



COMPARISON OF THE EFFECTIVE INTERACTIONS OF
ELECTRON LIQUIDS IN TWO AND THREE DIMENSIONS

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ABSTRACT

The effective interactions of electron liquids in two and three dimensions, which are constructed from the Monte Carlo data for the spin-dependent ground-state energy with the use of the compressibility and spin-susceptibility sum rules for response functions, are compared. The density dependences of the spin-parallel and antiparallel effective interactions in two dimensions are found to be remarkably similar to those in three dimensions over the entire liquid phase.

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Electron liquids serve as model systems for strongly-coupled Coulomb systems, which are realized under laboratory or astrophysical conditions. Such strongly-coupled Coulomb systems are represented by bulk metallic electrons, dense fusion plasmas, and ions in large planets, white dwarfs, and neutron stars in the case of three dimensions (3D), and by electron layer(s) in Si-MOSFETs, GaAs/AlGaAs and other semiconductor heterostructures, and on the surface of liquid helium in the case of two dimensions (2D). The many-body theoretical study of electron liquids in two and three dimensions thus provides a basis for understanding the physical properties of these Coulomb systems.^{1,2} So far the study has been carried out separately for each spatial dimensionality. Apparently, these systems possess certain qualitative similarities. In particular, in the case of degenerate systems in either dimension at high densities, the electrons interact weakly, and the random phase approximation (RPA) gives a satisfactory description of the system; whereas, at low densities, the systems crystallize, with either the body-centered cubic (3D) or triangular (2D) Wigner lattice formed as their ground states. The purpose of the present paper is to compare the ground-state properties of the two systems of different dimensionality and look for similarities and differences. In order to do so, it is necessary to examine some physical quantities which do not depend on the spatial dimensionality explicitly. Recent Monte Carlo calculations have given accurate numerical data on the ground-state properties of electron liquids in two and three dimensions^{3,4}. Subsequently, we have constructed

the dielectric functions and the spin susceptibilities of paramagnetic electron liquids in two and three dimensions at zero temperature in such a way that they are consistent with the Monte Carlo data in terms of the compressibility and the spin-susceptibility sum rules.⁵⁻⁷ In this work, the frequency moment sum rules provide exact relations that the response functions must satisfy, and which may be applied to systems of arbitrary coupling strengths⁸. The formulations in these terms are given such that the dielectric properties of both systems reduce to a small number of density dependent effective interactions. In the present paper, we find these effective interactions particularly suitable for comparing the two systems in order to answer the question as to whether there are any similarities between the systems. We then show that their density dependences of the two systems are strikingly similar.

At zero temperature, the electron system is characterized by only one parameter--the area density $n(2D)$ or volume density $n(3D)$. Equivalently, at zero temperature, the system can be characterized in terms of the dimensionless coupling constant $r_s(dD) \equiv r_0(dD)/a_B$, where $r_0(dD)$ is the mean-particle distance, $r_0(2D) \equiv 1/[\pi n(2D)]^{1/2}$ and $r_0(3D) \equiv [3/4\pi n(3D)]^{1/3}$, and $a_B \equiv \hbar^2/me^2$ is the Bohr radius.⁹ Here, the spatial dimensionality is denoted by "d" as in $n(dD)$, where $d = 2$ or 3 . Currently, the variational and fixed-node Green's function Monte Carlo calculations give the most accurate spin-dependent ground-state energy of these systems for the entire liquid regime. The

discrete Monte Carlo data points may be interpolated for the entire range of densities in the liquid phase,¹⁰ from which the compressibility may be calculated. It is found that, as the density is decreased, the compressibility diverges at $r_s(3D) \cong 5.2$ [$\cong r_s(\kappa, 3D)$]¹¹ and $r_s(2D) \cong 2.03$ [$\cong r_s(\kappa, 2D)$]³ and it becomes negative at lower densities.¹² Furthermore, the systems crystallize at $r_s(3D) \cong 100 \pm 20$ [$\cong r_s(W, 3D)$]⁴ and $r_s(2D) \cong 37 \pm 5$ [$\cong r_s(W, 2D)$].³

