Lattice model for the two-dimensional electron liquid

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Through comparison with Hockney and Brown's result of the molecular-dynamics computation of the radial distribution function, it is shown that a triangular-lattice model with a harmonic-oscillator potential provides a good account for the screening potential of the two-dimensional classical electron liquid. The radial distributuion function obtained in such a lattice model is then substituted in the calculation of the velocity autocorrelation time based on a sum-rule analysis of the self-motion of an electron; the resulting theoretical values correspond closely to the measured values of Zipfel, Brown, and Grimes.

I. INTRODUCTION

Recently, Zipfel, Brown, and Grimes[1] (ZBG) have measured the velocity autocorrelation time τ_c in a two-dimensional (2D) layer of electrons trapped on the surface of liquid helium and thereby discovered a strikingly close correspondence between τ_c^{-1} and

$$\omega_0 = 2.1(e^2/m)^{1/2}n^{3/4} \ ,$$

the harmonic-oscillator frequency for the electrons forming a triangular lattice, where n is the areal number density of electrons. This observation, providing important clues about the motion of electrons in a liquid state, has had a great impact on the theoretical study of such a 2D one-component plasma. The static properties of such a system have been investigated by Hockney and Brown[2] with the aid of molecular-dynamics computations. Their work provided a significant improvement upon the theory of Platzman and Fukuyama[3], revealing interesting features in the radial distributuion function of the 2D classical one-component plasma. After completion of the original manuscript of this paper, Totsuji's Monte Carlo study of the 2D electron liquid[4] was brought to the attention of the authors. Totsuji's result shows essential agreement with Hockney and Brown's result in the high-plasma-parameter region, and complements theirs in the low-plasma-parameter region.

In this paper we wish to point out that the detailed features of the radial distribution function clarified in the molecular-dynamics computations are closely related to the physical notion that the short-range order in the 2D classical plasma in its liquid phase is already very much like that in its lattice phase. This observation leads us to propose a lattice model, which provides an explicit expression for the short-range correlation function in such an electron liquid; Sec. II will be devoted to the construction of this model. In Sec. III we substitute the expression for the correlation function in a first-principles calculation of the velocity autocorrelation time based on a sum-rule analysis of the self-motion of an electron[5,6]; the numerical results so computed exhibit a close agreement with the measured values of ZBG. We thus intend to show that the harmonic-lattice model proposed here consistently accounts for those static and dynamic properties manifested in the molecular-dynamics computations and the ZBG experiments. Concluding remarks will be given in Sec. IV.

II. LATTICE MODEL

The screening potential $V_s(r)$ of the electron liquid with a uniform positive-charge background is related to its radial distribution function $g(r)$ via

$$g(r) = \exp\{-(1/k_BT)[e^2/r - V_s(r)]\} \ . \tag{1}$$

On analyzing the raw data of $g(r)$ obtained by Hockney and Brown,[2] we find that except in the vicinity of $r=0$ the screening potential is expressed in a linear form,

$$V_s(r) = (e^2/a)(c_0 - c_1 r/a) \ , \tag{2}$$

where $a = (\pi n)^{-1/2}$ is the radius of the Wigner-Seitz disk; the coefficients c_0 and c_1 satisfy the relationship

$$c_1 = (\tfrac{1}{2}c_0)^2 \ . \tag{3}$$

The values

$$c_0 = 1.13 \ , \quad c_1 = 0.32 \ , \tag{4}$$

satisfying (3), are found to fit Hockney and Brown's data for $33.1 \leq \Gamma \leq 1875.8$ within errors less than 5%, where Γ is defined by

$$\Gamma = e^2/ak_BT \ . \tag{5}$$

Hockney and Brown have shown that a λ-type phase transition occurs at $\Gamma = 95 \pm 2$. Linearity of the screening potential (2) and (4) is observed for $1.0 \lesssim r/a \lesssim 2.0$ in the case of $\Gamma = 33.1$, and for $1.65 \lesssim r/a \lesssim 2.0$ in the case of $\Gamma = 1875.8$. The precise values of the screening potential at short distances are very difficult to deduce from the computed values of $g(r)$; this function takes on extremely small values at short distances because of the bare Coulomb term e^2/r.

