Sum rule for the optical spectrum of a trapped gas

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(Received 1 October 2001; published 26 February 2002)

We develop an exact sum rule that relates the spectral shift of a trapped gas undergoing cold collisions to measurable quantities of the system. The method demonstrates the dependence of the cold collision frequency shift on the quantum degeneracy of the gas and facilitates extracting scattering lengths from the data. To illustrate the method, we consider optical shift for the Thomas-Fermi model of Bose-Einstein condensate in a harmonic optical trap.

PACS number(s): 03.75.Fi, 32.80.Pj

The broadening and shifting of spectral lines of a gas by collisions was among the earliest discoveries in the development of high-precision spectroscopy [1]. The pressure shift, which originates in interatomic perturbations [2], is particularly simple to interpret at low temperatures where the thermal de Broglie wavelength $\Lambda_T \equiv h/mv_T = h/(2mk_BT)^{1/2}$ is much larger than the scattering length a [3,4] and the interactions arise only through s-wave scattering. In this *cold collision* regime, the typical frequency shift $(4\pi\hbar/m)an$ with n the gas density is much larger than the collisional level broadening $4\pi a^2 v_T n$ [5].

The theory of the cold collision shift [6–8] has been developed to interpret hyperfine transitions in cryogenic hydrogen masers and laser cooled atomic fountains [9–13]. In this paper, we study the shift for optical excitation in a system that can be fully or partially quantum degenerate, and apply the results to a Thomas-Fermi model of Bose-Einstein condensate (BEC) in an optical trap. We also consider the case of fermions and demonstrate that the density shift disappears in the cold collision regime, well above Fermi degeneracy temperature.

For the case of a homogeneous sample of density n, and a coherent, weak excitation that couples two inner states of the atoms, we find

$$\hbar\Delta\omega_{\text{coll}} = g_2(\lambda_{12} - \lambda_{11})n, \quad \lambda_{\alpha\beta} = (4\pi\hbar^2/m)a_{\alpha\beta}. \quad (1)$$

Here g_2 is the equal point value of the second-order correlation function [14,15], $g_2 \equiv g^{(2)}(\mathbf{r}=0)$, the state 1 (2) is the ground (excited) state, and $a_{\alpha\beta}$ is the s-wave scattering length for $\alpha-\beta$ collisions.

Equation (1) shows that quantum correlations in the system are manifest in the collision shift. For a uniform Bose gas in thermal equilibrium $g_2 = 2 - (n_{\text{BEC}}/n)^2$ [16], where n_{BEC} is the density of condensed atoms. Above the condensation temperature, when $n_{\text{BEC}}=0$, g_2 equals two, in which case Eq. (1) is in agreement with previous work [6–8]. At zero temperature, for a pure condensate with $n_{\text{BEC}}=n$, the

collision shift is half of the shift for a noncondensed gas. Equation (1) generalizes the result of Refs. [6–8] to $T < T_{\text{BEC}}$ and relates the spectral shift to the condensate fraction.

It is quite remarkable that the factor g_2 in Eq. (1) multiplies *both* λ_{12} and λ_{11}. This results from correlations between an excited atom and other atoms. During the excitation, the internal states of the atoms are rotated: $\cos\theta(t)|1S\rangle + e^{-i\phi(t)}\sin\theta(t)|2S\rangle$. The angles $\theta(t)$, $\phi(t)$ depend on laser power and on the atom's trajectory in the laser field, specific for each atom. However, for small excitation power, the angle $\theta(t)$ is small, and thus the internal states of all atoms remain nearly identical while the laser is on, even if the excitation field is spatially nonuniform. Therefore, during the excitation the atoms interact as identical particles. This causes the short-range statistical correlations in the initial state to be replicated in the excited state of the gas, which results in the statistical factor g_2 in the first term of Eq. (1).

The transfer of spatial correlations to the excited state is not limited to weak excitation. For the case of strong excitation, spatial correlations in the ground state will also be transferred to the excited state, but only provided the excitation scheme is coherent [17]. The difference between coherent and incoherent cases can be illustrated by comparing two different states of a normal gas. One state is a coherent superposition of the ground and excited states obtained, e.g., by a $\pi/2$ pulse. The other is an incoherent mixture state resulting from saturating the Rabi transition. These states will both have equal populations in the two internal states, but quite different correlations. In the former case of a pure internal state the spatial correlation will be the same as for the ground state of indistinguishable particles. In the latter case of a mixed state the correlations will be reduced. Consequently, the interparticle interaction energy of the first state will exceed that of the second state by the factor g_2.