The formulation in both dimensions starts with the screened response function of the form⁵⁻⁷

$$\chi_{sc}(q, \omega) = \chi^0(q, \omega) / [1 + v(q)G(q)\chi^0(q, \omega)], \quad (1)$$

and the nonlocal spin susceptibility of the form

$$\chi_p(q, \omega) = -\mu_B^2 \chi^0(q, \omega) / [1 + v(q)G^a(q)\chi^0(q, \omega)], \quad (2)$$

where $v(q)$ [$\cong 2\pi e^2/q$ (2D) and $4\pi e^2/q^2$ (3D)] is the Coulomb interaction, $\chi^0(q, \omega)$ the Lindhard function in d dimensions,¹³ and μ_B the Bohr magneton. The spin-symmetric (antisymmetric) static local-field correction $G(q)$ ($G^a(q)$) takes into account the deviation of electron-electron interactions from those in the RPA. The local-field corrections are closely related to the effective interactions the electrons feel. To obtain these local-field corrections, we first express the effective potentials between electrons of parallel and antiparallel spin as a sum of the bare Coulomb potential and the deviation from it $v^{\uparrow\uparrow, \uparrow\downarrow}(q) = v(q) + f_q^{\uparrow\uparrow, \uparrow\downarrow}$; and define the spin symmetric and antisymmetric

effective potentials as

$$v_{\text{eff}}^{\text{S}}(\mathbf{q}) = (1/2)[v^{\uparrow\uparrow}(\mathbf{q}) + v^{\uparrow\downarrow}(\mathbf{q})] \equiv v(\mathbf{q}) + f_{\mathbf{q}}^{\text{S}}, \quad (3)$$

$$v_{\text{eff}}^{\text{A}}(\mathbf{q}) = (1/2)[v^{\uparrow\uparrow}(\mathbf{q}) - v^{\uparrow\downarrow}(\mathbf{q})] \equiv f_{\mathbf{q}}^{\text{A}}. \quad (4)$$

The local-field corrections are then given as $G^{\text{S},\text{A}}(\mathbf{q}) \equiv -f_{\mathbf{q}}^{\text{S},\text{A}}/v(\mathbf{q})$ with $G^{\text{S}}(\mathbf{q}) \equiv G(\mathbf{q})$.

One easily sees that the screened response function of the form (1) satisfies the f -sum rule⁸. The requirement that the response functions (1) and (2) satisfy the compressibility and spin-susceptibility sum rules determines the long-wavelength limit of the local-field corrections uniquely. Here, the spin-dependent ground-state energy from Monte-Carlo data gives numerical values for both the compressibility and the spin stiffness needed for applying these sum rules. We parametrize the effective interactions in Yukawa form in the Fourier space, $f_{\mathbf{q}}^{\uparrow\uparrow, \uparrow\downarrow}(2\text{D}) = -2\pi e^2/[q^2 + q_{\uparrow\uparrow, \uparrow\downarrow}(2\text{D})^2]^{1/2}$ and $f_{\mathbf{q}}^{\uparrow\uparrow, \uparrow\downarrow}(3\text{D}) = -4\pi e^2/[q^2 + q_{\uparrow\uparrow, \uparrow\downarrow}(3\text{D})^2]$. The parameters $q_{\uparrow\uparrow}$ and $q_{\uparrow\downarrow}$ may be determined from the two sum rules. The $f_{\mathbf{q}}$'s may be made dimensionless by multiplying them by the free-particle density of states $N^0(d,0)/V \equiv (d/2)n(d\text{D})/E_{\text{F}}^0(d\text{D})$, where $V \equiv L^d$ is the volume and $E_{\text{F}}^0(d\text{D})$ the free-particle Fermi energy in d dimensions. In the long-wavelength limit, the dimensionless effective interactions thus become $F^{\text{S}} \equiv \lim_{\mathbf{q} \rightarrow 0} f_{\mathbf{q}}^{\text{S}} N^0(d,0)/V$, etc.¹⁴ The compressibility sum rule then reduces to the form $F^{\text{S}} = \kappa_0/\kappa - 1$, where κ_0 is the free-particle compressibility and κ is the

compressibility calculated from the ground-state energy.

