

Force between jellium films at small separation in the linearized Thomas-Fermi approximation

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This Brief Report extends and complements the work of March and Paranjape [Phys. Rev. B **30**, 3131 (1984)] on the interaction between metallic systems, in various ways. Their analysis for jellium half-spaces, using the linearized Thomas-Fermi approximation, is generalized in the case of film geometries. This is essential in order to account for the intrinsic instability of jellium. Comparison of our results with exact (nonlinear) Thomas-Fermi results reveals successes and failures of the linearized Thomas-Fermi approximation. It is also pointed out that the generalization of the work of March and Paranjape in the case of arbitrary densities is provided by a known exact formula for the force between jellium films at small separation.

March and Paranjape¹ have recently studied the force $f(z)$, between jellium half-spaces a small distance z apart, using a linearized Thomas-Fermi approximation for the electrons at high densities. Their aim was to suggest a relationship between a linear term in z in their expression for the force between jellium systems and the elastic-cleavage force in real metals,

$$f_{\text{elastic}}(z) = -Az, \text{ for } z \rightarrow 0. \quad (1)$$

This elastic force plays an important role in a universal model for the surface energy of metals proposed recently by Kohn and Yaniv,² following earlier work by Zaremba.³

Here, we first generalize the model of March and Paranjape in the case of macroscopic jellium *films* bounded by vacuum. This is essential in order to recover the actual nonzero value of $f(0^+)$ responsible for the well-known instability of bulk jellium. This limiting force at vanishing separation, which is just the bulk electronic pressure, is indeed related to surface properties of jellium through the exact sum rule^{4,5} ($-e$ = electron charge)

$$f(0^+) = p = -e\rho_0\Delta V, \quad (2)$$

where ρ_0 is the uniform jellium density and ΔV is the electrostatic potential at the edge of a jellium half-space in vacuum relative to its bulk value. In contrast to this, the analysis of March and Paranjape yields $f(0^+) = 0$ because their model does not incorporate the effect of *external* boundaries of a jellium system in which a narrow planar vacuum gap of width z has been created.

By applying the linearized Thomas-Fermi approximation of Ref. 1 in the case of macroscopic films we obtain

$$f(0^+) = \frac{5}{6}p, \quad (3)$$

instead of Eq. (2). This shows that linearization of the Thomas-Fermi theory does not provide an internally consistent treatment of the limiting force $f(z \rightarrow 0^+)$.⁶ In this connection, it is comforting to note that the nonlinear Thomas-Fermi theory for an *isolated* planar jellium surface⁷ is compatible with Eq. (1). This is demonstrated by recalling the exact Thomas-Fermi expression for the electrostatic potential in the vacuum region of a jellium half-space con-

finied to the region $x < 0$:⁷

$$V(x) = \frac{400\epsilon_F}{e(x/\lambda + c)^4}, \quad (4)$$

where $c = \frac{2}{3}(15)^{3/4}$, $\lambda = (3\pi/8k_F)^{1/2}$, and ϵ_F and k_F are the Fermi energy and the Fermi wave vector, respectively. Here the potential deep inside the metal has been taken to be $V(-\infty) = e^{-1}\epsilon_F$. From these results one obtains

$$\Delta V = V(0) - V(-\infty) = -\frac{2}{3}e^{-1}\epsilon_F,$$

and by recalling the familiar expression for the pressure at high densities, $p = \frac{2}{3}\rho_0\epsilon_F$, one finds that Eq. (2) is identically verified in this case.

The main interest of March and Paranjape lies in the evaluation of the linear term in z in the expression for the force at small separation,⁸ using the linearized Thomas-Fermi approximation. This term is, however, given exactly at arbitrary density by^{4,9}

$$f(z) = p - az + \dots, \quad (5a)$$

$$a = 2e^2\rho_0^2 \int \frac{dk}{k^2\epsilon(k)}, \quad (5b)$$

where $\epsilon(k)$ is the static-bulk dielectric function. By inserting the Thomas-Fermi expression, $\epsilon(k) = 1 + q^2k^{-2}$, valid at high densities, we obtain

$$a \equiv a_{\text{TF}} = \frac{1}{3}\rho_0\epsilon_F q, \quad (6)$$

which coincides with the result obtained by March and Paranjape using the linearized Thomas-Fermi model. Here q^{-1} is the Thomas-Fermi screening length given by

$$q^2 = \frac{6\pi\rho_0e^2}{\epsilon_F}. \quad (7)$$

The Eq. (6) will be rederived below in the case of film geometries, again by using linearized Thomas-Fermi theory.

The attractive nature of the extra force $-az$, which arises when a jellium system is cleaved along a plane and the two parts are pulled slightly apart, is understandable: this physical operation leads to a readjustment of the electron distri-

bution towards lower densities and thus to a lowering of the electronic pressure in the vicinity of the cleavage plane. This fact, as well as the initial linear variation of $f(z)$, is the basis for the conjecture by March and Paranjape of the existence of a relation between the linear term in Eq. (5a) and the elastic-cleavage force (1) in real solids, in spite of the intrinsic instability of jellium expressed by the repulsive force $f(0^+) = p$.

