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Numerical investigation of the radial quadrupole and scissors modes in trapped gases

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Abstract – The analytical expressions for the frequency and damping of the radial quadrupole and scissors modes, as obtained from the method of moments, are limited to the harmonic potential. In addition, the analytical results may not be sufficiently accurate as an average relaxation time is used and the high-order moments are ignored. Here, we numerically solve the Boltzmann model equation in the hydrodynamic, transition, and collisionless regimes to study mode frequency and damping. When the gas is trapped by the harmonic potential, we find that the analytical expressions underestimate the damping in the transition regime. Furthermore, we demonstrate that the numerical simulations are able to provide reasonable predictions for the collective oscillations in the Gaussian potentials. The present method can also be used to study many other problems, e.g. formation of quantum shockwave, expansion of atom cloud, and effective heat conductivity in very elongated traps.

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Introduction. – The realization of quantum degeneracy in the ultracold atomic gases has attracted intensive research efforts to understand the interacting quantum systems [1,2]. The experimental controllability of the interactions, energy, and spin population makes these systems ideal to study the crossover from a Bose-Einstein condensation (BEC) to a Bardeen-Cooper-Schrieffer (BCS) superfluid, which is ubiquitous in high-temperature superconductivity, neutron stars, nuclear matter, and quark-gluon plasma [3]. And the study of the low-lying excitation modes is important for probing the properties of strongly correlated systems, revealing the underlying mechanisms of BEC-BCS crossover.

In the zero-temperature limit, the superfluid behavior of the quantum Fermi gases is well understood [2,4,5]. At high temperatures, the dilute quantum gases are in the normal phase and their dynamics can be described by the semi-classical Boltzmann equation [6]. On the other hand, when the temperature is below the critical temperature for superfluidity, the superfluid and normal phases coexist. In this case, the Boltzmann equation for the dynamics of the quasiparticle distribution function and the Euler equations for the superfluid order parameter can be combined to describe the quantum gas dynamics [7,8]. So far, however, the effects of temperature on the collective modes remain unclear. For instance, experimentally, in the same temperature range, Kinast et al. showed that the frequency of the radial compression mode stayed close to the hydrodynamic value [9], while Wright et al. measured the scissors mode and found a clear transition from the hydrodynamic to collisionless behavior [10]. This discrepancy motivated Riedl et al. to measure the frequency and damping of the radial compression, quadrupole, and scissors modes in a similar experimental condition and to compare the experimental data with the analytical prediction of the moment method [11]. However, there are discrepancies between the experimental and theoretical results, especially for the radial quadrupole mode.

The analytical expressions for the mode frequency and damping were obtained by applying the method of moments to the linearized Boltzmann equation [11–15]. However, the analytical method of moments may not provide accurate predictions for the two-component Fermi gases in the transition regime [11,16], which is caused by i) the spatially dependent relaxation time is replaced by the spatially average one and/or ii) only low orders of moments are included in the analytical method, which may not be adequate for capturing the important features
of the collective oscillations. For example, one needs to consider high-order terms for the cloud surface deformation at large radii in the quadrupole mode if using average relaxation time [16]. The other major drawback of the analytical method is that it is only limited to the external harmonic potentials, while experimentally anharmonic effects emerge at high temperatures where the external potential has a Gaussian profile [10,11]. Therefore, it is necessary to solve the Boltzmann equation numerically to get the accurate mode frequency and damping, which is the aim of the present paper.

Here we put forward a deterministic method to numerically solve the Boltzmann model equation in the hydrodynamic, transition, and collisionless regimes. We extract the frequency and damping of the radial quadrupole and dynamic, transition, and collisionless regimes. We extract the aim of the present paper.

\[
V(x,y) = V_0 \left[ 1 - \exp \left( -\frac{x^2}{a^2} - \frac{y^2}{b^2} \right) \right],
\]

where \( V_0 \) is trap depth and \( a, b \) are the trap widths. However, at low temperatures, the size of atom cloud is far smaller than the trap widths. In this case, the external potential is nearly harmonic

\[
V(x,y) = \frac{m}{2} \left( \omega_x^2 x^2 + \omega_y^2 y^2 \right),
\]

where the trap frequencies satisfy \( \Omega_x = \sqrt{2V_0/m} \) and \( \Omega_y = \sqrt{2V_0/m}/b \).

