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Comments and Addenda

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Thomas-Fermi Equation of State with Exchange, Correlation, and Quantum Corrections

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A method is given for computing the correlation and quantum corrections to the Thomas-Fermi-Dirac equation of state. Results for $_{26}$Fe show good agreement with shock-wave data.

In a recent paper, Salpeter and Zapolsky[1] (hereafter referred to as SZ) have computed equations of state for degenerate matter at extremely high pressures and densities on the basis of the zero-temperature Thomas-Fermi-Dirac (TFD) model of a solid with correlation energy corrections evaluated on the basis of the following three assumptions: (a) negligible correlation corrections, (b) local correlation corrections, and (c) average correlation corrections. They conclude, on the the basis of experimental data, that for all practical values of the atomic number Z, the assumption (c) is more realistic than the other two, and the prescription for computing the pressure on the basis of this assumption is simply to add to the TFD pressure, with proper sign, the correlation pressure of a uniform electron gas at the average electron density n. The pressure is thus given by the following expression (throughout, we use the notation of SZ and only new symbols, wherever introduced, are explained),

$$P_{\rm av}=P_0\lambda^5\left[1-\frac{5}{4\pi}\left(\frac{4}{9\pi}\right)^{1/3}s_0\right]-\frac{5}{6}\left(\frac{4}{9\pi}\right)^{2/3}P_0r_e^3\left[\frac{d}{ds}\bar{E}_c(s)\right]_{s=r_e}. \quad (1)$$

The first term on the R.H.S. of (1) is the TFD pressure, $P_{\rm TFD}$, and the second the correlation pressure, δP_c. δP_c can therefore be easily evaluated once we have an explicit expression for $\bar{E}_c(s)$.

We make use of the above prescription of SZ to compute the correlation energy corrections to the equation of state of high-density degenerate matter obtained on the basis of the more realistic TFDW model, i.e., TF model with exchange, and Weisczacker (also called inhomogeneity or quantum) correction terms.[2] We use the TFDW model, rather than the TFD model, because, as has been shown by several authors,[3] the first nonvanishing correction to TF model contains, in addition to the exchange term, another term called the quantum correction term. Kalitkin[4] has computed the exchange and quantum corrections to the TF pressure, and his results may be expressed as

$$P_{\rm TFDW}=P-|\delta P|, \quad (2)$$

where P is the pressure as given by the TF model and δP represents the contribution coming from the exchange and quantum corrections. Therefore, the total pressure, incorporating all the three corrections, viz., the exchange, the quantum, and the correlation, is given by

$$P_{\rm Total}=P-|\delta P|-|\delta P_c|. \quad (3)$$

Numerical values for P and δP (in dyn/cm^2) have been tabulated by Kalitkin in terms of a variable ZV, where V is the volume of each spherical cell in units of 10^{-24} cm^3, and Z is the atomic number. In order to evaluate the total pressure from (3) we need an explicit expression for $\bar{E}_c(s)$ so that δP_c may be calculated. Though for $\bar{E}_c(s)$ one can use the expression used by SZ, the correlation energy can quite accurately be expressed in a much simpler form given by Barnes[5] to be

$$\bar{E}_c(s)=-0.0842\left(\frac{3}{4\pi}\right)^{1/6}\frac{1}{s^{1/2}},\quad \text{in atomic units}. \quad (4)$$

In order to facilitate the computation of the total pressure from (3) and (4) using Kalitkin's tables for P and δP, we give below an expression for δP_c in terms of ZV, the variable used by Kalitkin,

$$|\delta P_c|=2.223\times10^{11}[Z^{7/3}/(ZV)^{7/6}]\ \text{dyn/cm}^2. \quad (5)$$

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[1] E. E. Salpeter and H. S. Zapolsky, Phys. Rev. **158**, 876 (1967).

[2] Various corrections to *TF* have been discussed by P. Gombas, Rev. Mod. Phys. **35**, 512 (1963).

[3] D. A. Kirznits, Zh. Eksperim. i Teor. Fiz. **32**, 115 (1957) [English transl.: Soviet Phys.—JETP **5**, 64 (1957)]; G. A. Baraff and S. Borowitz, Phys. Rev. **121**, 1704 (1961).

[4] N. N. Kalitkin, Zh. Eksperim. i Teor. Fiz. **38**, 1534 (1960) [English transl.: Soviet Phys.—JETP **11**, 1106 (1960)].

