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Equations of state and diagrams of two-dimensional liquid dusty plasmas

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Recently, the pressure of two-dimensional (2D) Yukawa liquids has been calculated from the simulations of isochores [Feng et al., J. Phys. D: Appl. Phys. 49, 235203 (2016)], which is applicable to 2D dusty plasmas. Thus, the equation of state for 2D strongly coupled liquid dusty plasmas is obtained. Isobars and isotherms of 2D liquid dusty plasmas are derived from this equation of state. For 2D liquid dusty plasmas, the surface corresponding to this equation of state has also been obtained in the 3D space of the pressure, the temperature, and the screening parameter which is related to the volume in the equilibrium state. Published by AIP Publishing.

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I. INTRODUCTION

Equations of state describe the relationship between various physical quantities of the studied matter, such as temperature, volume, and pressure. Equations of state are typically extracted from experimental observations and should be valid only within the studied parameter range. Within this parameter range, some properties of the matter can be derived directly from its equations of state. As typical examples of equations of state, the ideal-gas equation and the van der Waals equation are able to describe most behaviors of gases quite well. However, the equations of state for liquids and solids are much more complicated.

A dusty plasma is a mixture of highly charged micro-sized dust particles, free electrons, free ions, and neutral gas atoms. In laboratory conditions, these dust particles can self-organize into a single layer suspension, i.e., a 2D suspension, with negligible out-of-plane motion. Due to the shielding effects of free electrons and ions, within the single layer, the interaction between dust particles can be modeled as the Yukawa potential.

The Yukawa potential, also called the Debye-Hückel potential, has the form of 

\[ \phi(r) = \frac{Q^2}{4\pi\varepsilon_0ak_BT} \exp(-r/\lambda_D). \]

where \( Q \) is the particle charge and \( \lambda_D \) is the Debye screening length. Besides dusty plasmas, the Yukawa potential is also used to describe interparticle interactions in other physical systems, like colloids. Now, behaviors of 2D dusty plasmas are often studied using simulations of 2D Yukawa liquids and solids. To characterize 2D Yukawa systems, two dimensionless quantities, the coupling parameter \( \Gamma \) and the screening parameter \( \kappa \), are typically used. They are defined as

\[ \Gamma = \frac{Q^2}{(4\pi\varepsilon_0ak_BT)} \]

and

\[ \kappa = \frac{a}{\lambda_D}, \]

respectively. Here, \( a \) is the Wigner-Seitz radius for an areal number density of \( n \) for particles and \( T \) is the kinetic temperature of particles. The coupling parameter \( \Gamma \) is inversely proportional to the temperature, i.e., \( \Gamma \propto 1/T \). If the Debye screening length \( \lambda_D \) is assumed to be constant, then the screening parameter \( \kappa \) indicates the length scale of the space (or area for 2D systems) that one particle occupies. Thus, the screening parameter can be regarded as a quantity related to the “volume” of 2D Yukawa systems. Thus, we can use \( \Gamma \) and \( \kappa \) to replace the traditional physical quantities of temperature and volume in equations of state to study 2D Yukawa liquids. We choose the pressure as the third physical quantity for 2D Yukawa liquids.

The pressure \( p \) is typically an important physical quantity in thermodynamical procedures, which is not easy to be studied in dusty plasma experiments. Note that here the pressure is the internal force per unit length of the 2D lattice due to the interaction and collision of dust particles, not the plasma gas pressure. In our literature search, we have found previous studies of the pressure for 2D Yukawa liquids. Totsuji et al. obtained the pressure from their computed internal energy \( U \) from a simulation. Hartmann et al. calculated the pressure from the pair correlation function. Vaulina et al. got an expression of pressure using a semi-empirical jumps theory. In a recent paper, the pressure is calculated as exact values from the shear stress tensor obtained from molecular-dynamical (MD) simulations of 11 isochores for 2D Yukawa liquids, i.e., simulations of 2D liquid dusty plasmas, as briefly reviewed in Sec. II soon.

In the past two decades, the behaviors of 2D dusty plasmas have been investigated widely, from theories and simulations to experiments, as reviewed in Refs. 28–32. However, for 2D dusty plasmas, a concise analytical relationship between various physical quantities which can be easily used to derive other thermodynamical procedure is still lacking. Here, we combine the obtained equations in Ref. 1 and regard them as the equations of state for 2D liquid dusty plasmas to study other procedures of 2D strongly coupled dusty plasmas.

