Compressibility sum rule for the two-dimensional electron gas

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The authors establish formulas for the isothermal compressibility and long-wavelength static density-density response function of a weakly correlated two-dimensional electron gas in the $1 \ll \beta\varepsilon_F < \infty$ and $0 \leqslant \beta\varepsilon_F \ll 1$ degeneracy domains; $\beta\varepsilon_F = \pi n \hbar^2/(m k_B T)$. The calculation of the pressure in the former domain is based on the Isihara-Toyoda formula [A. Isihara and T. Toyoda, Phys. Rev. B **21**, 3358 (1980)] for the exchange-correlation energy at finite temperature. The pressure calculation in the latter domain is based on the Totsuji classical cluster-expansion formula for the correlation energy [H. Totsuji, J. Phys. Soc. Jpn. **40**, 857 (1976); Phys. Rev. A **19**, 889 (1979)].

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Satisfaction of the compressibility sum rule is recognized as an important test of the reliability of model static and dynamical theories of Coulomb systems in a strongly correlated (liquid) phase. The system of interest in this Brief Report is the two-dimensional electron gas (2DEG), an idealized model in which electronic motions in a uniform positive background are restricted to a two-dimensional plane of zero thickness; the electrons interact via the $1/r$ Coulomb potential, r being the in-plane separation distance. Examples of two-dimensional laboratory systems that the 2DEG emulates are (i) electrons trapped on the free surface of liquid helium [1,2,3], (ii) electron arrays on a thin helium film coating a dielectric substrate [3], and (iii) 2D electron states at the interface between GaAs and $Al_xGa_{1-x}As$. [2]

Compressibility sum rules for the static screened density response function $\chi_{sc}(\mathbf{q}) \equiv \chi_{sc}(\mathbf{q},\omega=0)$ have been formulated for the correlated 2DEG in the zero-temperature quantum and classical domains [4]. They have yet to be formulated, however, for arbitrary values of the 2D degeneracy parameter $\beta\varepsilon_F = \pi n \hbar^2/(m k_B T)$ owing to the lack of information about the internal energy. 2DEG internal energy calculations at low temperatures in the neighborhood of $T=0$ are nevertheless available in the weak coupling regime [5], making it possible to formulate the compressibility rule for $1 \ll \beta\varepsilon_F < \infty$. This is one goal of this Brief Report. The other is to formulate the 2D-compressibility rule for the weakly degenerate domain $0 \leqslant \beta\varepsilon_F \ll 1$ in the neighborhood of the classical limit also in the weak coupling regime.

The compressibility sum rule states that at long wavelengths the exact screened density response function is determined by the isothermal compressibility $K_T = [n(\partial P/\partial n)_T]^{-1}$:

$$\chi_{sc}(q \to 0) = -n^2 K_T, \tag{1}$$

For noninteracting charges, evaluation of the compressibility results in the familiar 2D static Lindhard function at long wavelengths:

$$\chi_0(q \to 0, \omega=0) = -n^2 K_T^0 = -\frac{n}{\varepsilon_F}(1 - e^{-\beta\varepsilon_F}). \tag{2}$$

For interacting charges, the calculation of K_T begins by specifying the total average energy per particle,

$$\langle E\rangle(n,T) = \langle E_{\mathrm{kin}}\rangle_0(n,T) + \langle E_x\rangle(n,T) + \langle E_c\rangle(n,T). \tag{3}$$

expressed in terms of the average kinetic energy per particle of a noninteracting system,

$$\langle E_{\mathrm{kin}}\rangle_0(n,T) = \frac{1}{\varepsilon_F}\int_0^\infty d\varepsilon \frac{\varepsilon}{1+\exp[\beta(\varepsilon-\mu_0)]}, \tag{4}$$

and $\langle E_x\rangle(n,T)$ and $\langle E_c\rangle(n,T)$, the Hartree-Fock (HF) exchange and correlation energies per particle.

