Microscopic Basis of Magnetism
Magnetism of Insulators Metals and Things-In-Between

Figures and Illustrations

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Random Phase approximation: Gell Mann Brueckner Sawada 1958-59. Inverse susceptibility as a function of $r_s$

$\lambda = r_s/6.03$


RPA predicts PM metal for $r_s \sim 18!$
In[5]:= \( e@rs, x \_ D = 2.21 \pm rs^2 \frac{HH_1 + xL^5 + 3H_1 - xL^5 + 3LL - 0.916 HH_1 + xL^4 + 3H_1 - xL^4 + 3LL \pm rs}{rs^2} \) \\
Out[5]= -0.916 HH_1 - xL^4 + 3H_1 + xL^4 + 3LL + 2.21 HH_1 - xL^5 + 3H_1 + xL^5 + 3LL rs^2

In[30]:= Plot \( e@e@, xD, e@5, xD, e@, xD, 8x, 0, 1D \) \\

In[32]:= Plot \( e@@rs, 0D - e@rs, 1D, 8rs, 4, 6D \) \\
Ground state of the fermion one-component plasma:  
A Monte Carlo study in two and three dimensions

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(Received 26 April 1978)

We have performed fermion Monte Carlo variational calculations to determine the equation of state of the uniform electron one-component plasma in two and three dimensions. The ground-state excess energies calculated by the Monte Carlo method are very precise and in agreement with those of other calculations in the metallic density range and in the very-low-density Wigner crystals. Three phases have been investigated: the Wigner crystal, the normal or unpolarized fluid, and the polarized fluid. The Wigner crystal has the lowest energy for \( r_e > 67 \) in three dimensions and \( r_e > 33 \) in two dimensions. The totally polarized quantum fluid is stable for \( 26 < r_e < 67 \) in three dimensions and for \( 13 < r_e < 33 \) in two dimensions, and the normal or unpolarized fluid is stable at higher densities, \( r_e < 26 \) in three dimensions and \( r_e < 13 \) in two dimensions. A pseudopotential with no adjustable parameters, derived from the random-phase approximation, is found to give excellent energies. The present results lend support to earlier conjectures that the ground state of the electron gas will be spin polarized at intermediate densities.

III. VARIATIONAL TRIAL FUNCTION

In this paper we will assume the trail function is of the Bijn-Dingle-Jastrow or product form:

\[
\Psi_f(R) = D(R) \exp \left(-\sum_{i<j} u(\mid \mathbf{r}_i - \mathbf{r}_j \mid) \right). \tag{4}
\]

The function \( D(R) \) is the "model" noninteracting term and serves to give the trail function the desired antisymmetry. For the fluid phase we take \( D(R) \) to be a Slater determinant of plane waves. In the unpolarized fluid there are separate determinants for spin-up and spin-down particles. For the polarized fluid there is a single determinant. In the crystal phase \( D(R) \) is a Slater determinant of single-particle orbitals centered around the lattice sites. The "pseudopotential," \( u(r) \) is repulsive and includes in an approximate way the effects of particle correlation.

FIG. 2. Minus the correlation energy times \( r_e \) vs \( r_e \) from our calculation (solid line) compared with perturbational calculations. The symbols represent the results of (1) the RPA approximation Freeman (Ref. 41), (2) Hubbard (Ref. 45), (3) Vashishta and Singwi (Ref. 43), (4) Freeman (Ref. 41), and (5) Lowy and Brown (Ref. 44).
Ground State of the Electron Gas by a Stochastic Method

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and

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(Received 16 April 1980)

An exact stochastic simulation of the Schrödinger equation for charged bosons and fermions has been used to calculate the correlation energies, to locate the transitions to their respective crystal phases at zero temperature within 10%, and to establish the stability at intermediate densities of a ferromagnetic fluid of electrons.