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obtained in Ref. 1 to achieve a single new equation, and we name it as the equation of state for 2D liquid dusty plasmas. Then, from this equation of state, we directly derive the relationship of isobars and isotherms for 2D liquid dusty plasmas and plot them in corresponding diagrams. Finally, also from this equation of state, we obtain a 3D surface plot in the space of their temperature, “volume,” and pressure, which provides a clear relationship between these physical quantities.

II. REVIEW OF ISOCHORES FOR 2D YUKAWA LIQUIDS

Here, we briefly review the results of the pressure for 2D Yukawa liquids from MD simulations in Ref. 1.

In Ref. 1, frictionless equilibrium MD simulations were performed to study 2D Yukawa liquids or 2D liquid dusty plasmas. The simulated \( N = 1024 \) particles are all constrained within a single 2D plane. The integration equation of motion is

\[
n \dot{\mathbf{r}} = -\nabla V, \quad \mathbf{F} = -\nabla V.\n\]

where \( \phi \) is the binary interparticle repulsion with a Yukawa potential.\(^8\) To study the liquid state of 2D Yukawa systems, the simulation conditions, i.e., eleven pairs of \( T \) and \( \rho \) values, were all chosen in the liquid regime. For 2D Yukawa systems, each \( \kappa \) value corresponds to one melting temperature, expressed as one \( \Gamma \) value.\(^{12}\) In Ref. 1, the simulated temperature \((1/\Gamma)\) value was chosen over a wide range: from nearly the melting point to 70 times higher than the melting point, for all specified eleven \( \kappa \) values. Since \( \kappa \) directly corresponds to the length scale or the area of 2D Yukawa systems while the environment length scale of the Debye length \( \lambda_D \) is assumed to be constant, the simulated conditions in Ref. 1 would form eleven isochores of 2D Yukawa liquids.

The pressure of 2D Yukawa liquids has been calculated from the shear stress tensor using the simulated particles’ positions, velocities, and interparticle forces.\(^4\) The two diagonal elements of the shear stress tensor \( P_{xx}(t) \) and \( P_{yy}(t) \) both fluctuate around a constant level of \( pA \) for 2D systems, where \( p \) is the pressure and \( A \) is the area of the total 2D system. To compare with other systems easily, we normalize both the temperature and pressure to be dimensionless. The temperature is normalized by the potential energy between two particles with a distance of the Debye length, i.e.,

\[
\bar{T} = k_B T / (Q^2/4\pi\epsilon_0\lambda_D^2). \quad \text{The pressure in the 2D system has the unit of the energy in unit area, so that it can be normalized by the energy of} \quad \langle Q^2/4\pi\epsilon_0\lambda_D^2 \rangle \text{divided by the area of} \quad \lambda_D^2, \text{i.e.,} \quad \bar{P} = p / \langle Q^2/4\pi\epsilon_0\lambda_D^2 \rangle = (p_0/\lambda_D^2) / Q^2. \quad \text{Other details of the method have been presented in Ref. 1. Alternatively, the dimensionless temperature} \quad \bar{T} \quad \text{and the dimensionless pressure} \quad \bar{P} \quad \text{can also be expressed using} \quad \Gamma \quad \text{and} \quad \kappa \quad \text{as} \quad \bar{T} = 1/\kappa \quad \text{and} \quad \bar{P} = \frac{p_0\lambda_D^2}{\kappa k_B T}, \text{respectively.} \]

In Ref. 1, it has been discovered that, for all simulated eleven isochores, the pressure of 2D Yukawa liquids can be analytically expressed as the sum of a potential term and a kinetic term

\[
\bar{P} = \bar{x} + \beta \bar{T}, \quad (1)
\]

using the normalized dimensionless pressure \( \bar{P} \) and dimensionless temperature \( \bar{T} \) defined above. In Eq. (1), \( \bar{x} \) and \( \beta \) are coefficients which can be determined from either MD simulations as in Ref. 1 or possible future experimental measurements. From Eq. (1), the first term \( \bar{x} \) is a simple multiple of the Coulomb potential energy at a distance of the Debye length, so that it should be attributed to the potential contribution of the particles, i.e., due to the lattice structure of particles. The second term \( \beta \bar{T} \) is a multiple of the average kinetic temperature of particles, so that it should come from the kinetic contribution. This kinetic term is comparable to the ideal gas equation, proportional to the temperature.