Addressing first the $\langle E_{\mathrm{kin}}\rangle_0$ kinetic energy contribution, the right-hand side of Eq. (4) can be cast in a more tractable form by observing that $\langle E_{\mathrm{kin}}\rangle_0$ satisfies the initial value problem

$$\left(\frac{\partial}{\partial n} + \frac{1}{n}\right)\langle E_{\mathrm{kin}}\rangle_0(n,T) = \frac{\pi\hbar^2}{m}\frac{1}{1-\exp(-\beta\varepsilon_F)}, \tag{5a}$$

$$\langle E_{\mathrm{kin}}\rangle_0(n \to 0,T) \to \frac{1}{\beta}k_B T, \tag{5b}$$

where the chemical potential μ_0 has been eliminated in favor of the 2D Fermi energy $\varepsilon_F = \pi n \hbar^2/m$ via the 2DEG relation for noninteracting particles [6(a)]

$$\beta\mu_0+\ln[1+\exp(-\beta\mu_0)]=\beta\varepsilon_F. \tag{6}$$

The uniqueness of the solution to Eq. (5),

$$\langle E_{\rm kin}\rangle_0(n,T)=\frac{1}{\varepsilon_F}\int_0^{\varepsilon_F}dx\,\frac{x}{1-\exp(-\beta x)}, \tag{7}$$

guarantees that Eqs. (7) and (4) are one and the same. It should be emphasized that this latter more tractable kinetic energy formula holds only in two dimensions. In the domain $1\ll\beta\varepsilon_F<\infty$, a denominator expansion of Eq. (7) in a geometric series gives [7]:

$$\begin{aligned}\langle E_{\rm kin}\rangle_0(n,T)&\cong\frac{1}{\varepsilon_F}\int_0^{\varepsilon_F}dx\,x\sum_{p=0}^{\infty}\exp(-p\beta x)\\&=\frac{\varepsilon_F}{2}+\frac{1}{\varepsilon_F}\sum_{p=1}^{\infty}\int_0^{\varepsilon_F}dx\,x\exp(-p\beta x)\\&=\frac{\varepsilon_F}{2}+\frac{1}{\beta^2\varepsilon_F}\sum_{p=1}^{\infty}\frac{1}{p^2}=\frac{\varepsilon_F}{2}\left[1+\frac{\pi^2}{3(\beta\varepsilon_F)^2}\right].\end{aligned} \tag{8}$$

The expression (8) is in agreement with Eq. (8.3) of Ref. [5], derived by application of the Sommerfeld expansion[6(b)] to the free-electron grand-partition function. In the weakly degenerate domain $0\leqslant\beta\varepsilon_F\ll1$, the 2D expression

$$\langle E_{\rm kin}\rangle_0(n,T)\cong\frac{1}{\beta}\left[1+\frac{1}{4}\beta\varepsilon_F\right] \tag{9}$$

results from expanding $[1-\exp(-\beta x)]$ in Eq. (7) in a Taylor series about $\beta x=0$ and retaining only the lowest-order $O(\beta\varepsilon_F)$ degeneracy correction.

We next consider the 2D-exchange contribution. In the domain $1\ll\beta\varepsilon_F<\infty$, the Isihara-Toyoda[5] formula for the finite-temperature correction to the HF exchange energy,[8] $\langle E_x\rangle(n,T=0)=-0.6(e^2/a)$, can be written in the form

$$\begin{aligned}\langle E_x\rangle(n,T)&=\langle E_x\rangle(n,T=0)\\&\quad+\frac{2\pi}{(\beta\varepsilon_F)^2}\left[0.0228-\frac{1}{12\sqrt{2}}\ln(\beta\varepsilon_F)\right]\frac{e^2}{a},\end{aligned} \tag{10}$$

where $a=1/\sqrt{\pi n}$ is the 2D interparticle distance. In the opposite domain $0\leqslant\beta\varepsilon_F\ll1$, the 2D-exchange energy is reasonably well approximated by the asymptotic formula[9]

$$\langle E_x\rangle(n,T)\approx0.632\sqrt{\beta\varepsilon_F}\langle E_x\rangle(n,T=0). \tag{11}$$