Salient features of the screening potential for $r \lesssim 2a$ which the molecular-dynamics computations have revealed may thus be summarized in the following three aspects[7]: its apparent linearity (2), the relationship (3), and the absolute magnitude of either c_0 or c_1 in (4). We now wish to show that those empirical features can be explained consistently in terms of a lattice model based on a harmonic-oscillator potential. In so doing, we shall first compare the screening potential in the liquid phase with that in the triangular-lattice phase.

In order to investigate the screening potential of the 2D classical electron liquid, based on a triangular-lattice model, we consider the 2D counterpart of the relaxed-lattice model due originally to Salpeter and Van Horn.[8-10] For this model we impose the condition that the screening potential tends to that of the harmonic lattice near the lattice points[11] and to one obtained from the Wigner-Seitz disk model near zero separation

$$V_s(0) = 4\left[\sqrt{2}-1\right]\left[1-\frac{4}{3\pi}\right]\frac{e^2}{a} = 1.8164\frac{e^2}{d} \ , \tag{6}$$

where $d = 1.9046a$ is the nearest-neighbor distance of the triangular lattice. The Wigner-Seitz disk is the 2D analogy of the Wigner-Seitz sphere. Expression (6) is simply the difference of energy between two separate Wigner-Seitz disks of radius a and one "fused" Wigner-Seitz disk of radius $\sqrt{2}a$ which contains two electrons at its center. Furthermore, in order to calculate the quadratic part of the screening potential near zero separation, we employ the 2D counterpart of Jancovici's model[12]; we place two electrons at the point $\frac{1}{2}\vec{r}$, $-\frac{1}{2}\vec{r}$ in the Wigner-Seitz disk of radius $\sqrt{2}a$ centered at the origin. The resulting potential turns out to be

$$V_s^{II}(r) = -e^2r^2/4\sqrt{2}a^3 \ . \tag{7}$$

Thus, we have two model potentials near the two extremes, and interpolate these two by a polynomial for intermediate distances. The screening potential in the relaxed lattice model is hence written

$$V_{rel}(\eta) = (e^2/d)[1.00 + 1.00(1-\eta) - 1.76(1-\eta)^2 + 6.26(1-\eta)^3 - 7.14(1-\eta)^4 + 2.46(1-\eta)^5] \ , \tag{8}$$

where η is the separation between the two electrons measured in units of d. In these units, the molecular-dynamics screening potential (2) and (4) reads

$$V_{MD}(\eta) = (e^2/d)[0.99 + 1.16(1-\eta)] \ . \tag{9}$$

The two screening potentials (8) and (9) are plotted in Fig. 1. We find a good agreement between them: The screening potential in the relaxed lattice model is nearly linear over the range $0.2 \lesssim \eta \lesssim 1.0$. The molecular-dynamics screening potential almost coincides with the prediction of the triangular-lattice model at the nearest-neighbor distance.

We have thus seen that the triangular-lattice model qualitatively accounts for the behavior of the screening potential for $0 \leq \eta \leq 1.0$.[13] To obtain additional, quantitative accounts for the remaining points (3) and (4), and thereby to provide a model describing the salient features of the screening potential in the liquid phase, we further investigate the harmonic-oscillator potential model in the vicinity of the nearest-neighbor distance.