In Ref. 1, eleven sets of coefficients \( \bar{x} \) and \( \beta \) have been determined by fitting to the MD simulation results. Also from these eleven sets of coefficients, analytical fits of both \( \bar{x} \) and \( \beta \) have also been obtained as

\[
\bar{x} = 2.29 e^{-2.45(a/\lambda_D)^2} + 0.34(a/\lambda_D)^5, \quad (2)
\]

\[
\beta = 0.14 e^{-0.37(a/\lambda_D)} + 1.30(a/\lambda_D)^2. \quad (3)
\]

In the studied parameter regimes, Eqs. (1)–(3) are able to describe the relationship among these thermodynamics parameters of 2D Yukawa liquids. These three equations, Eqs. (1), (2), and (3), were obtained from MD simulations of eleven isochores, or the conditions of constant volume (area), for 2D Yukawa liquids.

In this paper, we will extend the research findings in Ref. 1, as reviewed above. To investigate the thermodynamical procedures of 2D Yukawa liquids under the constant pressure or the constant temperature, we will derive analytical expressions of isochores and isotherms of 2D Yukawa liquids from the combination of the three equations reviewed above. We will plot these isochores and isotherms in corresponding diagrams and discuss the underlying physical mechanisms. To clearly demonstrate the strong coupling effect in dusty plasmas, we will compare our results with the isochores and isotherms for the ideal gas, i.e., the non-coupling case. Furthermore, to have a better understanding of the general relationship between these physical quantities, we will plot all three physical quantities of 2D Yukawa liquids, pressure, temperature, and length scale (related to “volume”) together, forming a 3D surface corresponding to these equations of state.

III. RESULTS

A. Equation of state

The equation of state for 2D Yukawa liquids, or 2D liquid dusty plasmas, can be obtained by combining the three equations, Eqs. (1), (2), and (3), as

\[
\bar{P} = \frac{(0.14 e^{-0.37\kappa} + 1.30/\kappa^2)\bar{T}}{(2.29 e^{-2.45\kappa^2} + 0.34/\kappa^2)} - (2.29 e^{-2.45\kappa^2} + 0.34/\kappa^2) = 0. \quad (4)
\]

For the three parameters of 2D Yukawa liquids, \( \bar{P} \), \( \kappa \), and \( \bar{T} \), only two of them are independent. When two of them are specified, Eq. (4) would determine the third parameter exactly. In the studied parameter regime of Ref. 1, Eq. (4) is able to describe the relationship among the thermodynamics parameters of 2D Yukawa liquids precisely.

To demonstrate the strong coupling effect of dusty plasmas, we will compare our results for 2D Yukawa liquids...
with those for the ideal gas. The equation of state for the ideal gas is \( P = N k_B T / V = n k_B T \). When we use the dimensionless pressure \( \Pi \) and the dimensionless temperature \( T \), the equation of state for the ideal gas would be changed to
\[
\Pi = n \lambda^2 T,
\]
which is the same as
\[
T = \pi k^2 \Pi. \tag{5}
\]
In later figures, we will add curves corresponding to this equation of state of the ideal gas (no coupling), Eq. (5), for comparison with the strongly coupled Yukawa liquids.

### B. Isobars

Isobars refer to curves corresponding to constant pressures in state diagrams. The equation of isobars for 2D Yukawa liquids can be derived in Eq. (4) while assuming the pressure to be a constant, \( C \Pi \). As a result, in principle, the analytical expression for isobars is
\[
C \Pi = (0.14 e^{-0.37 \kappa} + 1.30 / \kappa^2) T - (2.29 e^{-2.45 \kappa^2} + 0.34 / (\alpha / 2D)^2) = 0.
\]
Figure 1 shows the contour of isobars of 2D Yukawa liquids, where the dimensionless pressure \( \Pi \) changes from 0.001 to 20.0. From isobars in Fig. 1, when the Debye length is assumed to be constant, as the Wigner-Seitz radius or the lattice constant increases, the temperature would increase monotonically. It is equivalent to say, that, while the pressure is held to be constant, as the temperature increases, the volume would increase monotonically. This trend is not surprising for most forms of matter, similar to the ideal gas, although the analytical form is more complicated.

The main trend of isobars in the \( T - \kappa \) diagram is that as the temperature \( T \) increases gradually, the isobar curve goes to higher and higher values of \( \kappa \). One typical curve of the isobar of \( P = 0.02 \) is shown in Fig. 1. One interesting feature in Fig. 1 is that each isobar always starts from a specific \( \kappa \) value at nearly zero temperature \( T \to 0 \), and we call this \( \kappa \) value as the cutoff value of \( \kappa \) for this isobar. For example, for the isobar of \( P = 0.02 \) shown in Fig. 1, the cutoff of the \( \kappa \) value is \( \approx 1.8 \). It is equivalent to say, that \( P = 0.02 \) cannot be satisfied when \( \kappa < 1.8 \). Note that the cutoff value \( \kappa \approx 1.8 \) obtained from the isobar at \( T \to 0 \) is based on a smooth liquid-solid phase transition; however, whether this liquid-solid phase transition is smooth or not is beyond the scope of this paper.