For the 2D-correlation energy, the Ref. [5] calculation provides

$$\begin{aligned}\langle E_c\rangle(n,T)&=[-0.3496+0.865r_s-0.173r_s\ln r_s]\frac{e^2}{2a_0}\\&\quad+\frac{4\pi}{(\beta\varepsilon_F)^2}\left[-0.1824-0.0297\ln\beta\varepsilon_F\right.\\&\quad\left.+\frac{1}{24\pi}(\ln\beta\varepsilon_F)^2\right]\end{aligned} \tag{12}$$

for the domain $1\ll\beta\varepsilon_F<\infty$; $r_s=a/a_0\ll1$ (a_0 is the Bohr radius). The first right-hand-side member of (12) is the correlation energy at zero temperature; the second right-hand-side member is the finite-temperature correction. In the weakly degenerate quantum domain $0\leqslant\beta\varepsilon_F\ll1$, while the $O(\hbar^2)$ quantum correction $\Delta\langle E_c\rangle$ to the classical correlation energy was calculated some time ago for the 3D one-component plasma (OCP),[10] it has yet to be determined for the 2D OCP. If this correction is sufficiently small, then the *classical* Ref. [11] 2D cluster-expansion formula,

$$\langle E_c\rangle(n,T)=\frac{\gamma}{2\beta}[\ln(2\gamma)+0.1544]+O[(\gamma\ln\gamma)^2],$$

$$(\gamma=2\pi n\beta^2e^4\ll1) \tag{13}$$

should reasonably well represent the correlation energy in the $0\leqslant\beta\varepsilon_F\ll1$ domain. The error incurred by invoking the classical formula (13) can be roughly estimated by conjecturing that the Ref. [10] $\Delta\langle E_c\rangle|_{3\rm D}=-A_{3\rm D}(\varepsilon_F)_{3\rm D}\Gamma_{3\rm D}$ quantum correction to the 3D OCP correlation energy, expressed in terms of the classical coupling parameter $\Gamma_{3\rm D}=\beta Z^2e^2/a_{3\rm D}$, has the same form $\Delta\langle E_c\rangle|_{2\rm D}=-A_{2\rm D}\varepsilon_F\Gamma_{2\rm D}=-A_{2\rm D}\varepsilon_F\sqrt{\gamma/2}$ in two dimensions; $A_{3\rm D}=(1/2\pi)\times(16\pi/81)^{1/3}$ is a geometric constant; its 2D counterpart $A_{2\rm D}$ is also expected to be of order unity at most. Then ordering the smallness parameters so that $\beta\varepsilon_F\to0$ at the same rate as or faster than $\gamma\to0$ (to ensure the recovery of the classical Debye correlation energy in the $\hbar\to0$ limit), we see that the leading quantum correction is $O(\beta\varepsilon_F/\sqrt{\gamma})$ times smaller than the γ-dependent contributions to Eq. (13). Observe, however, that this correction is *always* $O(\sqrt{\beta\varepsilon_F})$ times smaller than the exchange energy (11), independently of the ordering of the smallness parameters. Thus, the rationale for leaving out of Eq. (13) the negligibly small quantum correction [and, consequently, the higher-order $(\gamma\ln\gamma)^2$ classical term], while at the same time retaining the exchange correction in the compressibility calculation below. This completes the specification of the total energy per particle $\langle E\rangle$ of the interacting system.

