Properties of the Trapped Dipolar Ultracold Gases at Finite Temperatures

Yuki Endo and Tetsuro Nikuni
Department of Physics, Faculty of Science, Tokyo University of Science, 1-3 Kagurazaka, Shinjuku-ku, Tokyo 162-8601, Japan
E-mail: a1208705@rs.kagu.tus.ac.jp

Abstract. We study the equilibrium and dynamical properties of dipolar Fermi gases at finite temperatures within the semiclassical treatment. The equilibrium property is discussed by introducing a variational ansatz for the phase-space distribution function. As for the dynamics, we apply the moment method to the kinetic equation to study quadrupole oscillation. We find that the quadrupole mode of polar molecules at high-temperature regime is in the hydrodynamic regime because of their large dipole moment.

1. Introduction
Interest in dipolar gases has been growing since the realization of Bose-Einstein condensates (BECs) of $^{52}$Cr atoms that have large magnetic dipole moments [1]. Recently, the experimental effort is put into creating heteronuclear polar molecules that have large electric dipole moments. The anisotropic and long-range nature of the dipolar interaction confers interesting properties to the equilibrium and dynamics of dipolar gases. There have been a number of theoretical studies in both dipolar BECs and Fermi gases, which have investigated the ground states and the stabilities, expansion dynamics, collective oscillation, and the properties in optical lattice potentials. For the dipolar Fermi gases, it was recently revealed that dipolar effects in the equilibrium can be detected with a typical electric dipole moment of the heteronuclear molecules [2, 3]. In experiments, however, many groups conducting experiments, no groups have succeeded in cooling polar molecules down to the quantum-degenerate regime [4]. It is thus important to investigate the equilibrium and dynamical properties and clarify whether the dipolar effects can be observable in the temperature regime of the current experiment.

In the present paper, we study the properties of dipolar Fermi gases at finite temperatures, especially the effect of dipolar interactions on thermal equilibrium and the quadrupole oscillation. In Sec.2, we derive a kinetic equation for dipolar Fermi gases. In Sec. 3, we discuss the thermal equilibrium by introducing a variational ansatz for the phase-space distribution function. In Sec. 4, we derive moment equations describing collective oscillations of quadrupole mode.
2. Kinetic equation for dipolar Fermi gases

We consider trapped dipolar fermions. The dipoles are assumed to be polarized along the z axis due to an external electric field. The second quantized Hamiltonian for this system is given by

$$\hat{H} (t) = \int d\mathbf{r} \hat{\Psi}^\dagger (\mathbf{r}, t) \left[ -\frac{\hbar^2}{2m} \nabla^2_{\mathbf{r}} + V_{\text{trap}} (\mathbf{r}) \right] \hat{\Psi} (\mathbf{r}, t) + \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \hat{\Psi}^\dagger (\mathbf{r}, t) \hat{\Psi}^\dagger (\mathbf{r}', t) V_{dd} (\mathbf{r} - \mathbf{r}', t) \hat{\Psi} (\mathbf{r}', t) \hat{\Psi} (\mathbf{r}) ,$$

where $\hat{\Psi} (\mathbf{r}, t)$ is the Fermi field operator in the Heisenberg expression, and the hat indicates a second quantized operator. The first term of Eq. (1) describes the Hamiltonian of a single particle in a harmonic trap $V_{\text{trap}} (\mathbf{r}) = (m/2) \left[ \omega_x^2 (x^2 + y^2) + \omega_z^2 z^2 \right]$, where $m$ is the particle mass.

The second term describes the two-body interaction Hamiltonian of the dipolar force, where $V_{dd} (\mathbf{r}) = (d^2/\rho^3) \left( 1 - 3z^2/r^2 \right)$. $d$ is the coefficient of the dipolar interaction and $\rho = p^2/4\pi\epsilon_0$, where $p$ is magnitude of the electric dipole moment and $\epsilon_0$ is the electric permittivity of a vacuum.