Instead of the Boltzmann equation, we begin with the kinetic model equation based on the relaxation-time approximation: this model can capture the essential physics of the problem and has been widely used to describe the rarefied gas dynamics [18]. It reads

\[
\frac{\partial f}{\partial t} + v_x \frac{\partial f}{\partial x} + v_y \frac{\partial f}{\partial y} + \alpha_x \frac{\partial f}{\partial v_x} + \alpha_y \frac{\partial f}{\partial v_y} = f_{le} - f_{\tau}(x,y),
\]

where \( f(x,y,v_x,v_y,t) \) is the reduced distribution function which neglects the axial motion, \( v_x \) and \( v_y \) are velocity components, \( (a_x, a_y) = -(\partial/\partial x, \partial/\partial y) V/m \) are the accelerations, \( \tau(x,y) \) is the local relaxation time, and \( f_{le} \) is the local equilibrium distribution function

\[
f_{le} = \frac{mn}{2\pi k_B T} \exp \left[ -\frac{m (v_x - u_x)^2 + (v_y - u_y)^2}{2k_B T} \right],
\]

which is defined in terms of the local particle density \( n(x,y) \), local temperature \( T(x,y) \), local macroscopic velocities \( u_x(x,y) \) and \( u_y(x,y) \), and the Boltzmann constant \( k_B \). When the system is in global thermal equilibrium, \( n = n_0 \exp[-V(x,y)/k_BT_0] \), with \( n_0 \) being the particle density at the trap center and \( T_0 \) the global equilibrium temperature.

The relaxation time can be determined by macroscopic properties such as shear viscosity or by microscopic information. The shear viscosity plays a dominant role in the collective oscillations; the atom cloud remains nearly isothermal and the experiment is not sensitive to the thermal conductivity [19,20]. Therefore, the local relaxation time can be determined by equating the shear viscosity with that derived from the kinetic model equation (3), yielding \( \tau = \eta/nk_BT \).

Using microscopic information, we have

\[
\tau(x,y) = 15\frac{m \pi}{k_BT} \frac{m \pi}{16 \pi n_0 \int_0^\infty d\xi \xi e^{-\xi^2} (1 + \xi^2 T/T_0)^{-1}},
\]

where \( \sigma = 4\pi a^2 \) is the total energy-independent cross-section and \( T_0 = k_B a^2/\hbar^2 \), with \( a \) the s-wave scattering length and \( \hbar \) the Planck constant [14]. Two limiting cases will be considered. When \( a \) is small, the scattering cross-section is energy-independent, and atoms behave like hard spheres. The local relaxation time is therefore given by [14,21,22]

\[
\tau(x,y) = \frac{5}{16\pi n(x,y)^2} \sqrt{\frac{m \pi}{k_B T(x,y)}}.
\]

In the unitarity limit where \( a \to \infty \), we have

\[
\tau(x,y) = \frac{15m^{3/2}}{64\hbar^2 n(x,y)} \sqrt{\frac{k_B T(x,y)}{\pi}}.
\]

**Numerical scheme.** – The relaxation time is a crucial parameter in the collective oscillations. A spatially uniform gas is in the hydrodynamic regime when \( \omega_\tau << 1 \). Here \( \omega_0 \) is the external trap frequency (the mode frequency is of the same order). In this circumstance, the Euler and Navier-Stokes equations can be derived from the Boltzmann equation by the Chapman-Enskog expansion [21]. On the contrary, the gas is collisionless when \( \omega_\tau \gg 1 \). When the gas is trapped, however, it could be in the hydrodynamical, transition (\( \omega_\tau \sim 1 \)), or collisionless regime in the central region of the trap, whereas in the surface region it is always collisionless. The different order-of-magnitude of \( \tau \) across the trap poses difficulty in numerical simulations: if one wants to resolve the details of the collision, the time step \( \Delta t \) should be smaller than \( \tau \), which is not practical for the long time behavior when the gas is in the hydrodynamic regime (\( \tau \to 0 \)). Therefore, in a calculation, it is desirable
to use a numerical scheme that can have practical time step across hydrodynamic and collisionless regimes as we are interested in the macroscopic behavior of the gas.