In the harmonic-oscillator potential model,[8] the effective potential between two electrons

$$V_{eff}(r) = e^2/r - V_s(r) \ ,$$

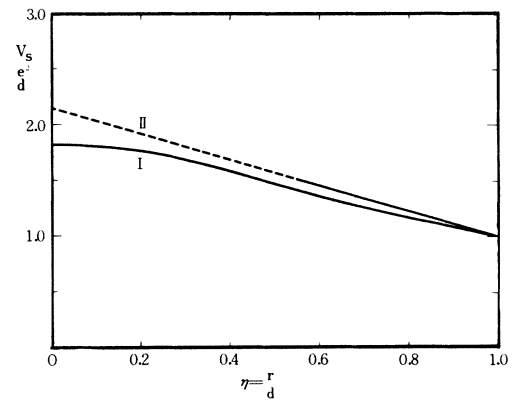

FIG. 1. Two screening potentials V_s as functions of η, the interparticle distance r measured in units of the nearest-neighbor distance d for the triangular lattice. I represents the screening potential in the relaxed lattice model (8); II, the molecular-dynamics result (9) in the liquid phase. The dashed line of the liquid-screening potential for $0 \leq \eta \leq 0.55$ is an extrapolation.

satisfies the conditions

$$V_{\rm eff}(d)=0 \ , \quad \left[\frac{dV_{\rm eff}(r)}{dr}\right]_{r=d}=0 \ , \tag{10}$$

at the equilibrium position $r=d$. The former condition arises from the assumption of perfect screening at the nearest-neighbor distance; the latter implies that the potential takes on an extremum (minimum) value there. Assuming linearity (2) for the screening potential, we obtain from (10),

$$c_1=(\tfrac{1}{2}c_0)^2 \ , \quad c_0=2a/d \ . \tag{11}$$

The former is identical to (3); the latter gives $c_0=1.0501$ for a triangular lattice. This value is again reasonably close to (4).

We have thus shown that the short-range order observed in the 2D classical one-component plasma is already very close to that predicted in a harmonic-lattice model for Γ as low as 33.1, as manifested by the similarity between the screening potential in the liquid phase and that in the lattice model.

III. VELOCITY AUTOCORRELATION TIME

The velocity autocorrelation time may be calculated from a sum-rule analysis of the dynamic structure factor $S_{\rm inc}(\vec{k},\omega)$ associated with the self-motion of a "tagged" electron

$$S_{\rm inc}(\vec{k},\omega)=\frac{1}{2\pi}\int_{-\infty}^{\infty}dt\,\langle\exp\{-i\vec{k}\cdot[\vec{r}_1(t)-\vec{r}_1(0)]\}\rangle e^{i\omega t} \ , \tag{12}$$

where $\vec{r}_1(t)$ is the position of the electron; $\langle\ \rangle$ denotes a statistical average. Defining the frequency moments of $S_{\rm inc}(\vec{k},\omega)$ by

$$\langle\omega^l\rangle_{\rm inc}\equiv\int_{-\infty}^{\infty}d\omega\,\omega^l S_{\rm inc}(\vec{k},\omega) \ , \tag{13}$$

one calculates with the aid of the rigorous equation of motion in the many-particle system[5,6]

$$\Omega^2\equiv\frac{\langle v_{1x}^2\rangle}{\langle v_{1x}^2\rangle}=\frac{\langle\omega^4\rangle_{\rm inc}}{\langle\omega^2\rangle_{\rm inc}}-3\langle\omega^2\rangle_{\rm inc}$$
$$=-\frac{\rho e^2}{m}\int d\vec{r}\left[\frac{\partial}{\partial x}\frac{1}{r}\right]\left[\frac{\partial}{\partial x}g(r)\right] \ . \tag{14}$$

Here ρ is the average number of electrons in a unit "volume" of the system; the x axis is chosen in the direction of $\vec{k}$; v_{1x} and $\dot{v}_{1x}$ are the velocity and the acceleration of the tagged electron in the x direction. It is clear from the definition of (14) that Ω^{-1} corresponds to the velocity autocorrelation time of an electron.

