotic (free) Hamiltonians for the incident photons and outgoing $m = 0$ atoms are $\hat{H}_{0ph} = \hbar c(k_1 \hat{N}_1 + k_2 \hat{N}_2)$ and $\hat{H}_{0a} = \sum_k [(\hbar^2 k^2 / 2m) + \Delta] \hat{N}_{k,m=0}$ where $\hat{N}_j = \hat{a}_{k_j,\lambda_j}^\dagger \hat{a}_{k_j,\lambda_j}$ and $\hat{N}_{k,m=0} = \hat{a}_{k,m=0}^\dagger \hat{a}_{k,m=0}$ are the occupation number operators for photons and $m = 0$ atoms in their electronic ground state and $\Delta$ is the energy difference between $m = -1$ and $m = 0$ atoms. The coherent laser state $|\text{laser}\rangle$ is not an exact eigenstate of $\hat{H}_{0ph}$, but its energy dispersion is negligible since the photon numbers are large.

The exact transition rate from a specified initial state to a specified final state is $(2\pi/\hbar)\langle f|T|i\rangle^2 \delta(E_f - E_i)$ where $E_f - E_i = E_{B_f} - E_{B_i} - \hbar \omega$ with $\hbar \omega = \hbar c(k_1 - k_2) - (\hbar^2 k^2 / 2m) - \Delta$, the energy transferred to the BEC; the momentum transferred is $\hbar \mathbf{q} = \hbar (k_1 - k_2 - \mathbf{k})$. Here $T$ is the exact transition operator $T = \hat{V} \hat{\Omega}^+ = \hat{\Omega} \hat{\Omega}^+$ where $\hat{\Omega}^\pm$ are the Möller wave operators $\hat{U}(0, \mp \infty)$ and $\hat{U}$ is the adiabatically switched evolution operator \[2\]. The angle-energy doubly differential cross section is then \[1\]

$$
\frac{d^2 \sigma}{d \theta \, d \omega} = \rho(\theta, \phi) \int_{-\infty}^{\infty} dt (\hat{U}^{-1} \hat{T}^\dagger(t) \hat{\mathcal{N}}_{k,m=0} \hat{T}(0) \hat{U})' \tag{1}
$$

where $\langle \cdot \cdot \rangle_B$ denotes an average over a statistical ensemble of BEC initial states $|B_i\rangle$ (reducing to an $N$-boson ground state average for temperature $T \to 0$) and the prime indicates that this expression is to be evaluated for an outgoing $m = 0$ atom with $k$ vector in the direction $(\theta, \phi)$ and with magnitude $k = \sqrt{(2m/\hbar^2) [\hbar c(k_1 - k_2) - \Delta - \hbar \omega]}$ consistent with a specified energy transfer $\hbar \omega$ to the BEC. Here $\rho(\theta, \phi)$ is the density of final states for an observation distance $D$ from the 1D gas which is much larger than the length $L$ of the trapped gas, $\phi$ is the angle of atomic ejection in the transverse plane, and $\theta$ the angle of ejection measured out of the transverse plane (see Figure 1). $\hat{T}^\dagger(t)$ is the Heisenberg operator

$$
\hat{T}^\dagger(t) = e^{it(\hat{H}_B + \hat{H}_{0ph} + \hat{H}_{0a})/\hbar} \hat{T}^\dagger e^{-it(\hat{H}_B + \hat{H}_{0ph} + \hat{H}_{0a})/\hbar} \tag{2}
$$

and the BEC final states have been eliminated by an exact closure summation $\sum_{B_f} |B_f\rangle |B_f\rangle = 1$ after introducing the integral representation of the energy delta function \[11\].

The terms in $\hat{T}(0) = \hat{T}$ contributing to the Raman process have the structure

$$
\sum_{k_1' k_2'} \hat{b}_{k_1' k_2'} \hat{a}_{k_2, m=0}^\dagger |k_2 \lambda_2, k_2' T| k_1 \lambda_1, k_1' \rangle \hat{a}_{k_1', m=-1}^\dagger \hat{b}_{k_1, \lambda_1} \tag{3}
$$