In order to have practical time step in hydrodynamic regime where $\tau$ is small, we adopt the concept of asymptotic preserving to solve the model equation (3) numerically [23,24]. The virtue of this scheme is that it can capture the macroscopic gas dynamics in the hydrodynamic limit even if the small scale determined by the relaxation time $\tau$ is not numerically resolved. The computational accuracy in the hydrodynamic regime is guaranteed by the fact that, using the Chapman-Enskog expansion [25], this numerical scheme yields the correct Euler equations when $\tau$ goes to zero while the spatial and time steps are fixed. Therefore, the computation of a hydrodynamic flow can be as fast and accurate as that of the transition and collisionless flows. This unique feature cannot be implemented by the probabilistic methods such as the direct simulation Monte Carlo and molecular dynamics simulation.

The terms at the left side of eq. (3) are treated explicitly, while the collision term at the right side is treated implicitly to overcome its stiffness in the hydrodynamic regime (the stiff means that, since $\tau(x,y) > 0$, numerical errors can be greatly amplified), yielding

$$\frac{f^{j+1} - f^j}{\Delta t} + Tr[f^j] = \frac{1}{\tau(x,y)} (f_{\text{le}}^{j+1} - f^{j+1}),$$  \hspace{1cm} (7)

where variables with superscript $j$ denote the values of these variables at the $j$-th time step and $Tr[f^j]$ represents the spatial and velocity discretization of the last four terms at the left side of eq. (3). If the spatial and velocity ranges are wide enough, $f$ is zero at the boundaries, so that $Tr[f^j]$ can be handled by the fast Fourier transformation. By using the conservative properties of the collision term, the nonlinear implicit equation (7) can be solved explicitly. That is, given $f^j$, one can get $n^{j+1}$, $u_x^{j+1}$, $u_y^{j+1}$, and $T^{j+1}$ from the following equations: $n^{j+1} = \int F dv_x dv_y/n^{j+1}$, and $T^{j+1} = m[\int (v_x^2 + v_y^2) F dv_x dv_y/n^{j+1} - (u_x^{j+1})^2 - (u_y^{j+1})^2]/2k_B$, where $F = f^j - \Delta T[f^j]$ and the numerical integration can be carried out by direct discrete sum or by the Simpson’s rule. The above four macroscopic quantities at the $(j+1)$-th time step determine $f_{\text{le}}^{j+1}$ according to eq. (4) and $\tau^{j+1}$ according to eq. (5) or (6). Therefore, $f^{j+1}$ can be solved explicitly.

In practice, since $n(x,y)$ is very small near the boundary, numerical error emerges when calculating the macroscopic velocity. Hence it is possible to get negative temperature, which is not physical. To tackle this problem, the collision term in eq. (7) is neglected near the spatial boundary. This is justified by the fact that far from the trap center the gas is in the collisionless limit so the collision term is negligible. Another point one should pay attention to is that, the maximum Courant-Friedrichs-Lewy (CFL) number

$\Delta t = \min \{ \Delta x/\omega_x, \Delta y/\omega_y \}$

must be smaller than 1.

**Numerical results for the harmonic potential.**

To validate the numerical scheme, we simulate the radial sloshing and breathing modes in the isotropic harmonic trap with $\omega_x = \omega_y = \omega_0$. The local relaxation time is given by eq. (5). However, the use of eq. (6) will give the same result because the cloud is nearly isothermal, i.e., after normalization, only $n(x,y)$ affects $\tau(x,y)$. The numerical results in fig. 1 show that, as expected, the sloshing and breathing modes oscillate with the frequency $\omega_0$ and $2\omega_0$, respectively [12,16]. Note that the simulations were carried out in the transition regime, where damped modes are suppressed rapidly. The two perfectly undamped modes prove the accuracy of the numerical scheme.