FIG. 2. The energy of the four phases studied relative to that of the lowest boson state times $r_s^2$ in rydbergs vs $r_s$ in Bohr radii. Below $r_s = 160$ the Bose fluid is the most stable phase, while above, the Wigner crystal is most stable. The energies of the polarized and unpolarized Fermi fluid are seen to intersect at $r_s = 75$. The polarized (ferromagnetic) Fermi fluid is stable between $r_s = 75$ and $r_s = 100$, the Fermi Wigner crystal above $r_s = 100$, and the normal paramagnetic Fermi fluid below $r_s = 75$. 
A "strong ferromagnet" has essentially filled majority band and partially filled minority band. (Ni, FeCo alloys)

A "weak ferromagnet" has partially filled majority as well as minority band. (Fe, Co)
Definitions:
- Paramagnet
- Weak ferrom.
- Strong ferrom.

- No polarisation: Ti, V
- Partially polarized: Fe, Co
- Fully polarized: Ni
Half metallic alloy with full polarisation:
Examples:
ferromagnetic oxide CrO2 and some intermetallic compounds (Heusler-alloys) PtMnSb, NiMnSb, Co2MnAl, Co2MnSb.
LDA Local Density Functional theory and its applications in Magnetism: Numerical procedure based on the Kohn Sham scheme and the Hohenberg Kohn variational principle

Stoner model of ferromagnetism and total-energy band theory

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(Received 7 March 1988)

The Stoner model of ferromagnetism in metals is generalized to reproduce the results of spin-polarized total-energy band calculations with the fixed-spin-moment procedure. The Stoner parameter for the exchange field is made a function of both volume and magnetic moment and evaluated from the band calculations. A generalized Stoner condition for the occurrence of ferromagnetism is derived and applied to fcc Fe. Our previous results on the high-spin and low-spin phases of fcc Fe are reproduced and differences from a recent Stoner analysis of fcc Fe are explained.

\[ \chi^{-1}(M,V) = \frac{\partial^2 E_T(M,V)}{\partial M^2} \]
\[ = \frac{1}{2\bar{N}} - \frac{M}{2\bar{N}^2} \bar{N}' - \frac{I}{2} - M I' - \frac{M^2}{4} I'' , \quad (3.10) \]

where \( \bar{N}' = (\partial \bar{N} / \partial M)_V, \quad I' = (\partial I / \partial M)_V, \quad I'' = (\partial^2 I / \partial M^2)_V \). Then

\[ \chi(0) = \frac{2\bar{N}(0,V)}{1 - \bar{N}(0,V) I(0,V)} = \frac{2N(\varepsilon_F,V)}{1 - N(\varepsilon_F,V)I(0,V)} . \]

\[ (3.11) \]
The spin-polarized Kohn-Sham equations may be written
\[ (-\nabla^2 + \phi_{\text{eff}}(n_u(r), n_d(r)))\psi_{ij}(r) = \varepsilon_{ij} \psi_{ij}(r), \]
\[ i = 1, 2, \ldots, N_j \text{ and } j = u, d, \tag{2.1} \]
where \( u \) and \( d \) designate up- and down-spin distributions, respectively, and the effective potential is
\[ \phi_{\text{eff}}(n_u(r), n_d(r)) = \phi_{\text{Coul}}(r) + \phi_{\text{xc}}(n_u(r), n_d(r)), \tag{2.2} \]
and the Coulomb part is the sum of a nuclear and an electronic part
\[ \phi_{\text{Coul}}(r) = \phi_{\text{nuc}}(r) + \phi_{\text{elec}}(r) = \sum_p \frac{Z_p}{|r - R_p|} + \int_V \frac{n(r')}{|r - r'|} d^3r', \tag{2.3} \]
with the electron number density for each spin
\[ n_j(r) = \sum_{i=1}^{N_j} |\psi_{ij}(r)|^2, \quad j = u, d, \tag{2.4} \]
and the total electron number density
\[ n(r) = \sum_{j=u,d} n_j(r). \tag{2.5} \]