We interpret that the feature of the cutoff \( \kappa \) in the isobars comes from the potential contribution \( \alpha \) of the pressure. For the simulated temperature range of each \( \kappa \) value, i.e., from about the melting point to 70 times higher than the melting point, the potential contribution is mostly dominant in the pressure expression, as shown in Fig. 3 of Ref. 1, especially for lower \( \kappa \) values. In Eq. (2), or Fig. 4 of Ref. 1, the value \( \alpha \) diminishes drastically about four orders of magnitude as \( \kappa \) increases from 0.5 to 3.0. For one specific dimensionless pressure \( P_0 \), the corresponding cutoff of this isobar in the \( T - \kappa \) diagram should be at the value of \( k_0 \) when \( \alpha = 2.29 e^{-2.45 (k_0)^2} + 0.34 / (k_0)^3 \) is satisfied. For lower values of \( \kappa \), the corresponding \( \alpha \) (its pressure while the dimensionless temperature \( T \) is zero) would be definitely larger than \( P_0 \), so that it is impossible to achieve the lower pressure of \( P_0 \) at this \( \kappa \) value. However, for higher values of \( \kappa \), the corresponding \( \alpha \) is smaller than \( P_0 \), so that we can increase the temperature, i.e., the kinetic term, to achieve a higher pressure \( P_0 \). Thus, for one constant pressure, it is reasonable that, at higher \( \kappa \) values, the corresponding isobar should be at higher temperature, which is just the main trend of Fig. 1.

The liquid-solid phase transition line can also be observed in Fig. 1. It starts from around the center of left to about the lower right corner. The solid regime is below this line, while the liquid state is above this phase transition line. The isobar of \( P = 0.02 \) for the ideal gas is shown as the straight dashed line on the upper portion of Fig. 1. This isobar is a straight line in the log-log plot, which is due to the equation of state of the ideal gas, Eq. (5), so that for one specific \( P \), the dimensionless temperature \( T \propto \kappa^2 \). Due to the lack of the potential contribution on the pressure for the ideal gas, for the same level of \( P \), the ideal gas needs a higher temperature, i.e., isobar of the ideal gas is on the upper portion.

### C. Isotherms

Isotherms are curves corresponding to constant temperature in the state diagram, and it can be also reflected in Eq. (4) while holding the temperature to be constant. Replacing the temperature \( T \) using the constant of \( C T \), then the equation of state for 2D Yukawa liquids, Eq. (4), would be changed to
\[
P = (0.14 e^{-0.37 \kappa} + 1.30 / \kappa^2) C T - (2.29 e^{-2.45 \kappa^2} + 0.34 / (\alpha / 2D)^2) = 0,
\]
which is the analytical expression of the isotherm curve in the \( P - \kappa \) diagram. Figure 2 shows the contour of the isotherm curve of 2D Yukawa liquids, where the dimensionless temperature \( T \) changes from 0.001 to 1.0.

The main trend of the isotherms in the \( P - \kappa \) diagram is that the pressure diminishes monotonically as \( \kappa \) increases. This trend means that, while the temperature is held constant, when the 2D Yukawa liquid system size increases, its pressure would diminish monotonically, as one typical isotherm
FIG. 2. The isotherm contour plot for 2D Yukawa liquids, with the temperature $T$ changing from $1e-3$ to 1.00. As $\kappa$ increases, the pressure $P$ diminishes monotonically for each isotherm curve. Even when the temperature changes three orders of magnitude, the difference in $P$ is less than one order of magnitude for any value of $\kappa$. The small difference of various isotherms is caused by the potential term, which mainly dominates the pressure, especially for lower $\kappa$ values. One typical isotherm of $T = 0.01$ is shown. For comparison, the isotherm of $T = 0.01$ for the ideal gas is shown as the straight dashed line.

of $T = 0.01$ shown in Fig. 2. Although this trend is similar to the ideal gas, the analytical expression of the isotherm in the previous paragraph is more complicated than that for the ideal gas.