We now proceed to the calculation of the pressure from the well-known thermodynamic formula[12]

$$\left(\frac{\partial}{\partial\beta}\beta P\right)_n=n^2\left(\frac{\partial}{\partial n}\langle E\rangle\right)_\beta \tag{14}$$

$$= -n\langle E_{\rm kin}\rangle_0 + \frac{n\varepsilon_F}{1-\exp(-\beta\varepsilon_F)} + n^2\left(\frac{\partial}{\partial n}[\langle E_x\rangle + \langle E_c\rangle]\right)_\beta . \qquad (15)$$

Here, it is instructive to isolate for the moment the contribution from the free-particle kinetic energy; integrating the first two right-hand-side members of Eq. (15) over β gives

$$\beta P_0 = n - n\int_0^\beta \langle E_{\rm kin}\rangle_0(n,\beta')d\beta' + n\varepsilon_F\int_0^\beta \frac{d\beta'}{1-\exp(-\beta'\varepsilon_F)} . \qquad (16)$$

Differentiating Eq. (16) and making use of the differential equation (5a) for the noninteracting 2D Coulomb gas, one readily obtains

$$\left(\frac{\partial P_0}{\partial n}\right)_\beta = \frac{\varepsilon_F}{1-\exp(-\beta\varepsilon_F)}, \qquad (17)$$

consistent with the long-wavelength Lindhard expression (2) for arbitrary degeneracy.

We can now construct the 2DEG equations-of-state in the two domains $1 \ll \beta\varepsilon_F < \infty$ and $0 \leq \beta\varepsilon_F \ll 1$. On substituting the expressions from Eqs. (8), (10), and (12) into Eq. (14) and integrating, one readily obtains for the first domain:

$$P - P_0 = \frac{n}{2}\langle E_x\rangle(n,T=0) - \frac{ne^2}{4a_0}[0.692 r_s - 0.173 r_s \ln r_s] + \frac{\pi n e^2}{a(\beta\varepsilon_F)^2}[0.0095 - 0.1768\ln\beta\varepsilon_F] + \frac{2\pi n e^2}{a_0(\beta\varepsilon_F)^2} \times[-0.368 - 0.0328\ln\beta e_F + 0.0265(\ln\beta\varepsilon_F)^2]; \qquad (18)$$

$$P_0 = n\langle E_{\rm kin}\rangle_0(n,\beta) = \frac{n\varepsilon_F}{2}\left[1+\frac{\pi^2}{3(\beta\varepsilon_F)^2}\right] \quad (1 \ll \beta\varepsilon_F < \infty). \qquad (19)$$

The first two right-hand-side members of Eq. (18) are identified as the exchange-correlation part of the pressure at $T = 0$.[4] The third and fourth right-hand-side members are their respective low-temperature corrections. Repeating this procedure for the weakly degenerate domain and dropping the $O(\gamma \ln \gamma)^2$ term in Eq. (13), one obtains

$$P - P_0 = \tfrac{1}{2} n\langle E_c\rangle(n,T) + \tfrac{2}{3} n\langle E_x\rangle(n,T), \qquad (20)$$

$$P_0 \cong n\langle E_{\rm kin}\rangle_0(n,\beta) \cong \frac{n}{\beta}[1+\tfrac{1}{4}(\beta\varepsilon_F)] \quad (0 \leq \beta\varepsilon_F \ll 1). \qquad (21)$$

The first right-hand-side member of Eq. (20) is given by Eq. (13) and the second by Eq. (11).

The inverse compressibility formulas

$$\frac{1}{K_T} = n\varepsilon_F + \tfrac{3}{4} n\langle E_x\rangle(n,T=0) - \frac{ne^2}{8a_0}(0.865 r_s - 0.173 r_s \ln r_s) + \frac{\pi n e^2}{2a(\beta\varepsilon_F)^2}(-0.363 + 0.177\ln\beta\varepsilon_F) + \frac{2\pi n e^2}{a_0(\beta\varepsilon_F)^2}[0.335 + 0.086\ln\beta\varepsilon_F - 0.0265(\ln\beta\varepsilon_F)^2] \quad (1 \ll \beta\varepsilon_F < \infty), \qquad (22)$$

$$\frac{1}{K_T} = \frac{n}{\beta}(1+\tfrac{1}{2}\beta\varepsilon_F) + \frac{\gamma n}{2\beta}(\ln 2\gamma + 0.654) + (0.632\sqrt{\beta\varepsilon_F})\tfrac{4}{3} n\langle E_x\rangle(n,T=0) \quad (0 \leq \beta\varepsilon_F \ll 1), \qquad (23)$$

then follow from Eqs. (18)–(21).