In (2.3), \( \mathbf{R}_p \) is the lattice vector of the nucleus of charge \( Z_p \) and the sum is over all nuclei. In (2.2)
\[ \phi_{\text{xc}}(n_u, n_d) = \frac{\partial[n \varepsilon_{\text{xc}}(n_u, n_d)]}{\partial n_j}, \quad j = u, d, \tag{2.6} \]
where \( \varepsilon_{\text{xc}}(n_u, n_d) \) is a known function in the local-density approximation. The equations (2.1) are solved self-consistently under the two constraints
\[ \int_V n_j(r) d^3r = N_j, \quad j = u, d, \tag{2.7} \]
where \( N_u \) and \( N_d \) are specified separately and the total number of electrons per atom is
\[ N = \sum_{j=u,d} N_j. \tag{2.8} \]
If the system is neutral, \( N \) is fixed by the \( Z \) values and only the difference
\[ M = N_u - N_d \tag{2.9} \]
can vary; \( M \) is then the magnetic moment of the system in Bohr magnetons.

The total energy of the system is a function of \( M \) and of the set of nuclear coordinates \( \{ \mathbf{R}_p \} \), and is given by
\[ E_T(M, \{ \mathbf{R}_p \}) = \sum_{j,i} \varepsilon_{ij} - \frac{1}{2} \int_V n(r) \phi_{\text{elec}}(r) d^3r \]
\[ + \int_V \left[ n(r) \varepsilon_{\text{xc}}(r) - \sum_j n_j(r) \phi_{\text{xc}}(r) \right] d^3r. \tag{2.10} \]

This doubly constrained self-consistent ground-state calculation, which fixes both \( N \) and \( M \), is called the fixed-spin moment procedure. For cubic bulk crystals it leads to a thermodynamic function \( E_T(M, V) \), which contains information about the stable and metastable ferromagnetic bulk phases and their stability ranges in \( V \). We note
TABLE I. Theoretical equilibrium lattice constants $a_{\text{eq}}$ (in a.u.), spin magnetic moments (in $\mu_B$) and total hyperfine field $B_{\text{hf}}$ (in kG) as well as their core and valence parts, $B_{\text{core}}$ and $B_{\text{val}}$, for bcc Fe, fcc Co, and fcc Ni, respectively. In addition the decomposition of $B_{\text{core}}$ into its contributions from the 1s, 2s, and 3s shells is given. The last line represents the ratio of the core hyperfine field $B_{\text{core}}$ and the spin magnetic moment $\mu_{\text{spn}}$ in kG/\(\mu_B\), respectively. As explained in the text the abbreviations VBH and so on denote the various parametrizations for the used exchange-correlation potentials. All results have been obtained assuming a nucleus of finite radius $r_0$ with $r_0 = 8.22, 8.33, \text{ and } 8.44 \times 10^{-5}$ a.u. for Fe, Co, and Ni, respectively. The corresponding experimental values for the lattice constant are 5.406, 6.707, and 6.658 a.u., 2.13 $\mu_B$, 1.52 $\mu_B$ and 0.57 $\mu_B$ for the magnetic moment and $-339$, $-215$, and $-75$ kG for the total hyperfine field, respectively.

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FIG. 3. A replot of the data of Weiss and Forrer to conform to the variables of Eq. (1).

FIG. 2. Arrott plots for alloy V at eight temperatures between 45 and 80 K.

Arrott Noakes: Ni
(1967 PRL)
Na Cl structure of MO, where M= transition metal.
Note the M surrounded by O octahedra.
## 3d Transition Metal Monoxides

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<th>Compound</th>
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<th>Electrical Properties</th>
<th>Magnetic Properties</th>
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<td>2.94 Å</td>
<td>Metallic</td>
<td>Pauli Paramagnetic</td>
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<tr>
<td>VO ($d^3$)</td>
<td>2.89 Å</td>
<td>Intermediate</td>
<td>Intermediate</td>
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AFM = Antiferromagnetic

Example of t$_{2g}$ overlap with oxygen p levels

Example of e.g. overlap of Cu d levels with oxygen p levels