To emphasize the nontrivial character of the result (1), let us point out that $\hbar\Delta\omega_{\text{coll}}$ differs from the thermodynamic work needed to transfer one atom from the state 1 to the state 2. The latter work, calculated by removing one atom from the sample, and then introducing an atom in state 2 from far away, ignoring entropy, is given by $(\lambda_{12} - g_2\lambda_{11})n$. Here $\lambda_{12}n$ is the energy of interaction of the excited atom with the atoms in the state 1, and $g_2\lambda_{11}n$ is the chemical potential of

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a Bose gas. The key difference between this process and optical excitation, resulting in the different dependence on g_2, is the incoherence of the state of the added atom with the initial state of the sample.

To calculate the full optical spectrum shape of a trapped gas in the cold collision regime, other factors would have to be considered in addition to the effects of statistical correlations. Optical coherence can be lost via dephasing elastic collisions, giving rise to collisional broadening. One would have also to take into account atomic motion in the trap and the effects of the inhomogeneous density distribution in the sample, especially in the Bose-Einstein condensate. In addition, the interaction may give rise to a doublet structure of the spectrum [18]. Altogether, these effects can lead to a complicated broadened spectrum with asymmetric lines [19–21]. However, we demonstrate below that the spectrum's center of mass obeys a simple and exact sum rule and is insensitive to these additional effects.

We lay out the theory of the shift by deriving a sum rule [Eq. (12)] that relates the center of mass of the observed spectrum to measurable experimental parameters. The sum rule bridges between the uniform density result (1) and experimentally measured spectra. The sum rule accounts for all interactions between atoms occurring in the s-wave scattering channel, which includes the s-wave collisional broadening. It follows from the sum rule that collisional broadening as well as the time of flight broadening resulting from atomic motion in the trap do not contribute to the spectral shift. At the same time, the effects on the shift of inhomogeneity in the gas density and nonuniformity in the excitation field are expressed in the sum rule (12) in an exact and straightforward way. The sum rule is applicable both to Doppler-free and Doppler-sensitive spectra.

We start by considering a homogeneous Bose gas and derive Eq. (1). Then for the realistic situation of a trapped gas sample we derive the sum rule (12), a generalization of Eq. (1). Finally, to illustrate usage of the sum rule, we consider the Thomas-Fermi model of BEC in a harmonic optical trap and analyze optical shift in this case.

I. THE SYSTEM

To provide the context for the theory, we briefly describe a recent experiment, in which optical spectroscopy was used to identify BEC in spin-polarized hydrogen [19,20]. In this experiment, the temperature of the hydrogen is $100–500$ μK, well below the cold collision threshold $T \simeq 1$ K [3,4]. The atoms are spin polarized and interact in the triplet channel. Calculated values of the $1S$-$1S$ and $1S$-$2S$ triplet scattering lengths are $a_{11} = 0.0648$ nm [22] and $a_{12} = -2.3$ nm [23]. We neglect $2S$-$2S$ scattering because the excitation rate is assumed low (in the experiment typically 10^{-4} of the sample is excited and no atom has more than a few percent excitation probability) so the background gas is essentially pure $1S$ [24]. Since $|a_{12}| \gg a_{11}$, collisions between $1S$ and $2S$ atoms dominate the shift, which is to the red.

Each atom will be in some superposition of the ground-

state $1S$ and the excited-state $2S$. In the second quantization formalism, the atoms are described by the canonical Bose operators $\psi_1(r)$ and $\psi_2(r)$. The Hamiltonian is $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{int}}$, where $\mathcal{H}_0$ describes atoms freely moving in the trap, and $\mathcal{H}_{\text{int}}$ is the interaction term

$$\mathcal{H}_0 = \int \sum_{\alpha=1,2} \psi_\alpha^\dagger(r) \left(-\frac{\hbar^2 \nabla^2}{2m} + U(r) \right) \psi_\alpha(r) d^3 r, \quad (2)$$

$$\mathcal{H}_{\text{int}} = \frac{1}{2} \int \sum_{\alpha,\beta=1,2} \lambda_{\alpha\beta} \psi_\alpha^\dagger(r) \psi_\beta^\dagger(r) \psi_\beta(r) \psi_\alpha(r) d^3 r. \quad (3)$$

Here $U(r)$ is the trap potential (essentially the same for the $1S$ and the $2S$ states).