To examine the validity of the use of (14) for comparison with the experimental values of ZBG, we have carried out numerical integration of (14) by substituting the exact molecular-dynamics[2] and Monte Carlo[4] values of $g(r)$. The result is shown in Table I. The measured values τ_c of the velocity autocorrelation time by ZBG have been interpolated or slightly extrapolated to make a comparison at the same values of Γ where the molecular-dynamics[2] or Monte Carlo[4] data exist. The agreement is within the experimental error of ZBG ($\pm10\%$). Hence, this comparison provides additional confirmation that the τ_c of ZBG corresponds to Ω^{-1} defined by (14).[14]

To obtain an analytical expression of (14) for a 2D electron liquid ($\rho=n$) in the harmonic-lattice model, we use the radial distribution function (1) as given by (2) and (11) for the short-range domain $r\leq d$. For $r>d$, the radial distribution funtion generally exhibits a damped-oscillatory behavior around unity. Contributions from the peaks and troughs of $g(r)$ tend to cancel each other in the integration of (14). We may thus take

$$g(r)=\begin{cases}\exp\left[-\dfrac{e^2}{k_BTD}\left(\dfrac{d}{r}-2+\dfrac{r}{d}\right)\right] & (r\leq d) \ , \\ 1 \quad (r>d) \ , \end{cases} \tag{15}$$

as an approximate expression, to be substituted in (14); the result for $\Gamma\gg1$ is

$$\Omega^2=\frac{\pi e^2 n^{3/2}}{\alpha m}\left(1+\frac{\alpha^{1/2}\pi^{3/4}}{2\Gamma^{1/2}}\right)$$
$$=0.66\omega_0^2(1+1.223\Gamma^{-1/2}) \ , \tag{16}$$

where $\alpha=1.0746$.

The theoretical values Ω^{-1} of the velocity autocorrelation time are computed from (16) for the values of the electron density studied by ZBG; the

TABLE I. Comparison of the interpolated or extrapolated experimental values τ_c of the velocity autocorrelation time by Zipfel *et al.* (Ref. 1) and the molecular-dynamics (Ref. 2) and Monte Carlo (Ref. 4) values based on the fundamental relationship (14). Temperature is fixed at 1.2 K.

Γ	τ_c (10^{-11} sec)	Ω^{-1} (10^{-11} sec)
7.1	16.0	17.5[a]
15.8	5.1	5.5[a]
22.4	3.2	3.3[a]
33.1	1.9	1.9[b]
46.8	1.00	1.08[b]
50.0	0.95	1.01[a]

[a]Reference 4.
[b]Reference 2.

TABLE II. Comparison of the measured values τ_c of the velocity autocorrelation time by Zipfel *et al.* (Ref. 1) and the theoretical values Ω^{-1} based on a harmonic-lattice model (16).

n (10^8 cm^{-2})	Γ	τ_c (10^{-11} sec)	Ω^{-1} (10^{-11} sec)
0.15	9	9.9	13.1
0.20	11	7.2	10.6
0.51	17	4.8	5.4
1.4	29	2.1	2.7
2.2	36	1.4	1.9

results are listed in Table II together with the measured values of τ_c. Here we observe a good correspondence between the two sets of values. It is also proved that the velocity autocorrelation time in an electron liquid is, in fact, intimately related to the harmonic-oscillator frequency ω_0, as pointed out by ZBG.

IV. CONCLUDING REMARKS

We have shown that the harmonic-lattice model correctly accounts for the salient features of the radial distribution function in the 2D electron liquid obtained from the molecular-dynamics computations. The measured values of the velocity autocorrelation time are explained consistently in terms of such a lattice model. These results strongly indicate that the short-range order in the 2D classical plasma in its liquid phase is already very much like that in its lattice phase.

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[13]The linear relationship (2) of the screening potential does not hold in the vicinity of $\eta=0$; its expansion takes the form $a_0-a_1\eta^2+\cdots$ there. We here intend to remark on similarity in magnitude between the two. These errors involved in the use of (2) around $\eta=0$ do not affect subsequent calculation leading to (16).
[14]One might argue that the actual shapes of the absorption line contain features much richer than the reported values of the velocity autocorrelation time deduced from the experimental linewidths; information on the velocity autocorrelation function would be obtained from such a lineshape measurement. When results of such a measurement become available, it may become necessary to reexamine the validity of the use of (14), which is based on the short-time behavior of the velocity autocorrelation function.