To obtain the relevant terms in $\hat{T}^\dagger(t)$ we take the hermitian conjugate of (3) and propagate each of its annihilation and creation operators to time $t$ in accordance with (2). Heisenberg propagation of $\hat{b}_{k_1}^\dagger$ and $\hat{a}_{k', m=0}^\dagger$ gives only trivial phases since the target BEC contains only atoms with $m = -1$, whereas the propagation of $\hat{a}_{k', m=-1}^\dagger$ is nontrivial and leads to inclusion of effects of energy and momentum transfer to the target BEC. Noting that the $T$-matrix elements $\langle k_2 \lambda_2, k_2' T| k_1 \lambda_1, k_1 \rangle$ contain a momentum conservation factor $\delta_{k_1 + k_1', k_2 + k_2'}$ and performing Wick’s theorem algebra after evaluating the coherent laser unitary transformation $\hat{U}^{-1} \cdots \hat{U}$ in Eq. (1), one finds

\[2\]
\[
\frac{d^2\sigma}{d\Omega d\omega} = n_1(n_2 + 1)\rho(\theta, \phi)
\times \left| \langle k_2, \lambda_2, k | T | k_1, \lambda_1, k - k_1 + k_2 \rangle \right|^2
\times \int_{-\infty}^{\infty} \langle \hat{a}^\dagger_{k - k_1 + k_2}(t) \hat{a}_{k - k_1 + k_2}(0) \rangle \beta e^{i\omega t} dt \tag{4}
\]

where the annihilation and creation operators refer to atoms in the BEC target, their \( m = -1 \) subscript having been dropped for simplicity in notation. Physically, Eq. (3) reflects that fact that outgoing \( m = 0 \) atoms with momentum \( \hbar k \) originate from transfer of momentum \( \hbar (k_1 - k_2) \) from the Raman photons to the target bosons of momentum \( \hbar (k - k_1 + k_2) \) and the differential cross section at the corresponding angle is related to the number of such target bosons.

**1D trapped gases:** The expression (4) is exact. We now introduce approximations appropriate to tightly confined 1D gases where only the ground transverse mode is occupied (3). When an atom is transferred by the Raman transition from the \( m = -1 \) trapped state to the \( m = 0 \) untrapped state it is ejected and undergoes radial expansion in the transverse plane \( r_T = (y, z) \) in addition to the momentum kick \( \hbar (k_1 - k_2) \) in the forward direction \( z \) from the Raman process. In the limit that the transverse mode \( u_g(r_T) \) of the trapped atoms has a width \( w_T \) much less than both the length \( L \) of the sample and the Raman laser wavelength, the ejected atom wave function will predominantly propagate out radially as a cylindrical wave concentrated along the direction \( \theta = 0 \). The density of final states \( \rho(\theta, \phi) \) may then be replaced by a constant (we assume the atoms can be detected before gravity significantly changes the final density of states).

In addition, writing the field operator for the trapped target atoms as \( \psi(r, t) = u_g(r_T)\hat{v}(x, t) \) to reflect their single-transverse mode structure, and setting \( k = k_T + x \bar{k}_T \) with \( k_x = k \sin(\theta) \) the longitudinal component of the wavevector, we find, for example

\[
\hat{a}_{k - k_1 + k_2}(t) = \int d^3 r \hat{\psi}(r, t) e^{-i(k - k_1 + k_2)\cdot r},
\]

\[
\approx \hat{u}_g(K_T) c(k_x, t). \tag{5}
\]

Here \( \hat{u}_g(K_T) \) is the Fourier transform over the transverse plane of the transverse mode evaluated at \( K_T = (k_T - k_1 + k_2) \), that may be approximated by its value \( \hat{u}_g(0) \) at zero momentum under tight confinement conditions \( 2\pi/w_T >> |k_T - k_1 + k_2| \), and \( \hat{c}(k_x, t) = \int dx \hat{v}(x, t) \exp(-ik_{x}x) \) is the Fourier transform of the longitudinal field operator. Putting this together in Eq. (4) and treating the T-matrix elements as constants (see below) yields an expression proportional to the Fourier transform of the longitudinal one-particle momentum-time correlation function:

\[
\frac{d^2\sigma}{d\Omega d\omega} \approx \alpha \int_{-\infty}^{\infty} \langle \hat{c}^\dagger(k_x, t) \hat{c}(k_x, 0) \rangle_B \beta e^{i\omega t} dt \tag{6}
\]

where \( \alpha \) is a constant. Thus, measurement of the doubly differential cross section for the ejected atoms gives access to a one-particle momentum-time correlation function of the trapped atoms.