Inelastic collisions, such as collisions in which the hyperfine level of one or both of the colliding partners changes, may contribute additional shifts which are not accounted for in this formalism. However, these effects, as well as the three-body collision effects, are small in the experiment and can be neglected [25,26].

The two-photon $1S$-$2S$ spectrum consists of Doppler-free and Doppler-sensitive excitations. In the Doppler-free situation, the transition results from absorbing two counter-propagating photons with equal frequencies and zero net momentum. In the absence of interactions, the resonance condition is $2\omega_{\text{laser}} = \omega_0$, where ω_0 corresponds to the resonance of a single free atom. In the Doppler-sensitive situation, the transition is caused by two photons propagating in the same direction. For a free atom, the resonance frequency is shifted by the recoil energy: $2\hbar\omega_{\text{laser}} = \hbar\omega_0 + (2k)^2/2m$, where $k = \hbar\omega/c$ is photon momentum and m is the atom mass.

Radiative excitation in a many-particle system is described by adding to the Hamiltonians (2),(3) the term

$$\mathcal{H}_{\text{rad}} = \int d^3 r [A(r) e^{-i\omega t} \psi_2^\dagger(r) \psi_1(r) + \text{H.c.}], \quad (4)$$

where $\omega = 2\omega_{\text{laser}} - \omega_0$. The two-photon excitation field $A(r)$ is equal, up to a constant factor, to the square of the electric field. Spatial variation of $A(r)$ in the Doppler-free case occurs on a scale set by the focused laser beam diameter, and in the Doppler-sensitive case is given by $\tilde{A}(r)\cos[2kr + \phi(r)]$, where $\tilde{A}(r)$ and $\phi(r)$ are slowly varying functions.

II. EXAMPLE

Before discussing the general case, here we derive the mean frequency shift for the Doppler-free transition caused by a uniform excitation field $A(r) = A_0$, ignoring the $1S$-$1S$ interactions ($\lambda_{11} = 0$). To that end, consider a gas of N atoms confined in a box of volume V. Since we ignore the $1S$-$1S$ interaction, the many-body state ground state of the system Φ_0 is simply a symmetrized product of single-particle states. It can be characterized by occupation numbers n_j of the single-particle plane-wave states $V^{-1/2} e^{ik_j r}$, $\Sigma_j n_j = N$. Initially, the internal state of all atoms is $1S$.

The excited state, to lowest order in the excitation, is

given by $\Phi_1 = \mathcal{H}_{rad}\Phi_0$. We consider the norm $\|\Phi_1\|^2$ and the expectation value of the interaction $\langle\Phi_1|\mathcal{H}_{int}|\Phi_1\rangle$. The ratio of these quantities gives the mean frequency shift. Because Φ_0 is the product of plane-wave states in a box, the frequency shift can be evaluated exactly.

The norm $\langle\Phi_1|\Phi_1\rangle$ of the excited state is given by

$$|A_0|^2 \int \langle\Phi_0|\psi_1^\dagger(r)\psi_2(r)\psi_2^\dagger(r')\psi_1(r')|\Phi_0\rangle d^3r d^3r'. \quad (5)$$

To evaluate the norm one first puts the operators $\psi_2(r)$ and $\psi_2^\dagger(r')$ in Eq. (5) in normal order by using the commutation relation $[\psi_2(r),\psi_2^\dagger(r')] = \delta(r-r')$. Noting that $\psi_2(r)|\Phi_0\rangle = 0$, the norm is given by

$$\|\Phi_1\|^2 = |A_0|^2 \int \langle\Phi_0|\psi_1^\dagger(r)\psi_1(r)|\Phi_0\rangle d^3r = |A_0|^2 N. \quad (6)$$

To obtain the frequency shift $\Delta\omega_{coll}$, we consider the expectation value $\langle\Phi_1|\mathcal{H}_{int}|\Phi_1\rangle$, keeping in $\mathcal{H}_{int}$ only the $1S$-$2S$ interaction λ_{12}. After arranging in normal order, as in the calculation of the norm $\|\Phi_1\|^2$, one has

$$\langle\Phi_1|\mathcal{H}_{int}|\Phi_1\rangle = \lambda_{12}|A_0|^2$$

$$\times \int \langle\Phi_0|\psi_1^\dagger(r)\psi_1^\dagger(r)\psi_1(r)\psi_1(r)|\Phi_0\rangle d^3r. \quad (7)$$