[5] J. F. Barnes, Phys. Rev. 140, A721 (1965).

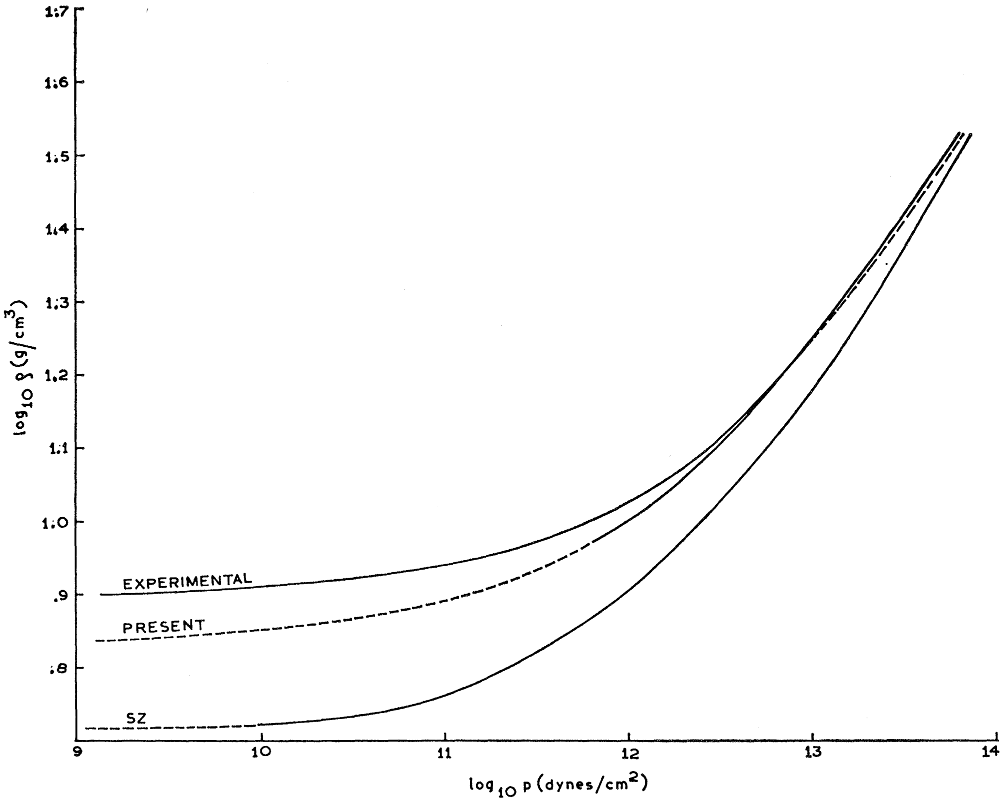

FIG. 1. Density versus pressure curve for $_{26}$Fe. The experimental curve represents the reduced shock-wave data (taken from Ref. 1). The curve SZ is based on TFD plus average correlation corrections (Ref. 1). The present curve is based on TFD plus the quantum and the average correlation corrections.

The matter density is given by

$$\rho = 1.664[AZ/(ZV)] \text{ g/cm}^3, \tag{6}$$

where A is the atomic mass in physical atomic-mass units.

Results for the equation of state of $_{26}$Fe are shown in Fig. 1 along with the experimental data (taken from SZ) and the results of SZ. From the figure we see that the simple procedure outlined in this note improves the agreement with experimental data.

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Reaction-Rate Kinetics and Distribution of Activation Energies

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In the problem of the determination of the characteristics of reaction-rate kinetics through the analysis of isothermal (or isochronal) data, we show that (1) it is impossible to determine both the order of reaction and, concurrently, the distribution of activation energies, and that (2) without prior knowledge of one of these—either the order of the reaction or the distribution of activation energies—the other cannot be determined in a unique manner.

A SYSTEMATIC study of the kinetics of processes distributed in activation energy was made by Primak,[1] who also gave an impressive list of fields in physics where this concept has been applied. We follow, in general, the notation of Primak to write the kinetic equation

$$-\frac{dq}{dt} = \lambda q^n, \tag{1}$$

where q is the concentration of the reactant, t is the

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[1] W. Primak, Phys. Rev. **100**, 1677 (1955).