To facilitate comparison with mean field theories, we introduce the local field correction $G(\mathbf{q})$ via

$$\chi_{\rm sc}(\mathbf{q}) = \frac{\chi_0(\mathbf{q})}{1+\nu(q)G(\mathbf{q})\chi_0(\mathbf{q})}, \qquad (24)$$

where $\nu(q) = 2\pi e^2/q$ is the Fourier transform of the 2D Coulomb potential energy. From Eqs. (1), (2), (22), (23), and (24), one obtains

$$G(q\to 0) = \frac{1}{\nu(q)\chi_0(q\to 0)}\left(\frac{K_T^0}{K_T} - 1\right) = \frac{q}{k_F}\left\{\frac{1}{\pi} + r_s^2(0.0765 - 0.0153\ln r_s) + \frac{1}{(\beta\varepsilon_F)^2}(0.4032 - 0.1963\ln\beta\varepsilon_F) - \frac{r_s}{(\beta\varepsilon_F)^2} \times[1.489 + 0.3815\ln\beta\varepsilon_F + 0.1179(\ln\beta\varepsilon_F)^2]\right\} \quad (1 \ll \beta\varepsilon_F < \infty), \qquad (25)$$

$$G(q\to 0) = \frac{q}{\kappa}\left\{-\frac{\gamma}{2}(\ln 2\gamma + 0.6544) - (0.632\sqrt{\beta\varepsilon_F})\tfrac{4}{3}\beta\langle E_x\rangle(n,T=0)\right\} \quad (0 \leq \beta\varepsilon_F \ll 1); \qquad (26)$$

$k_F = \sqrt{2\pi n}$ is the Fermi wave number and $\kappa = 2\pi e^2\beta n$ is the 2D Debye wave number. The first two right-hand-side members of Eq. (25) comprise the zero-temperature exchange-correlation contribution; the last two are the respective temperature corrections. Equation (26) exhibits the exchange correction to the classical correlation energy. Observe that the respective pure quantum and classical local field corrections of Ref. [4] are indeed recovered in the zero-temperature and classical limits.

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[7] The $\cong$ sign in Eq. (8) is there to indicate that care must be taken at $x=0$ where the expansion in a geometric series breaks down. To deal with this, rewrite Eq. (7) as:

$$\langle E_{\rm kin}\rangle_0=\varepsilon_F\int_0^1 dy\,\frac{y}{1-\exp(-\beta\varepsilon_F y)}.$$

Then divide the interval [0, 1] into two subintervals, one going from 0 to δ and the other from δ to 1, where δ can be chosen arbitrarily small. Integration over the first subinterval gives δ/β, which vanishes in the limit $\delta=0$. Integration over the second subinterval gives

$$\frac{\varepsilon_F}{2}(1-\delta^2)+\frac{\delta}{\beta}\sum_{p=1}^{\infty}\frac{1}{p}\exp(-p\beta\varepsilon_F\delta)$$

$$+\frac{1}{\beta^2\varepsilon_F}\sum_{p=1}^{\infty}\frac{1}{p^2}\exp(-p\beta\varepsilon_F\delta).$$

For $\delta\ll 1/(\beta\epsilon_F)\ll 1$, we then see that

$$\lim_{\delta\to 0}\delta\sum_{p=1}^{p_{\rm max}}\frac{1}{p}\exp(-p\beta\varepsilon_F\delta)\ll\frac{1}{\beta\varepsilon_F}\sum_{p=1}^{p_{\rm max}}\frac{1}{p^2}\exp(-p\beta\varepsilon_F\delta)$$

for $p_{\rm max}\ll 1/(\beta\varepsilon_F\delta)$ thereby guaranteeing the Eq. (8) outcome in the $\delta=0$ limit.

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