Similarly, the spin-susceptibility sum rule takes the form $\chi^a = \chi_p^0 / \chi_p - 1$, where χ_p^0 is the free-particle spin susceptibility and $\chi_p \equiv \lim_{q \rightarrow 0} \chi_p(q, 0)$.

The density dependence of the effective interactions F in two dimensions calculated in Ref. 7 are plotted in Fig. 1. Since the plot is made for one dimensionless quantity (F^S , for example) against another [$r_s(2D)$], it is possible as well as illuminating to compare the present results with those of the three dimensional case.^{5,6} The density dependences of the F 's in three dimensions are taken¹⁵ from Ref. 5, and are plotted in Fig. 2. From the comparison of Figs. 1 and 2, one finds the following features that are remarkably similar for two and three dimensions:

(i) Both the spin-parallel and spin-antiparallel effective interactions are negative and become stronger approximately linearly as r_s increases.

(ii) For a given value for r_s , the spin-parallel interaction is stronger (in absolute values) than the spin-antiparallel interaction, while the relative difference between the strengths of these interactions becomes smaller as r_s increases.

(iii) Because of (i) and (ii), the spin-symmetric interaction also increases approximately linearly (with negative values) as r_s increases, while the spin-antisymmetric interaction takes on small negative values for the entire range of r_s in the figure and its density dependence is very weak.

In addition to the above overall similarities, one finds the following quantitative differences between two and three dimensions:

(iv) The strengths of the interactions for a given value of r_s are different between two and three dimensions: For a given value of r_s , the effective interaction is stronger in two dimensions than in three dimensions. For example, $F^S = -5.98$ (2D) and $F^S = -2.03$ (3D) for $r_s(2D) = r_s(3D) = 10$, and $F^S = -27.64$ (2D) and $F^S = -9.52$ (3D) for $r_s(2D) = r_s(3D) = 40$. In other words, a given value of the effective interaction is reached with a smaller value of r_s in two dimensions than in three dimensions. For example, $F^S = -5.98$ [$r_s(2D) = 10$] and $F^S = -5.89$ [$r_s(3D) = 26$]; $F^S = -12.96$ [$r_s(2D) = 20$] and $F^S = -12.99$ [$r_s(3D) = 53$].

One thus concludes that the electron-electron correlation is stronger in two dimensions than in three dimensions for a given value of r_s . A similar conclusion has been reached by Jonson¹⁶, who examined the RPA, the Hubbard approximation (HA), and the Singwi-Tosi-Land-Sjölander approximation¹⁷ in two dimensions. He found that the RPA and HA are less satisfactory for two dimensions than for three dimensions because the pair correlation function near zero separation calculated in these two approximations take on larger negative values in two dimensions.

(v) From the above values of the F 's at different densities, one can be more quantitative in comparing the two and three dimensional systems. In particular, as far as the strengths of

the electron-electron correlations are concerned, the two dimensional system at a given value of $r_s(2D)$ corresponds to the three dimensional system at about $r_s(3D) \approx 2.5r_s(2D)$. This ratio ≈ 2.5 is consistent with both the ratio of the coupling strengths where the compressibility diverges