In order to describe time evolution of the nonequilibrium system, we introduce the Wigner operator: $\tilde{W} (\mathbf{p}, \mathbf{r}, t) = \int d\mathbf{r}' e^{-i\mathbf{p}\cdot\mathbf{r}'/\hbar} \hat{\Psi}^\dagger (\mathbf{r} - \mathbf{r}'/2, t) \hat{\Psi} (\mathbf{r} + \mathbf{r}'/2, t)$, and define the semiclassical Wigner distribution function as $W (\mathbf{p}, \mathbf{r}, t) \equiv \text{tr} \tilde{W} (\mathbf{p}, \mathbf{r}, t)$, where $\text{tr}$ is the statistical density operator. Using a semiclassical approximation to describe atomic motion in terms of a phase-space distribution function, we obtain the semiclassical kinetic equation for $W (\mathbf{p}, \mathbf{r}, t)$ as

$$\frac{\partial W}{\partial t} + \nabla_{\mathbf{p}} \left( \frac{\mathbf{p}^2}{2m} - U_{dd}^{\text{ex}} \right) \cdot \nabla_{\mathbf{r}} W - \nabla_{\mathbf{r}} V_{\text{trap}} \cdot \nabla_{\mathbf{p}} W - \nabla_{\mathbf{r}} (U_{dd}^{H} - U_{dd}^{\text{ex}}) \cdot \nabla_{\mathbf{p}} W = \left( \frac{\partial W}{\partial t} \right)_{\text{coll}} ,$$

where we defined the dipolar potential of the Hartree term $U_{dd}^{H} (\mathbf{r}, t)$ and the Fock exchange term $U_{dd}^{\text{ex}} (\mathbf{r}, t)$ as

$$U_{dd}^{H} (\mathbf{r}, t) \equiv \int d\mathbf{r}' V_{dd} (\mathbf{r}' - \mathbf{r}) \ n (\mathbf{r}', t) , \quad U_{dd}^{\text{ex}} (\mathbf{p}, \mathbf{r}, t) \equiv \int \frac{d\mathbf{p}'}{(2\pi\hbar)^3} \tilde{V}_{dd} (\mathbf{p} - \mathbf{p}') \ W (\mathbf{p}', \mathbf{r}, t) .$$

One important feature of the dipolar gases is that the Fock exchange term of the dipolar energy makes the single-particle energy anisotropic as shown in the second term of Eq.(2). The term on the right-hand side of Eq.(2) is the collision term. This collision term depends on the dipolar potential in momentum space. Therefore, the collisional relaxation between the particles become anisotropic. Explicit form and detailed derivation of the collision integral will be given elsewhere [5].

3. Equilibrium properties

We briefly summarize the result for the thermal equilibrium of dipolar fermions trapped in a harmonic potential. The system has a metastable state at finite temperatures under certain conditions even if a dipolar interaction is partially attractive and causes collapse of the gas. To find this metastable state, we introduce a variational Wigner distribution function [3] consistent with the kinetic equation (2). We assume the Maxwell–Boltzmann regime at relatively high temperatures:

$$W^0 (\mathbf{p}, \mathbf{r}) = \exp \left( - \frac{\theta^2}{2m} \left( \frac{\mathbf{p}_x^2 + \mathbf{p}_y^2}{\alpha} + \alpha^2 \mathbf{p}_z^2 \right) + \lambda^2 \frac{m\omega^2}{2} \left[ \beta (x^2 + y^2) + z^2 \right] - \mu_0 \right) / k_B T ,$$

where $\omega \equiv \left( \omega_x^2 \omega_y^2 \right)^{1/3}$. Here, the positive parameters $\alpha$ and $\beta$ represent deformations of density distributions in momentum and real space. $\lambda$ and $\theta$ characterizes isotropic compressions in real
and momentum space respectively \[3\]. We note that $\alpha$ indicates the anisotropy of the effective kinetic energy induced by the dipolar interaction, as showed in the second term of Eq.(2). The expression of the free energy in terms of the variational parameters is described as

$$F = \left\{ \frac{f(\alpha)}{2\theta^2} + \frac{g(\beta)}{2\pi^2} + \frac{CA^3}{(k_BT)^{3/2}} [I(\beta) - I(\alpha)] - 3 + \ln \left[ N (\lambda \theta \omega_h)^3 \right] - 3 \ln (k_BT) \right\} N k_B T \tag{5}$$