Evaluating the expectation value for Φ_0 chosen as a symmetrized product of plane-wave states, one expresses Eq. (7) in terms of the occupation numbers of the ground and excited states as

$$\langle\Phi_1|\mathcal{H}_{int}|\Phi_1\rangle = \frac{\lambda_{12}|A_0|^2}{V}\left(2\sum_{i\neq j} n_i n_j + \sum_i n_i(n_i-1)\right). \quad (8)$$

The mean frequency shift is then given by the ratio of Eq. (8) and the norm (6)

$$\hbar\Delta\omega_{coll} = \frac{\lambda_{12}}{VN}\left(2N^2 - \sum_i n_i(n_i+1)\right). \quad (9)$$

The formal reason for the factor 2 to appear in Eqs. (8) and (9) and, eventually for g_2 to appear in Eq. (1), is the following. In taking the average in Eq. (7) by Wick's theorem [27], there are two essentially different ways to pair the operators, analogous to the Hartree and Fock contributions to the energy. For short-range interaction between bosons, the Hartree and Fock contributions are equal and as a result the frequency shift is twice as large as the "mean density" result.

In the thermodynamic limit, $V,N\rightarrow\infty$, $n=N/V$ constant, the second term in Eq. (9) contributes only when there are states filled by a macroscopic number of particles. For example, in thermodynamic equilibrium at $T<T_{BEC}$, the shift (9) is $\lambda_{12}(2n-n_c^2/n)$, whereas in a nondegenerate gas, at $T>T_{BEC}$, the shift is $2\lambda_{12}n$.

III. THE SUM RULE

We turn now to deriving a sum rule that generalizes the result (1) to nonhomogeneous samples and spatially varying excitation field (and $\lambda_{11}\neq 0$). We start with the Golden Rule formula for the absorption spectrum,

$$\mathcal{I}(\omega) = \frac{2\pi}{\hbar}\sum_{E_i,E_f}\delta(\hbar\omega + E_i - E_f)|\langle f|\mathcal{H}_{rad}|i\rangle|^2 p_i, \quad (10)$$

where $|i\rangle$ and $|f\rangle$ are eigenstates of the Hamiltonian $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{int}$ with the energies E_i and E_f and p_i is the statistical occupation of the states $|i\rangle$.

The sum rule for the spectrum $\mathcal{I}(\omega)$ is found by evaluating the first moment

$$\int \omega\mathcal{I}(\omega)\frac{d\omega}{2\pi} = \frac{1}{\hbar^3}\sum_{E_i,E_f}(E_f-E_i)|\langle f|\mathcal{H}_{rad}|i\rangle|^2 p_i$$

$$= \frac{1}{\hbar^3}\sum_{E_i,E_f}\langle i|\mathcal{H}_{rad}|f\rangle\langle f|[\mathcal{H},\mathcal{H}_{rad}]|i\rangle p_i$$

$$= \frac{1}{\hbar^3}\sum_{E_i}\langle i|\mathcal{H}_{rad}[\mathcal{H},\mathcal{H}_{rad}]|i\rangle p_i. \quad (11)$$

In obtaining this result we first integrated the delta function, then wrote the result as a matrix element of the commutator $[\mathcal{H},\mathcal{H}_{rad}]$ and, finally, used the completeness relation.

Now we consider contributions of the different terms of the Hamiltonian to the sum rule. The potential-energy operator $\int(\psi_1^\dagger\psi_1 + \psi_2^\dagger\psi_2)\,U(r)d^3r$ commutes with $\mathcal{H}_{rad}$, and thus does not contribute. There are two contributions, first from the interaction Hamiltonian, second from the kinetic-energy operator, denoted by F_{int} and F_{kin}, respectively. The sum rule becomes

$$\int \omega\mathcal{I}(\omega)\frac{d\omega}{2\pi} = F_{int} + F_{kin}. \quad (12)$$

For Doppler-free excitation the term F_{kin} in Eq. (12) is small compared to F_{int}, whereas for Doppler-sensitive excitation it contributes the larger shift.