$$r_s(\kappa, 3D)/r_s(\kappa, 2D) \approx 2.6 \quad (5)$$

and the ratio of the Wigner crystallization points^{18,19}

$$r_s(W, 3D)/r_s(W, 2D) = 2.70 \pm 0.65. \quad (6)$$

In summary, the effective interactions of electron liquids in two and three dimensions, which are constructed from the Monte Carlo results for the spin-dependent ground-state energy together with the compressibility and spin-susceptibility sum rules are compared. The strengths of the dimensionless effective interactions are found to be stronger in two dimensions than in three dimensions for the same value of the dimensionless coupling constant $r_s(2D) = r_s(3D)$. More quantitatively, a particular value of the dimensionless effective interaction in two dimensions with the dimensionless coupling constant $r_s(2D)$ is attained for three dimensions at a larger coupling constant $r_s(3D) \approx 2.5r_s(2D)$. It is to be stressed that the present analysis is based on the exact sum rules combined with the accurate Monte Carlo data. While we have parametrized the effective interactions within the framework of our model, the static properties in the long-wavelength limit so far discussed are exact and thus model independent.

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FOOTNOTES

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1. For reviews on two dimensional electron systems, see, e.g.,
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 2. For three dimensional systems see, e.g., K. S. Singwi and
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A. Benjamin, New York, 1966), Vol. I.
 9. The physical quantities in two and three dimensions are
given in N. Iwamoto, Phys. Rev. A 30, 3289 (1984).
 10. The interpolation formula in the Padé form for the

correlation energy of the electron liquid in three dimensions is given by S. H. Vosko, L. Wilk, and M. Nusair (VWN) [Can. J. Phys. 58, 1200 (1980)] from the Monte Carlo data of D. M. Ceperley and B. J. Alder (Ref. 4). The interpolation formula for two dimensions is given in Ref. 3.

11. This value is obtained in Ref. 5 from VWN's interpolation formula for the correlation energy (Ref. 10).
12. The negative compressibility has been observed experimentally in a modulation-doped GaAs/AlGaAs heterostructure by J. P. Eisenstein, L. N. Pfeiffer, and K. W. West [Phys. Rev. Lett. 68, 674 (1992)]. Due to the finite thickness of the quantum wells (and the electron layers), the experimental data are in qualitative agreement with the Monte Carlo results of Tanatar and Ceperley (Ref. 3).
13. The Lindhard functions in two and three dimensions are given by F. Stern [Phys. Rev. Lett. 18, 546 (1967)] and by J. Lindhard [K. Dan. Vidensk. Selsk. Mat. Fys. Medd. 28, 8 (1954)], respectively.
14. These quantities are closely related to the Landau parameters [L. D. Landau, Zh. Eksp. Teor. Fiz. 30, 1058 (1956); 32, 59 (1957); Sov. Phys. JETP 3, 920 (1957); 5, 101 (1957)], the difference being that the effective mass enters into Landau theory through the interacting-particle density of states.
15. The analysis in Ref. 5 has been extended to $r_s = 80$. We use

VWN's correlation energy in the Padé form (Ref. 10). For the spin stiffness, we use their Padé fit to the four values for $\alpha_c(r_s)_{III}$ ($r_s = 10, 20, 50$ and 100), i.e., their scheme V for the spin-dependent correlation energy $\Delta\epsilon_c(r_s, \zeta)_V$.

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17. K. S. Singwi, M. P. Tosi, R. H. Rand, and A. Sjölander, Phys. Rev. 176, 589 (1968).
18. Here we are concerned neither with the geometric details of the crystalline structure (the bcc lattice for three dimensions and a triangular lattice for two dimensions) nor with the different magnetic properties of the liquid (paramagnetic, ferromagnetic phases, etc.).
19. The uncertainties in this ratio are calculated by regarding the uncertainties in the Wigner crystallization points as one-sigma uncertainties. cf. P. R. Bevington, Data Reduction and Error Analysis for the Physical Sciences (McGraw-Hill, New York, 1969), Chap. 4.

FIGURE CAPTIONS

FIG. 1. The dimensionless effective interactions that characterize the effective potentials in the long-wavelength limit in two dimensions for $0 \leq r_s \leq 40$.

FIG. 2. The dimensionless effective interactions in three dimensions for $0 \leq r_s \leq 80$.