Now we simulate the radial quadrupole mode and compare the results with the analytical and experimental ones. Analytically, replacing the local relaxation time by the average relaxation time $\bar{\tau} = 2\sqrt{2}\tau(0,0)$ and applying the method of moments up to the second-order, one find that the mode frequency $\omega_r$ and damping rate $\omega_l$ satisfy [13,26]

$$\omega^2 - 2\omega_0^2 - i\omega \bar{\tau}(\omega^2 - 4\omega_0^2) = 0,$$  \hspace{1cm} (8)

where $\omega = \omega_r - i\omega_l$. This equation clearly shows that in the hydrodynamic regime, the mode frequency is $\Omega_r = \sqrt{2}\omega_0$, while in the collisionless regime, it is $\omega_r = 2\omega_0$.

As mentioned above, the analytical solution (8) are not accurate due to the local relaxation time is replaced by the average one and/or only the second-order moments are included. To see which factor affects the accuracy of
the analytical results, we use both the local and average relaxation times in the numerical simulations. Numerically extracted mode frequency and damping are depicted in fig. 2. When the average relaxation time is used, the numerically obtained mode frequency, damping, and their relations (stars) agree with the analytical results very well, indicating that it is sufficient to include up to the second-order moments. The inaccuracy of the analytical results is therefore caused solely by replacing the local relaxation time with the average one. Comparing the analytical results with the numerical (squares, when the local relaxation time is used) and experimental ones (solid circles), one finds that the analytical mode frequency coincides with the numerical one (fig. 2(a)), while the analytical method underestimates the damping, especially in the transition regime (fig. 2(b) and (c)). The numerical results (squares) agree better with the experimental data than the analytical results reported in refs. [11].

Finally, we simulate the radial scissors mode in the elliptical harmonic potential with $\omega_x = 2\omega_y = 4$. Analytically, the method of moments up to second-order predicts the following relation between the mode frequency and damping [15]

$$i\omega(\omega^2 - \omega_{x1}^2) + \tilde{\tau}(\omega^2 - \omega_{x2}^2)(\omega^2 - \omega_{y1}^2) = 0,$$

where $\omega_{i} = (\omega_{x1}^2 + \omega_{y1}^2)^{1/2}$ is the frequency in the hydrodynamic limit and $\omega_{x1} = \omega_x + \omega_y$, $\omega_{x2} = |\omega_x - \omega_y|$ are the frequencies at the collisionless limit.

Typical oscillation scenarios of the radial scissors mode are shown in fig. 3. In the collisionless limit ($\sqrt{\Omega_x\Omega_y\tilde{\tau}} = 28$), the angle of atom cloud oscillates with two frequencies of 5.999 and 2, and the damping rate is 0.036. As the value of $\sqrt{\Omega_x\Omega_y\tilde{\tau}}$ decreases, both the frequencies decrease, with the larger one gradually reducing to $2\sqrt{2}$ (fig. 4(a)) and the smaller one quickly approaching zero. For example, when $\sqrt{\Omega_x\Omega_y\tilde{\tau}} = 0.316$, $\omega_r = 4.609$ and the smaller frequency is already 0.012; however, the damping corresponding to the larger frequency decreases with an initial increase (fig. 4(b)). The largest damping is achieved when $\sqrt{\Omega_x\Omega_y\tilde{\tau}} = 0.72$, where the scissors mode damps out within 2 oscillations. When the average relaxation time is used in the numerical simulation, the mode frequency (stars) overlaps with the analytical prediction (fig. 4(a)), while the damping agrees with the analytical prediction only in the hydrodynamic and collisionless regimes (fig. 4(b)); in the transition regime the damping is slightly larger than that of the analytical prediction. This implies that, unlike the radial quadrupole mode, the
Numerical results for the Gaussian potential. – Instead of the harmonic potential, the gases are trapped in the Gaussian potential at higher temperatures. The moment method fails to provide analytical solution for the Gaussian potential, so we have to rely on numerical simulations. To calculate the collective frequency and damping of the radial quadrupole mode, the following experimental data are used [11]: $V_0 = 50 k_B \mu K$, $a, b = 32.8 \mu m$, with the corresponding trap frequency $\omega_z, \omega_r = 1800 \times 2 \pi$ Hz. The trap frequency in the $z$ direction is $\omega_z = 32 \times 2 \pi$ Hz, and the total number of atoms is $N = 6 \times 10^5$. In numerical simulations, the time, spatial coordinates, velocity, and temperature are respectively normalized by $a \sqrt{m/k_B T_F}$, $a \sqrt{k_B T_F/m}$, and the Fermi temperature $T_F = 2.73 \mu K$. The distribution function is also normalized by the particle density at the trap center. Therefore, the normalized accelerations in the $x$ and $y$ directions are respectively $-36.6 x \exp(-x^2 - y^2)$ and $-36.6 y \exp(-x^2 - y^2)$, and at the unitarity limit, the normalized local relaxation time is $\tau(x, y) = 0.09 (T/T_F)^2/\mu(n(x, y))$. 

