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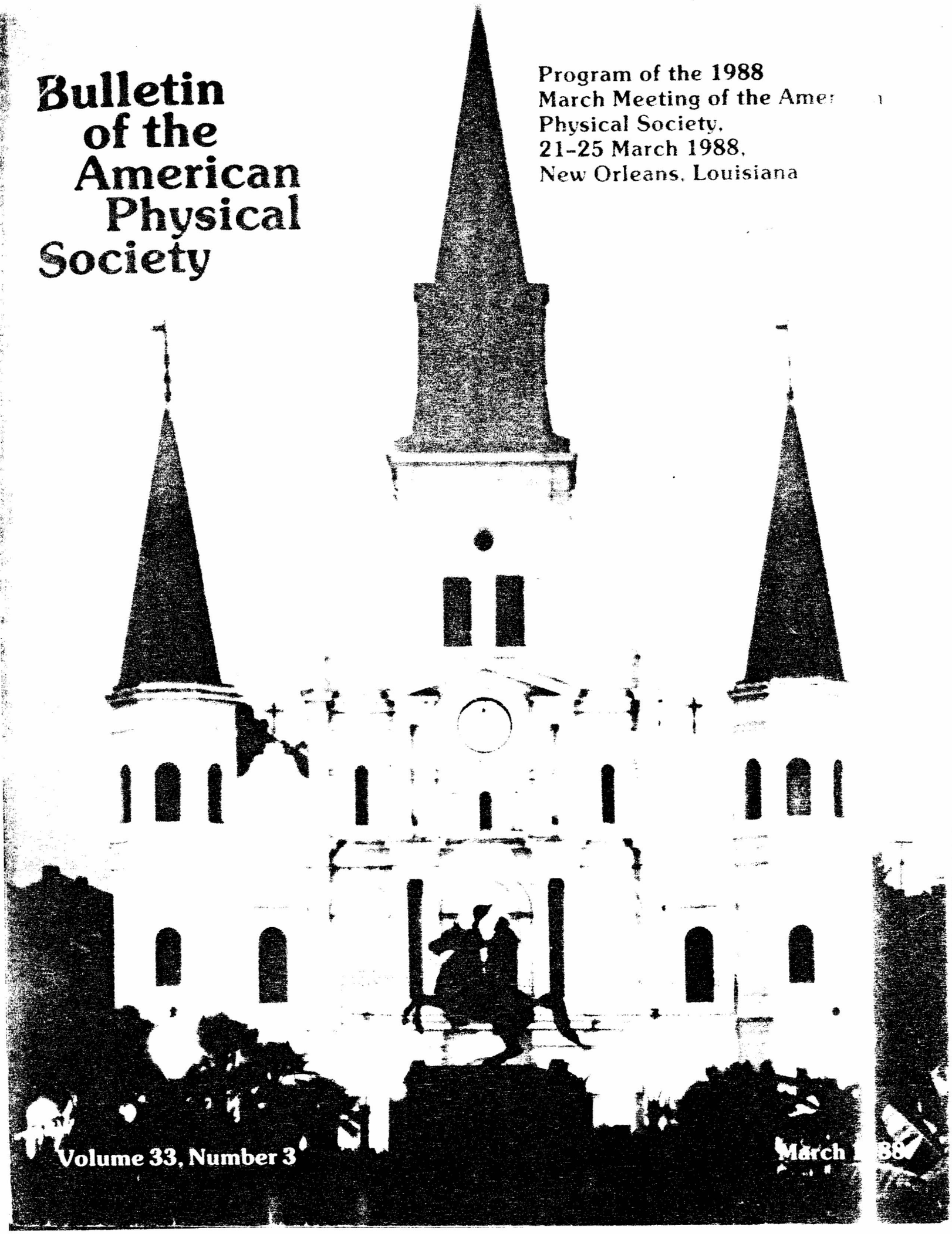

Volume 33, Number 3 March 1988

SESSION A18: THEORY I: DENSITY FUNCTIONAL METHOD
Monday morning, 21 March 1988
Mardi Gras J at 8:00
P. Vashishta, presiding

8:00
A18 1 **Density Functional Theory for Ensembles of Fractionally Occupied States I: Basic Formalism.*** E. K. U. GROSS, L. N. OLIVEIRA†, W. KOHN, UC Santa Barbara.—The Rayleigh-Ritz minimization principle is generalized to ensembles of unequally weighted states. Given the M lowest eigenvalues $E_1 \leq E_2 \leq \ldots \leq E_M$ of a Hamiltonian, and given M real numbers $w_1 \geq w_2 \geq \ldots \geq w_M > 0$, an upper bound for the weighted sum $w_1E_1 + w_2E_2 + \cdots + w_ME_M$ is established. The ground state Rayleigh-Ritz principle and the variational principle for equiensembles are recovered as special cases. Based on this generalized Rayleigh-Ritz principle, a Hohenberg-Kohn theorem is proven and a Kohn-Sham scheme involving fractionally occupied single-particle states is derived. The exact excitation energies are expressed in terms of differences of the Kohn-Sham single-particle energies and a correction term, directly obtainable from the ensemble exchange-correlation energy functional.