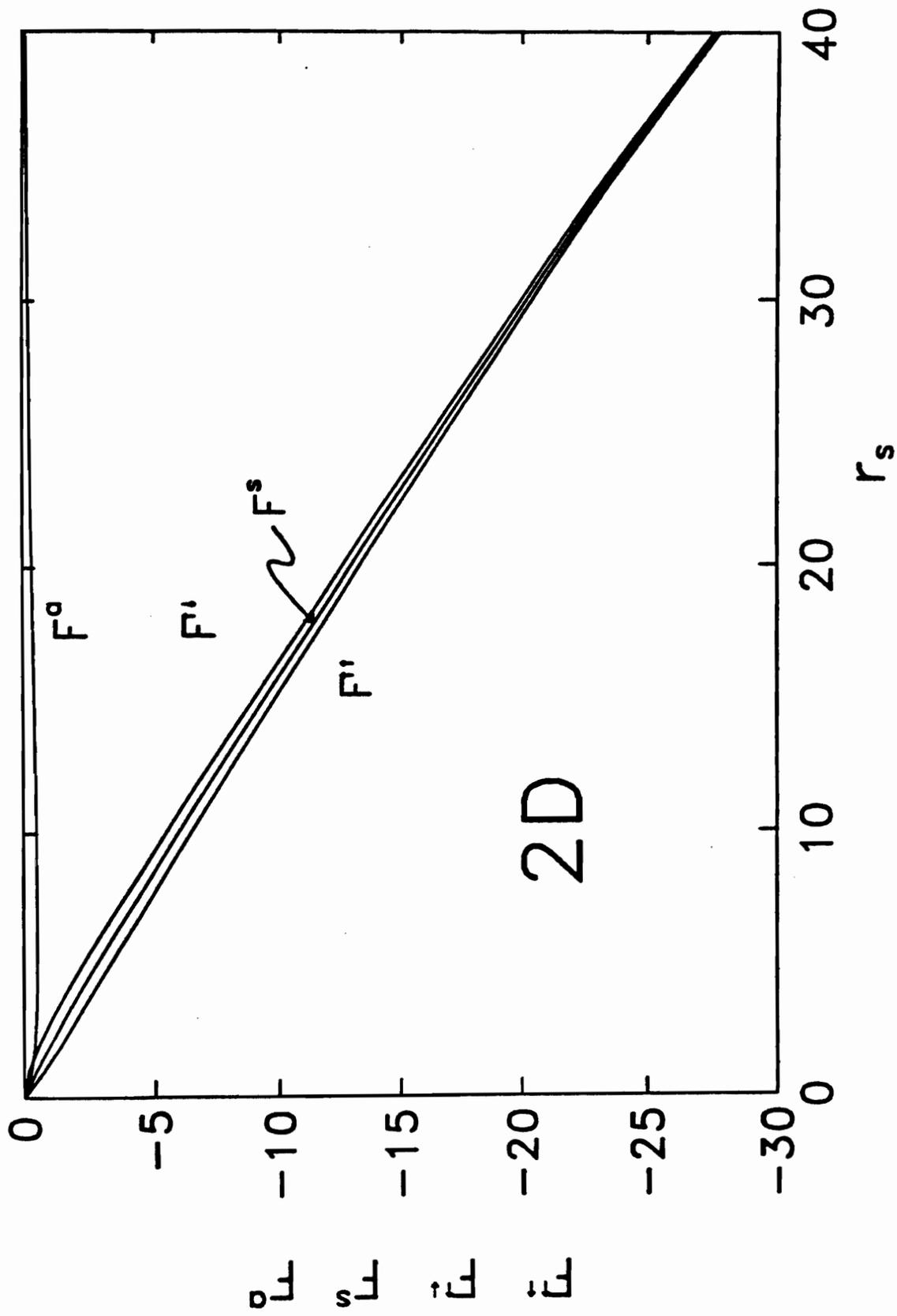


FIGURE 1