First, consider the interaction $\mathcal{H}_{int}$, and calculate F_{int}. After evaluating the commutator in Eq. (11), one follows the same procedure as in the above calculation of the norm $\|\Phi_1\|$. The result is

$$F_{int} = \left\langle \int (\lambda_{12}-\lambda_{11})|A(r)|^2\psi_1^\dagger(r)\psi_1^\dagger(r)\psi_1(r)\psi_1(r)\frac{d^3r}{\hbar^3}\right\rangle, \quad (13)$$

where $\langle\cdots\rangle$ means $\Sigma_{E_i}\langle i|\cdots|i\rangle p_i$. The expectation value $\langle:[\psi_1^\dagger(r)\psi_1(r)]^2:\rangle = G_2(r)$, the two-particle density. (Here $:\cdots:$ indicates canonical normal ordering.) Finally, using the statistical factor $g_2 = G_2/n^2$, the result is

$$F_{int} = \int (\lambda_{12}-\lambda_{11})|A(r)|^2 g_2 n^2(r)\frac{d^3r}{\hbar^3}. \quad (14)$$

Next, we calculate F_{kin}, the contribution to the sum rule coming from the kinetic-energy operator $-(\hbar^2/2m)\int(\psi_1^\dagger\nabla^2\psi_1+\psi_2^\dagger\nabla^2\psi_2)d^3r$. After evaluating the commutator with $\mathcal{H}_{\text{rad}}$, one has

$$F_{\text{kin}}=-\frac{\hbar^2}{2m}\left\langle\int\psi_1^\dagger(r)A*(r)[\nabla^2,A(r)]\psi_1(r)\frac{d^3r}{\hbar^3}\right\rangle. \tag{15}$$

Integrating by parts, and writing the excitation field as $A(r)=|A(r)|e^{i\theta}$, yields

$$F_{\text{kin}}=\int\left(\frac{\hbar^2}{2m}|\nabla A|^2 n-\hbar|A|^2\mathbf{j}\cdot\nabla\theta\right)\frac{d^3r}{\hbar^3}, \tag{16}$$

where n and $\mathbf{j}$ are the particle number and flux densities

$$n(r)=\langle\psi_1^\dagger(r)\psi_1(r)\rangle, \tag{17}$$

$$\mathbf{j}(r)=-\frac{i\hbar}{2m}\langle\psi_1^\dagger(r)\nabla\psi_1(r)\rangle+\text{H.c.}$$

The first term in Eq. (16) generalizes the ordinary momentum recoil energy shift to the trapped gas problem [28]. The second term represents the Doppler shift due to possible macroscopic gas flow in the sample. To clarify this, consider $A(r)=A_0 e^{ipr/\hbar}$, which would describe Doppler-sensitive excitation. Then $F_{\text{kin}}=|A_0|^2\int(p^2/2m-\mathbf{p}\cdot\mathbf{v})n\ d^3r/\hbar^3$, where $\mathbf{v}=\mathbf{j}/n$ is the local velocity. The sensitivity of the frequency shift to motion within the sample, manifest in the second term in Eq. (16), makes it possible, in principle, to detect vortices in the condensed state.

To employ the sum rule, one needs to relate the integrated spectral power to $A(r)$ and $n(r)$. Repeating the steps that led to Eq. (12), one obtains

$$\mathcal{I}_{\text{tot}}=\int\mathcal{I}(\omega)\frac{d\omega}{2\pi}=\int|A(r)|^2 n(r)\frac{d^3r}{\hbar^3}. \tag{18}$$

Combining Eq. (18) with the sum rule (12), one obtains an exact expression for the spectrum's "center of mass" $\bar\omega=\int\omega\mathcal{I}(\omega)d\omega/\int\mathcal{I}(\omega)d\omega$.

For example, consider a uniform density sample, and ignore the spatial variation of the laser field $A(r)$. Equation (14) gives $F_{\text{int}}=(\lambda_{12}-\lambda_{11})g_2 n^2\int|A(r)|^2 d^3r/\hbar^3$. In the experiment [19,20] the kinetic contribution F_{kin} is small and thus we can neglect it. After pulling constant density $n(r)\equiv n$ out of integral in Eqs. (14) and (18), and dividing one equation by the other, one obtains the frequency shift (1).