where $C \equiv \left( d^2 m^3 / 2 \omega_1^3 N \right) / \left( 3 \cdot 2^2 \pi^1 / 2 \right)$. In the above expression, we have defined the scaling functions $f(\alpha) = 2\alpha + 1 / \alpha^2$ and $g(\beta) = 2\beta/\beta^2 + \beta_0^2$, where $\beta_0 \equiv (\omega_\parallel / \omega_\perp)^{2/3}$. The deformation function $I(\alpha)$ is defined in Ref. [2], which indicates the deformation for the gases in terms of the dipolar interaction. By minimizing the free energy (5), we reveal that the momentum space distribution is always elongated in the $p_z$ direction and the real-space distribution tends to be stretched in the $z$ direction as is shown in Fig.1-3 in Ref. [3]. In addition, we found that the partial attraction of the interaction causes instability of the gas to collapse.

We also studied a dipolar Bose gas above the Bose-Einstein transition temperature $T_{\text{BEC}}$. It was found that the different statistics of Fermi and Bose gases gives rise to different signs for the Fock exchange energy. The different signs of the Fock exchange energy causes opposite properties: the momentum distribution is stretched in the $p_x - p_y$ plane in a Bose gas. More detailed discussion of the dipolar Bose gases can be found in Ref. [6].

### 4. Quadrupole oscillation for the trapped dipolar Fermi gases

In this section, we consider the quadrupole oscillation for the dipolar Fermi gases in the collisional regime. In this paper, we consider the mode at relatively high temperature regime, where the equilibrium distribution is given by the Maxwell-Boltzmann distribution as discussed in Sec. 3. The quadrupole mode of the dipolar gases is of particular interest because of their ellipsoidal momentum distribution. First, we linearize the kinetic equation around the equilibrium state derived in Sec. 2 by substituting $W(p, r, t) = W^0(p, r) + \delta W(p, r, t)$ and using analogous treatments for $U^H_{dd}$ and $U^\text{ex}_{dd}$ into (2). Next, we take moment of the linearized kinetic equation for general quantity $\chi_a(r, p)$. We define the following expectation values:

$$\langle \chi_a \rangle \equiv \frac{1}{N} \int dr \int \frac{dp}{(2\pi \hbar)^3} \chi_a \delta W(p, r, t) \quad , \quad \langle \chi_a \rangle^{\text{eq}} \equiv \frac{1}{N} \int dr \int \frac{dp}{(2\pi \hbar)^3} \chi_a W^0(p, r) \quad , \quad \langle \chi_a \rangle^{\text{coll}} \equiv \frac{1}{N} \int dr \int \frac{dp}{(2\pi \hbar)^3} \chi_a \left( \frac{\partial \delta W}{\partial t} \right)^{\text{coll}} \tag{6}$$

Using the above moments, we can derive the general moment equation from the linearized kinetic equation. After some algebra, we obtain the generalized moment equation as

$$\frac{\partial \langle \chi_a \rangle}{\partial t} - \langle \nabla_r \chi_a \cdot \frac{p}{m} \rangle - \langle \nabla_r \chi_a \cdot \nabla_p W^0 \rangle - \langle \nabla_r \chi_a \cdot \nabla_p \delta U \rangle^{\text{eq}}$$

$$+ \langle \nabla_p \chi_a \cdot \nabla_r U^0 \rangle + \langle \nabla_p \chi_a \cdot \nabla_r \delta U \rangle^{\text{eq}} = \langle \chi_a \rangle^{\text{coll}} \tag{7}$$

where $U^0$ and $\delta U$ are the equilibrium part and fluctuation part of $U(p, r, t) \equiv V_{\text{trap}}(r) + U^H_{dd}(r, t) - U^\text{ex}_{dd}(p, r, t)$. Considering quadrupole modes, we prepare the following quantities:

$$\chi_0 = 1, \quad \chi_1 = z^2, \quad \chi_2 = z p_z / m, \quad \chi_3 = z^2 / m^2, \quad \chi_4 = r_\perp^2, \quad \chi_5 = r_\perp \cdot p_\perp / m, \quad \chi_6 = p_\perp^2 / m^2 \tag{8}$$