In the remainder of this paper, we sketch our derivation of $f(z)$ for two identical-macroscopic jellium films separated by a small distance z . The two interacting films, which are unbounded in the y and z directions, are represented schematically in Fig. 1. In the linearized Thomas-Fermi approximation the electrostatic potential $V(x)$ and the electron density $\rho(x)$, are related by the equations

$$\frac{d^2 V(x)}{dx^2} = \begin{cases} -4\pi e[\rho_0 - \rho(x)], & \text{regions 1, 3} \\ 4\pi e\rho(x), & \text{regions 2, 4, 5} \end{cases} \quad (8a)$$

$$\rho(x) = \rho_0 \left(1 + \frac{3e}{2\epsilon_F} V(x) \right) \quad (9)$$

The potential and its first derivative are required to be con-

$$V(x) = \begin{cases} -\frac{2\epsilon_F}{3e} [1 + (e^{-qL} - e^{-qz/2}) \cosh(qx)], & -\frac{z}{2} \leq x \leq \frac{z}{2} \\ -\frac{\epsilon_F}{3e} \left\{ e^{q(x-L)} + \left[e^{-qL} + 2 \sinh\left(\frac{qz}{2}\right) \right] e^{-qx} \right\}, & \frac{z}{2} \leq x \leq L \\ -\frac{2\epsilon_F}{3e} \left\{ 1 + \left[\sinh\left(\frac{qz}{2}\right) - \sinh(qL) \right] e^{-qx} \right\}, & x \geq L \end{cases} \quad (10a)$$

$$V(x) = \begin{cases} -\frac{\epsilon_F}{3e} \left\{ e^{q(x-L)} + \left[e^{-qL} + 2 \sinh\left(\frac{qz}{2}\right) \right] e^{-qx} \right\}, & \frac{z}{2} \leq x \leq L \end{cases} \quad (10b)$$

$$V(x) = \begin{cases} -\frac{2\epsilon_F}{3e} \left\{ 1 + \left[\sinh\left(\frac{qz}{2}\right) - \sinh(qL) \right] e^{-qx} \right\}, & x \geq L \end{cases} \quad (10c)$$

Finally, the force per unit area exerted by one jellium film on the other is simply^{4,10}

$$f(z) = -e\rho_0 \int_{z/2}^L \frac{dV}{dx} dx, \quad (11a)$$

$$= -e\rho_0 [\Delta V - \Delta V(z)], \quad (11b)$$

where

$$\Delta V = V(L) - V, \quad (12a)$$

$$\Delta V(z) = V\left(\frac{z}{2}\right) - V, \quad (12b)$$

are the electrostatic potentials at the jellium edges relative to the potential V , in the bulk region deep inside each film. Since the film thicknesses are macroscopic there is no electrostatic coupling between the dipole layers near $x = z/2$ and $x = L$, so that ΔV is given by Eq. (2). On the other hand, the explicit evaluation of the force (11a), using Eq. (10b),

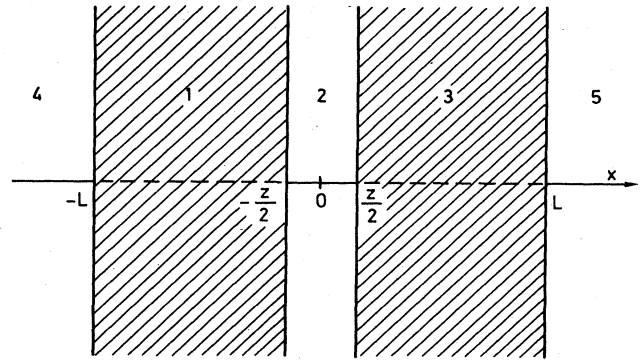


FIG. 1. Showing regions 1 and 3 occupied by jellium films, a distance z apart, placed in vacuum.

tinuous at the edges of the various regions of Fig. 1, and $V(x)$ is required to decay exponentially beyond the exterior-film boundaries at $x = \pm L$. The details of the calculation of $V(x)$ are similar to those given in Ref. 1 for jellium half-spaces. For brevity's sake we only list the final solutions in regions 2, 3, and 5. These are

leads to

$$f(z) = \frac{1}{3}\rho_0\epsilon_F [e^{-qz} + e^{-qL}(e^{-qL} - 2e^{-qz/2})], \quad (13a)$$

$$= \frac{5}{6}p [1 - qz + O(z^2)], \quad qz \ll 1, \quad qL \gg 1, \quad (13b)$$

where p is the high-density electronic pressure. The significance of the two terms in Eq. (13b) and their comparison with the exact result, Eqs. (5a) and (5b), has been fully discussed above. In particular, the coefficient of the linear term coincides with the exact result of Eq. (6).

Finally, we recall that while the validity of (6) is restricted to high densities, the behavior of a at arbitrary density could be obtained from Eqs. (5a) and (5b). Therefore, if one accepts the argument of March and Paranjape¹ concerning the relation between a and the parameter A , describing the elastic force at short distances in real metals, one could use these expressions to discuss the form of A over the entire density range.

¹N. H. March and B. V. Paranjape, Phys. Rev. B 30, 3131 (1984).

²W. Kohn and A. Yaniv, Phys. Rev. B 20, 4948 (1979).

³E. Zaremba, Solid State Commun. 23, 347 (1977).

⁴H. F. Budd and J. Vannimenus, Phys. Rev. Lett. 31, 1218; 31,

1430(E) (1973).

⁵J. Heinrichs and N. Kumar, Phys. Rev. B 12, 802 (1975); Solid State Commun. 18, 961 (1976).

⁶See, especially, the Erratum in Ref. 4.

⁷See, e.g., the reviews by N. D. Lang, in *Solid State Physics*, edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic, New York, 1973), Vol. 28; A. Sommerfeld and H. Bethe, in *Handbuch der Physik*, 2nd ed., edited by H. Geiger and K. Scheel, (Springer-Verlag, Berlin, 1933), Vol. 24, Sec. 14.

⁸In Refs. 1, 2, and 4 one introduces the quantity $F(z) = -f(z)$ but

here we follow Refs. 3 and 5 in dealing with the force $f(z)$, itself.

⁹J. Vannimenus and H. F. Budd, *Solid State Commun.* 17, 1291 (1975).

¹⁰Note that our general straightforward evaluation of the force avoids considerations about the virial theorem for inhomogeneous systems developed in Ref. 1.