Further simplification is possible if measuring the energy transferred to the BEC is not feasible, and only the angular distribution is measured. We consider that the 1D gas is confined longitudinally in a harmonic trap of frequency \( \omega_T \), in which case the maximum energy transfer to the BEC that can occur is \( \hbar \omega_{\max} = N \hbar \omega_T \). If we arrange that the Raman transition is detuned such that \( \hbar \omega_{\max} \ll \hbar \delta = e|k_1 - k_2| - \Delta \), then for all relevant energy transfers \( k \approx k_0 = \sqrt{2m\delta/\hbar} \), and the implicit dependence of \( \langle \cdot \cdot \cdot \rangle_B \) on \( \omega \) may be neglected. Then the integral over \( \omega \) yields a delta function of time, and one obtains an expression for the singly differential angular cross section in terms of the static longitudinal momentum distribution of the target:

\[
\frac{d\sigma}{d\Omega} \approx \beta \langle \hat{c}^\dagger(k_0 \sin(\theta), 0) \hat{c}(k_0 \sin(\theta), 0) \rangle_B, \tag{7}
\]

where \( \beta \) is a constant. Measurement of the differential cross section as a function of angle \( \theta \) out of the transverse plane will then yield the structure of the longitudinal momentum distribution of the target atoms. For a longitudinal trap of frequency \( \omega_T \) the characteristic longitudinal momentum is \( k_{\text{osc}} = 2\pi/x_{\text{osc}} \), with \( x_{\text{osc}} = \sqrt{\hbar/m\omega_T} \) the ground state width. If \( k_0 >> k_{\text{osc}} \) then we may approximate \( k_0 \sin(\theta) \approx k_0 \theta \) for all angles of interest, in which case the differential angular cross section will directly mirror the momentum distribution.

**Evaluation of T-matrix:** Although the expressions (6) and (7) do not require explicit evaluation of the T-matrix, it is helpful to examine its leading term to verify that it can be absorbed into constant prefactors. The Raman process is of second order in the interaction between the atoms and the laser field, so we approximate \( T \) by the second term in its Born series: \( T \approx H' G_0 H' \). Here \( H' \) represents the interaction of the atomic electrons and nuclei with the quantized electromagnetic field and \( G_0 = (E + ic - H_0)^{-1} \) with \( E = E_i = E_f \) (remembering the energy delta function in the cross section) and \( c \to 0^+ \). \( H_0 \) is the Hamiltonian of free atoms and quantized electromagnetic field. We use the electric field gauge with quantized electric field operator

\[
\hat{E}(r) = i \sum_{k\lambda} \sqrt{\frac{\hbar c k}{V}} \left( e_{k\lambda} \hat{b}_{k\lambda} e^{i k r} - \text{h.c.} \right), \tag{8}
\]

where \( e_{k\lambda} \) are the unit polarization vectors and \( V \) is the quantization volume. It is assumed that the Raman lasers are tuned close to resonance for a single S-P transition from the atomic ground state to an electronically excited state \( \nu \) with electronic excitation energy \( \epsilon_{\nu 0} \), i.e., \( \hbar c k_1 \approx \hbar c k_2 \approx \epsilon_{\nu 0} \). Then the dominant contribution to the T-matrix element in Eq. (4) is
\[(k_2 \lambda_2, k | T | k_1 \lambda_1, k - k_1 + k_2) \approx -(hc/\gamma) \sqrt{k_1 k_2} \times (e_{k_2 \lambda_2} \cdot d_{0\nu})(e_{k_1 \lambda_1} \cdot d_{0\theta})/(\epsilon_{\nu \theta} - \hbar c \epsilon_k), \quad (9)\]

where \(d_{0\theta}\) is the corresponding dipole matrix element. The contributions \(k^2 k^2/2m\) (kinetic energy of ejected atom) and \(\Delta\) (Zeeman splitting) to the energy denominator have been dropped since they are much less than the electronic transition energy. Assuming that the Raman laser parameters are held constant, the expression (10) is indeed a constant.

**Discussion:** Figure 2 shows numerical results for the angular cross section versus angle for both a 1D system of fermions [23] (solid line), where we chose \(\omega_r = 2\pi \times 1\) Hz, \(\delta = 2\pi \times 10^3\) Hz, so that \(k_0 = 7.3k_{osc}\).