To obtain a closed coupled equation for the quadrupole mode, we expand the distribution function: $\delta W(p, r, t) \equiv W^0(p, r) \left( \alpha_0 + \alpha_1 z^2 + \alpha_2 z p_z + \alpha_3 z^2 / m^2 + \alpha_4 r_\perp^2 + \alpha_5 r_\perp \cdot p_\perp + \alpha_6 p_\perp^2 \right)$. The coefficients in these expansion can be related back to the set of moments. Inserting (8) into
Figure 1. (Color online) Frequency of the quadrupole mode as functions of the dipole moment $p$ at the temperature $T = 2.0T_F^0$ for a trap asymmetry $\beta_0 = 0.5$ (red line). We also plotted the quadrupole frequencies in the hydrodynamic limit (dashed line) and in the collisionless limit (dotted-dashed line).

the general moment equation (6), we obtain the closed set of coupled moment equations for the quadrupole mode. Considering the normal mode solutions $\langle \chi_a \rangle \propto e^{-i\Omega t - \Gamma t}$, the moment equations are reduced to the eigenvalue equation. Solving the eigenvalue equation, we obtain the frequency $\Omega$ and damping rate $\Gamma$. We find that the damping rate damping rates are proportional to the fourth power of their dipole moment. Therefore their damping rates are about $10^6$ times larger than that of the damping rates of the typical Bose gases with s-wave interatomic interaction above the Bose-Einstein transition temperatures. In Fig.1, we plot the frequencies as a function of the dipole moment $p$ for a oblate traps ($\beta_0 = 0.5$) with a fixed temperature $T = 2.0T_F^0$, where $T_F^0 = (6N)^{1/3} \hbar \omega/k_B \approx 188 \text{nK}$ is the ideal gas Fermi temperature. We take the following values for the physical quantities: $m = 100 \text{ a.u.m.}$, $\omega = 5\pi \times 10^2 \text{ Hz}$, and $N = 10^4$. We plotted the optimized values for $p > p_c$, where $p_c$ is the critical dipole moment below which the variational free energy (5) has no local minimum and the system becomes unstable to collapse. We note that these frequencies suddenly decrease at the critical value. For reference, we plot the frequencies of the dipolar Fermi gases both in the hydrodynamic and collisionless regimes. Comparing these modes, we found that the frequencies of the dipolar Fermi gases are almost in the hydrodynamic regime. This results are understood by a large coefficient of the two-body interparticle interaction derived from the electric dipole moment. This result are quite different at zero temperature. In addition, we note that these frequencies suddenly decrease at the critical value. We find that these phenomena can be seen in any trap aspect ratios.

5. Conclusion
In this paper, we have studied the equilibrium and the collective oscillation in dipolar Fermi gases at finite temperatures. First, we derived the kinetic equation. We studied the equilibrium properties at finite temperatures by using a variational method. As in the zero temperature case, the anisotropic nature of the dipolar interaction leads to deformations in momentum. Next, starting from the kinetic equation, we derived the moment equation given in Eq.(6). Solving this equation for the quadrupole mode in the collisional regime, we found that the modes of the dipolar Fermi gases are in the hydrodynamic regime because the collisional relaxation rate increases with the fourth power of the dipole moment.

References
[1] Griesmaier A, Werner J, Hensler S, Stuhler J and Pfau T 2005 Phys. Rev. Lett. 94 160401
[2] Miyakawa T, Sogo T and Pu H 2008 Phys. Rev. A 77 061603 R
[3] Endo Y, Miyakawa T and Nikuni T 2010 Phys. Rev. A 81 063624
[4] Ni K K, Ospelkaus S, Wang D, Quéméner G, Neyenhuis B, de Miranda M H G, Bohn J L, Ye J and Jin D S 2010 Nature 464 1324
[5] Endo Y and Nikuni T unpublished
[6] Endo Y, Miyakawa T and Nikuni T 2011 J. Phys. Soc. Jpn. 80 044006