There are two comments concerning the generality of the sum rule. First, note that in deriving the sum rule (12), we do not assume thermodynamic equilibrium. The result is exact and applies to nonequilibrium systems for which the factor g_2 may differ from its equilibrium value. Second, the above derivation of the sum rule assumes coherence of the excitation described by Eq. (4). One can see, however, that the results (14), (16), and (18) hold as well for an incoherent excitation field of the form $A(r)e^{i\omega t+i\phi(t)}$ with a fluctuating phase $\phi(t)$. Also, it is straightforward to generalize the results for the excitation field with different spatial dependence of different frequency components.

IV. FREQUENCY SHIFT IN THE THOMAS-FERMI MODEL

To demonstrate the use of the sum rule for a nonhomogeneous system, we apply it to a condensate in a parabolic trap with cylindrical symmetry

$$V(r)=\frac{1}{2}m\omega_\perp^2(x^2+y^2)+\frac{1}{2}m\omega_z^2 z^2. \tag{19}$$

We consider the situation when the trap is so soft in the z direction, $\omega_z\ll\omega_\perp$, that the gas sample is quasi-one-dimensional. This corresponds to the hydrogen system studied in Refs. [19,20]. The BEC density distribution in such a trap can be calculated in the Thomas-Fermi approximation, $n(\mathbf{r})=[\mu-V(\mathbf{r})]/\lambda_{11}$. Since the trap is elongated, the gas sample near the trap center is cylindrical. The density as a function of the distance $r_\perp$ from the trap axis is

$$n(\mathbf{r})=\begin{cases}n_0(1-r_\perp^2/d^2) & r_\perp<d\\ 0 & r_\perp>d,\end{cases} \tag{20}$$

where $n_0=\mu/\lambda_{11}$ is the BEC density at the trap center and $d=\sqrt{2\mu/m\omega_\perp^2}$ is the BEC sample radius.

We take the excitation field $A(\mathbf{r})$ to be a Gaussian beam aligned with the trap axes

$$A(\mathbf{r})=A_0\exp\left(-\frac{r_\perp^2}{2a^2}-\frac{z^2}{2b^2}\right). \tag{21}$$

To keep the discussion simple we further assume that the size b of the beam in the z direction is much smaller than the gas sample length $L=\sqrt{2\mu/m\omega_z^2}$.

Excitation spectrum in this case is rather complicated, because of the combination of factors such as the nonhomogeneous gas density (20), nonuniform distribution of the excitation power (21), as well as, the last but not the least, interactions in the gas. However, the sum rule (12) enables one to write an exact expression for the spectrum center of mass. Below we calculate the interaction and kinetic contributions (14) and (16) to the frequency shift for an arbitrary ratio of the sample radius d and the beam radius a, and study the shift as a function of d/a.

First, consider the frequency shift due to interactions. It is given by the ratio of Eqs. (14) and (18) as

$$\hbar\Delta\omega_{\text{coll}}=(\lambda_{12}-\lambda_{11})\frac{\langle n^2(\mathbf{r})\rangle}{\langle n(\mathbf{r})\rangle}, \tag{22}$$

where $\langle\cdots\rangle$ stands for $\int\cdots|A(\mathbf{r})|^2 d^3 r$. Neglecting the dependence of $n(\mathbf{r})$ on z and changing the integration variable to $u=r_\perp^2/d^2$ we obtain
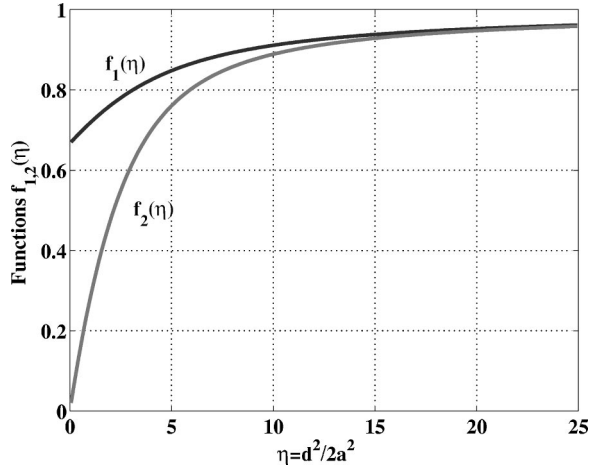
FIG. 1. The mean frequency shift is reduced due to spatial non-uniformity of the BEC sample density and laser beam power. The interaction (f_1) and recoil (f_2) reduction factors are shown as a function of $\eta = d^2/2a^2$, where d is the BEC Thomas-Fermi distribution radius [Eq. (20)] and a is the excitation beam width [Eq. (21)]. The functions $f_{1,2}(\eta)$ are defined by Eqs. (25) and (29).