![Angular cross section versus angle](image)

**FIG. 2.** Angular cross section versus angle \(\sin(\theta) \approx \theta\) for \(N = 10\). The dashed line is for the 1D gas of impenetrable bosons and the solid line is for the corresponding system of non-interacting fermions [23].

These results highlight the difference between the momentum distributions for Fermi and Bose gases: The central peak characteristic of a Tonks gas gets sharper as \(N\) increases [24], whereas the fermionic momentum distribution, which shows the rounded Fermi sea due to the trapping potential with Friedel oscillations superposed [23], broadens with increasing \(N\). We remark again that this difference in angular distribution arises even though both the fermionic and bosonic atoms have the same dynamic structure factor. This highlights the need for a measurement technique that accesses the momentum distribution directly. One could measure the momentum distribution by simply releasing the atoms from the trap and letting them expand, but this leaves open the possibility of many-body interactions obscuring the results as the gas expands. The momentum distribution could also in principle be reconstructed from the single-particle reduced density matrix \(\rho_{ij}(x, x')\) as measured in the experiment of Bloch et al. [11], and it will be of interest to see how our approaches compare.

We thank Profs. Poul Jessen and Pierre Meystre for helpful discussions. MDG also thanks Profs. S. Stringari and L.P. Pitaevskii for pointing out that the Tonks and Fermi gases have the same dynamic structure factor, and for support during his stay at the Dipartimento di Fisica, Universita di Trento. This work was supported at the University of Arizona by Office of Naval Research grant N00014-99-1-0806.

[1] P.C. Hohenberg and P.M. Platzman, Phys. Rev. 152, 198 (1966).
[2] L.P. Pitaevskii and S. Stringari, Phys. Rev. Lett. 83, 4237 (1999).
[3] F. Zambelli et al., Phys. Rev. A 61, 063608 (2000).
[4] M. Girardeau, J. Math. Phys. 1, 516 (1960); Phys. Rev. 139, B500 (1965).
[5] M. Olshanii, Phys. Rev. Lett. 81, 938 (1998).
[6] D. S. Petrov et al., Phys. Rev. Lett. 85, 3745 (2000).
[7] E. A. Hinds et al., Phys. Rev. Lett. 80, 645 (1998); M. Key et al., Phys. Rev. Lett. 84, 1371 (2000).
[8] J. H. Thywissen et al., Eur. Phys. J. D 4, 57 (1998); Phys. Rev. Lett. 83, 3762 (1999).
[9] K. Bongs et al., cond-mat/0007381 (2000).
[10] D.A. Micha, Chem. Phys. Lett. 81, 517 (1981); D.A. Micha, Intern. J. Quantum Chem. Quantum Chem. Symp. 15, 643 (1981).
[11] M.D. Girardeau and C.I. Ivanov, Chem. Phys. Lett. 131, 389 (1986).
[12] L. van Hove, Phys. Rev. 95, 249 (1954).
[13] G.M. Moy, J.J. Hope, and C.M. Savage, Phys. Rev. A 55, 3631 (1997).
[14] E.W. Hagley et al., Science 283, 1706 (1999).
[15] Mark Edwards et al., J. Phys: B: At. Mol. Opt. Phys. 32, 2935 (1999).
[16] I. Bloch et al., Nature 403, 166 (2000).
[17] J. Stenger et al., Phys. Rev. Lett. 82, 4569 (1999).
[18] D. M. Stamper-Kurn et al., Phys. Rev. Lett. 83, 2876 (1999).
[19] A.B. Kuklov and B.V. Svistunov, Phys. Rev. A 60, R769 (1999).
[20] E.V. Goldstein and Pierre Meystre, Phys. Rev. Lett. 80, 5036 (1998).
[21] Charles J. Joachain, Quantum Collision Theory, 3rd edn. (North-Holland Publishing Co., Amsterdam, 1983), Chaps. 14 and 15.
[22] M. D. Girardeau et al., to be published in Phys. Rev. A (2001). Restriction to \(N = 10\) is limited by our computational resources for the Tonks gas, but in general Tonks gases are restricted to relatively small numbers of atoms, see Ref. [15].
[23] F. Gleisberg et al., Phys. Rev. A 62, 063602-1 (2000).