Even for different temperatures, the corresponding isotherms do not vary too much. For various isotherms in Fig. 2, we change the temperature $T$ in three orders of magnitude, from 0.001 to 1.0. However, at any value of $\kappa$, the difference in $P$ is less than one order of magnitude, as shown in Fig. 2. Especially in the range of lower $\kappa$ values, the relative difference between various isotherms is even smaller. This phenomenon can be interpreted as the two contributions of pressure, potential and kinetic terms. From the previous results of Fig. 3 of Ref. 1, the potential term is mostly larger than the kinetic term, i.e., the potential term mainly dominates the pressure, especially for lower $\kappa$ values. Thus, in the isotherms, the kinetic term contribution of the pressure is small, in fact, mostly negligible for lower $\kappa$ values. As a result, the relative difference in isotherms is small, and in the lower $\kappa$ range, these isotherms almost cannot be distinguished. For higher $\kappa$ values, the potential term is much smaller, so that the kinetic term might suppress the potential term at higher temperatures. As a result, isotherms at higher $\kappa$ values can be easily distinguished. Note that another important reason that isotherms can be easily distinguished at higher $\kappa$ values is due to the exaggerate effect of extremely small values on the log plot of the pressure data.

The isotherm of $T = 0.01$ for the ideal gas is shown as the straight dashed line on the lower portion of Fig. 2. In the log-log plot, the isotherm of the ideal gas is a straight line, which is also due to its equation of state, Eq. (5). For one specific $T$ the dimensionless pressure $P \propto \kappa^{-2}$. Also, due to the lack of the potential contribution on the pressure, for the same dimensionless temperature $T$, $P$ of the ideal gas is much lower than that of the 2D Yukawa liquids, i.e., isotherm of the ideal gas is on the lower portion.

D. Isochores

In Ref. 1, eleven data sets of isochores, corresponding to eleven values of $\kappa$, for 2D Yukawa liquids have been simulated and reported. Then, analytical expressions of 2D liquid dusty plasmas, combined as Eq. (4), have been achieved by fitting these isochores as discussed above. From the analytical expression of Eq. (4), by substituting more values of the screening parameter $\kappa$ and the dimensionless temperature $T$, more isochores curves can be obtained, as the contour plot shown in Fig. 3. In Fig. 3, it is not surprising that, for each specific $\kappa$, when the temperature increases, the pressure always increases monotonically.

The pressure of 2D Yukawa liquids does change drastically as the screening parameter changes. From Fig. 3, as well as the simulated results in Ref. 1, the pressure changes about four orders of magnitude, while the $\kappa$ value only changes from 0.5 to 3.0 and the temperature is at around the melting points.

E. Surface of equation of state

The equation of state for 2D liquid dusty plasmas, Eq. (4), defines a surface in the 3D space of their three parameters, $P$, $\kappa$, and $T$, as shown in Fig. 4. The color on this surface shows the value of $\kappa$ there. The projection of this surface on the $P - T$ plane forms the isochore contour plot, as on the left portion of Fig. 4, which is exactly the same as the isochore contour plot of Fig. 3 above. Similarly, the surface projection on the $T - \kappa$ plane would form the contour of isobars as in Fig. 1, and the surface projection on the $P - \kappa$ plane would form the contour of isotherms as in Fig. 2.

IV. SUMMARY

In summary, we have systematically studied the equations of state for 2D strongly coupled dusty plasma liquids, as the development of the previous study of pressure for 2D Yukawa liquids.1 We have derived the expressions for isobars, isotherms, and isochores of 2D liquid dusty plasmas and plot them in corresponding diagrams. Finally, we also plot the surface corresponding to the equation of state for 2D

FIG. 3. The isochore contour plot for 2D Yukawa liquids. For each specific $\kappa$, as the temperature increases, the pressure always increases monotonically. Note that as the screening parameter $\kappa$ changes only from 0.5 to 3.0, the dimensionless parameter $P$ changes about four orders of magnitude.
FIG. 4. The surface of the three parameters, \( P \), \( \kappa \), and \( T \), for 2D Yukawa liquids, with the color showing the \( \kappa \) values. The projection of this surface on the \( P - T \) plane forms the isochore contour plot, as shown on the left.

liquid dusty plasmas in the 3D space of the three system parameters: \( P \), \( \kappa \), and \( T \). These results provide a clear picture of the relationship between three quantities of 2D liquid dusty plasmas, and they are applicable in providing a quantitative estimation or prediction of some physical quantities of 2D dusty plasmas. Following the similar derivation procedure presented here, other thermodynamical processes or some physical quantities for 2D liquid dusty plasmas can also be derived.

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