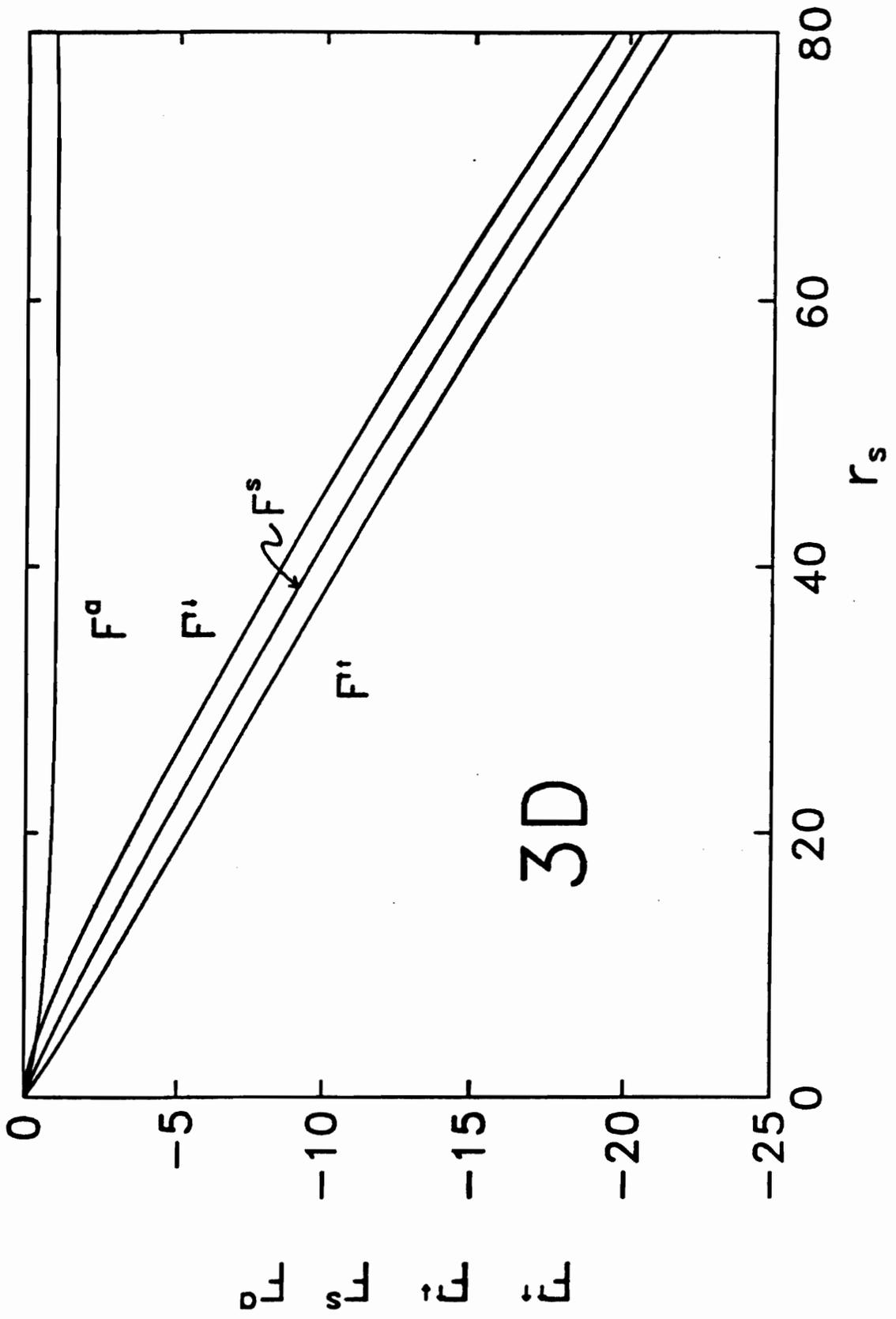


FIGURE 2