$$\hbar\Delta\omega_{\mathrm{coll}} = (\lambda_{12} - \lambda_{11})n_0 \frac{\int_0^1 (1+\partial_\eta)^2 e^{-\eta u} du}{\int_0^1 (1+\partial_\eta) e^{-\eta u} du}, \qquad (23)$$

where $\eta = d^2/2a^2$. Here powers of $r_\perp^2$ are represented in Eq. (23) using partial derivatives with respect to η to facilitate calculation. Performing the integral over u we obtain

$$\hbar\Delta\omega_{\mathrm{coll}} = (\lambda_{12} - \lambda_{11})n_0 f_1(d^2/2a^2), \qquad (24)$$

$$f_1(\eta) = \frac{(1+\partial_\eta)^2 \eta^{-1}(1-e^{-\eta})}{(1+\partial_\eta)\eta^{-1}(1-e^{-\eta})}.$$

The function $f_1(\eta)$ is readily evaluated

$$f_1(\eta) = \frac{\partial_\eta^2 \eta^{-1}(e^\eta - 1)}{\partial_\eta \eta^{-1}(e^\eta - 1)} \equiv \frac{\eta^2 - 2\eta + 2 - 2e^{-\eta}}{\eta(\eta - 1 + e^{-\eta})}. \qquad (25)$$

The resulting function f_1 is shown in Fig. 1. There are two limiting cases corresponding to a well-focused and completely defocused beam. The first case when only the central part of the BEC distribution is illuminated ($a \ll d$) is described by $f_1(\eta \to \infty) = 1$. In the second case the entire cross section of the BEC sample is illuminated uniformly ($a \gg d$), which corresponds to $f_1(\eta \to 0) = 2/3$. The 1/3 reduction of the mean frequency shift (24) for a defocused beam can be understood as a result of averaging over local densities in the BEC sample ranging from 0 to the maximal density n_0.

The kinetic contribution (16) to the frequency shift is a sum of two parts: a recoil term due to nonzero momentum transfer at excitation by a narrow beam and a Doppler term describing the effect of current flux in the BEC sample. Here

we consider a static BEC sample for which the second contribution is zero. The recoil contribution is given by the first term in Eq. (16),

$$F_{\mathrm{kin}} = \frac{\hbar^2}{2m} \int |\nabla A(\mathbf{r})|^2 n(\mathbf{r}) d^3\mathbf{r} = \frac{\hbar^2}{2ma^4} \langle r_\perp^2 n \rangle, \qquad (26)$$

where $\langle \cdots \rangle$ means $\int \cdots |A(\mathbf{r})|^2 d^3\mathbf{r}$ as above. Taking the ratio of the expressions (26) and (18) one finds

$$\hbar\Delta\omega_{\mathrm{kin}} = \frac{\hbar^2 d^2}{2ma^4} \frac{\int_0^1 u(1-u)e^{-\eta u} du}{\int_0^1 (1-u)e^{-\eta u} du}, \qquad (27)$$

where the notation $\eta = d^2/2a^2$ is the same as above. The result can be written in the form

$$\hbar\Delta\omega_{\mathrm{kin}} = \frac{\hbar^2}{ma^2} f_2(d^2/2a^2), \qquad (28)$$

$$f_2(\eta) = \eta \frac{-\partial_\eta(1+\partial_\eta)\eta^{-1}(1-e^{-\eta})}{(1+\partial_\eta)\eta^{-1}(1-e^{-\eta})}.$$

The function f_2 can be evaluated as

$$f_2(\eta) = \frac{(1-\partial_\eta)\partial_\eta \eta^{-1}(e^\eta - 1)}{\eta^{-1}\partial_\eta \eta^{-1}(e^\eta - 1)} \equiv \frac{(\eta-2)e^\eta + \eta + 2}{(\eta-1)e^\eta + 1} \qquad (29)$$

(see Fig. 1). The two limiting cases of a focused and defocused beam can be understood as follows. Qualitatively, as the beam becomes more defocused the recoil momentum decreases. For a well-focused beam ($a \ll d$) the function $f_2(\eta \to \infty) = 1$, which corresponds to a recoil momentum of the order of $\Delta p \approx \hbar/a$. For a defocused beam of the width much larger than the BEC sample radius ($a \gg d$) the function $f_2(\eta \ll 1) \propto \eta$ describes recoil with small transferred momentum $\Delta p \approx \hbar d/a^2$. Accordingly, for a defocused beam the recoil frequency shift decreases from $\hbar^2/ma^2$ to $\hbar^2 d^2/ma^4$.