* Supported in part by the National Science Foundation under grant DMR 87-03434.
† On leave from the University of São Paulo; fellow of the Brazilian Council for Scientific and Technological Development.

8:12
A18 2 **Density Functional Theory for Ensembles of Fractionally Occupied States II: Application to the He Atom.*** L. N. OLIVEIRA†, E. K. U. GROSS, W. KOHN, UC Santa Barbara.—The density functional formalism described in the preceding abstract is applied to the excitation spectrum of the He atom. On the basis of the quasi-local-density approximation[1] for the equiensemble exchange-correlation energy functional, the Kohn-Sham equations for the ensemble density are solved and the excitation energies are computed. The splittings between nearly degenerate levels with different angular momenta (*e.g.*, between the $2S$ and $2P$ levels) are overestimated, but the averages over angular momentum and spin of the experimental excitation energies (*e.g.*, the average of the $2S$ and $2P$ energies) measured from the ionization threshold are reproduced within a few percent.

* Supported in part by the National Science Foundation under grant DMR 87-03434.
† On leave from the University of São Paulo; fellow of the Brazilian Council for Scientific and Technological Development.
1. W. Kohn, Phys.Rev.A 34, 737 (1986).

8:24
A18 3 **Fundamental Constraints on Correlation Functions.*** A. H. KRIMAN and D. K. FERRY, Center for Solid State Electronics Research, Arizona State University-- Inequalities are derived that constrain one-time correlation functions. These follow from exchange symmetry and require no assumption about the time behavior of the particle distribution. In particular, they are valid out of equilibrium and for general interactions. Identical forms obtain for Fermi and Bose statistics. We study two-particle correlations in detail and find various linear functionals of the correlation function which are bounded by the inverse density. In equilibrium, these constraints are associated with mechanical stability. Higher-order constraints involve linear functionals of two- through 2n-particle correlations. These can be used as a test of the Kirkwood Superposition principle.

* Supported by US Office of Naval Research.

8:36
A18 4 **Inequality Based Constraints on the Static Structure Factor of the Homogeneous Electron Gas.*** K. RAPCEWICZ† and N. W. ASHCROFT *Cornell University*.– We present zero and finite temperature results for the static structure factor, $S(q)$, for the homogeneous interacting electron gas. These results follow from the use of Schwarz-based and other inequalities and provide qualitative insights about the behaviour of the exact results that are not obtainable by other methods. In particular, we have examined the small q, small r_s expansion[1,2] of the exchange-correlation kernel, $K_{XC}(q)$, to obtain a rigorous upperbound on the next to leading order correction to the small q, small r_s expansion of $S(q)$. We show that this term is of order q^4 and negative. Further, these inequalities provide constraints that approximate solutions must satisfy.

* Supported by the National Science Foundation
† Natural Sciences and Engineering Research Council of Canada Post-Graduate Fellow
1 D. Langreth and S. Vosko, *Phys. Rev. Lett.* 59, 497, (1987).
2 L. Kleinman, *Phys. Rev. B* 30, 2223 (1984).

8:48
A18 5 Density-Functional Theory in Strong Magnetic Fields.* G. VIGNALE† and MARK RASOLT, Oak Ridge National Laboratory, Oak Ridge, TN. — We formulate the current-density functional theory for systems in arbitrarily strong magnetic fields. A set of self-consistent equations comparable to the Kohn-Sham equations for ordinary density functional theory is derived, and proved to be gauge-invariant and to satisfy the continuity equation. We prove that the exchange-correlation energy functional $E_{xc}[n,j_p]$ ($n(r)$ is the density, and $j_p(r)$ is the 'paramagnetic' current density) depends on the current via the combination $v(r) = \nabla\times\{j_p(r)/n(r)\}$. An explicit formula for E_{xc} is derived, which is local in $v(r)$.

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†Also Department of Physics, University of Tennessee, Knoxville, TN.

9:00
A18 6 Jellium Work Function for All Electron Densities. Y. WANG and J. P. PERDEW, Tulane U.* -- The work function of the jellium surface has been calculated self-consistently within the local density approximation for bulk densities in the range $1 \leq r_s \leq 12$. The results have been fitted to an analytic formula based upon the displaced-profile change-in-selfconsistent-field expression[1] for the work function. The $r_s \to 0$ limit of this formula is close to the value 1.2 eV predicted by Peuckert[2] for the high-density limit.

*Supported by NSF Grant DMR84-20964.
[1]J. P. Perdew and V. Sahni, Solid State Commun. 30, 87 (1979).
[2]V. Peuckert, J. Phys. C 7, 2221 (1974).

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