Figure 5(a) shows the frequency of the sloshing mode decreases as the temperature increases, which coincides with the experimental observations. This can be explained by the fact that the anharmonicity becomes stronger and stronger as the cloud size increases due to the temperature rise. Also, we find that the frequency decreases as the cloud’s initial center $x_0$ increases. Note that the sloshing mode is excited by shifting the Gaussian potential by $x_0$ in the $x$ direction.

Figure 5(b) demonstrates the relation between the mode frequency and damping, where the local relaxation time is $\tau(x, y) = a \tilde{T}^2/n(x, y)$, the initial distribution function is $f = \exp[-18.3 \{1 - e^{-x^2/1.05^2-1.05^2y^2}/\tilde{T}\} \exp[-(u_x^2 + v_y^2)/2\tilde{T}]/2\pi\tilde{T}$, and $\tilde{T} = T/T_F$. In the numerical simulation we use two values of $\alpha$, because if the repulsive mean-field potential is presented in the experiment, the atom density at the trap center will decrease and hence the coefficient will be larger than 0.09. When $\alpha = 0.09$, as the temperature increases (corresponding to the data from left to right), the mode frequency first increases, remains almost unchanged at $\omega_r/\omega_z \approx 1.8$, and then slightly decreases. The constant frequency is due to the balance between

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the anharmonic and collisionless effects: the anharmonic effect reduces the effective trap frequency (and hence the mode frequency) while the collisionless effect increases the mode frequency. When \( \alpha = 0.18 \), the trend of the relation between the mode frequency and damping agrees with the experimental finding reasonably well. That is, from the hydrodynamic regime to the collisionless regime, the mode frequency first increases and then decreases. These results indicate that our numerical scheme can provide reasonable predictions for the collective oscillations in the Gaussian potentials. Also, it indicates that the difference between the numerical and experiment results may be a consequence of the approximation of the relaxation rate or the neglected mean-field potential term in eq. (3), rather than the anharmonic effect [11].

**Outlook.** – In summary, to improve the accuracy and overcome the limitation of the method of moments, we have demonstrated a computationally efficient numerical scheme to solve the Boltzmann model equation. The extracted mode frequency and damping of the radial quadrupole and scissors modes provide better agreement with the experimental data than the analytical solutions obtained from the method of moments. The advantage of this numerical approach is that it can deal with the harmonic and Gaussian potentials, as well as other forms of the potential, including the mean-field and other self-energy terms, which will help us to understand the properties of strongly interacting particles. In particular, the asymptotic preserving nature of the numerical scheme makes the computation of a hydrodynamic flow as fast and accurate as that of the transition and collisionless flows, which cannot be implemented by the probabilistic methods.

In addition to the study of collective oscillations, the present method can be useful for investigation of many other problems. For example, one can use it to study the expansion of the atom cloud after the trap being switched off; to examine the collision of two initially separated atom clouds to see the formation of quantum phase transitions or the neglected mean-field potential term in eq. (3), i.e., the damping of superfluid flow by a thermal cloud [28].

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