To summarize, the mean frequency shift is given by the sum of the interaction and kinetic terms

$$\hbar\Delta\omega_{\mathrm{total}} = (\lambda_{12} - \lambda_{11})n_0 f_1(\eta) + \frac{\hbar^2}{ma^2} f_2(\eta), \qquad (30)$$

where $\eta = d^2/2a^2$ and the functions $f_{1,2}(\eta)$ are defined by Eqs. (25) and (29). In the hydrogen system [19,20] the 1S-2S interaction λ_{12} is negative and $|\lambda_{12}| \gg \lambda_{11}$. At the high densities n_0 reported in Refs. [19,20] the first (negative) term in Eq. (30) is much larger in magnitude than the second (positive) term. The resulting shift is therefore negative in sign. At present, due to the lack of precise knowledge of the parameters of the hydrogen system, we are not able to compare the numerical value of the observed shift with the result (30).

V. CONCLUSION

In summary, we have shown that quantum statistical correlations of a cold gas sample are imprinted in the collisional shift of the center of mass of an optical absorption spectrum. In the cold collision regime the sum rule (12) can be applied to determine the statistical correlation factor g_2 from optical spectrum. The sum rule is valid for any gas in the cold collision regime. It takes into account possible inhomogeneities in the sample and the excitation field, and it is valid above and below T_{BEC}. Also, the sum rule is valid for a nonequilibrium system, with g_2 values possibly different from those in equilibrium. By considering an example of a Thomas-Fermi BEC distribution we have demonstrated how the sum rule could in principle be applied to extract the $1S$-$2S$ scattering length for hydrogen from experimental data.

It should be pointed out that our results, the frequency shift (1) and the sum rule (12), are only valid at small mixing angles of the $1S$ and $2S$ states. The cold collision shift at large angle mixing [17] is an important problem, particularly for atomic clocks [9–13]. The generalization of the result (12) for such systems is an interesting open problem.

ACKNOWLEDGMENTS

APPENDIX: THE ABSENCE OF THE INTERACTION SHIFT FOR FERMI PARTICLES

Here we briefly discuss how the sum rule will look for a trapped Fermi gas. Effective inter-particle interaction at short distances depends very strongly on particle statistics. Identical fermions, due to the Pauli principle, can never be found at one point. Thus in the cold collision regime, when only the s-wave scattering can take place, interacting fermions effectively turn into a noninteracting Fermi gas. Evidently, this means that in a cold gas of fermions there will be no interaction shift.

This conclusion is true when the thermal de Broglie wavelength $\Lambda_T = h/(2mk_BT)^{1/2}$ is larger than the two-particle scattering length a, i.e., at $k_BT \lesssim \hbar^2/ma^2$. Similar to the case of Bose particles, this condition is considerably weaker than the Fermi degeneracy criterion $\Lambda_T n^{1/3} \simeq 1$. Therefore, degeneracy is not required for the absence of the interaction shift.

To verify this quantitatively, we derive a sum rule for the center of mass of the spectrum by using the same method as for Bose particles. Since the derivation proceeds in exactly the same steps as for the Bose gas, there is no need to discuss it in detail. The operator products that arise in the derivation can be bilinear or quartic. In both cases the difference between Bose and Fermi commutation relations is unimportant. The resulting expressions for F_{int} and F_{kin} are the same as Eqs. (14) and (16) above. However, the value of g_2 in Eq. (14) in this case should be calculated using Fermi statistics. For fermions with spin s one has $g_2 = 1 - 1/(2s+1)$. Accordingly, $g_2 = 0$ for spinless fermions, as well as for fully spin-polarized particles in a magnetic trap. Therefore in the case of Fermi particles the spectral shift is determined solely by the kinetic contribution (16).

The absence of the interaction shift for fermions is an interesting result from the point of view of designing atomic clocks. The value of the kinetic shift is typically small and independent of particle density. If necessary, it can be further reduced by increasing spatial uniformity of the excitation field.

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