Mean field approach - introduction

Computational Physics

4. október 2010

Ising - many-spin - single-spin description

The Ising Hamiltonian

$$H = -\frac{J}{2}\sum_{\langle i,j\rangle} s_i s_j - B\sum_i s_i$$

is a real many-body Hamiltonian. Can we approximate it by a single-spin Hamiltonian?

Denote the mean value of s_i by $\langle s_i\rangle$, then

$$s_i s_j = s_i\langle s_j\rangle + \langle s_i\rangle s_j - \langle s_i\rangle\langle s_j\rangle + (s_i - \langle s_i\rangle)(s_j - \langle s_j\rangle)$$

without an approximation. The system is homogeneous
$\rightarrow \langle s_i\rangle = \langle s\rangle$ independent of i.

Thus we can rewrite the Hamiltonian

$$H = -\frac{J}{2}\sum_{\langle i,j\rangle}\left[s_i\langle s\rangle + \langle s\rangle s_j - \langle s\rangle\langle s\rangle + (s_i - \langle s\rangle)(s_j - \langle s\rangle)\right] - B\sum_i s_i$$

Two terms are identical, and one is pure correlation term.

We make the approximation

$$H \approx -Jq\langle s\rangle\sum_i^N s_i + J\frac{q}{2}N\langle s\rangle^2 - B\sum_i s_i$$

q is the number of nearest neighbors, coordination number.
This can be simplified as

$$H \approx J\frac{q}{2}N\langle s\rangle^2 - (B^{\mathrm{mf}} + B)\sum_i s_i$$

with $B^{\mathrm{mf}} = qJ\langle s\rangle$

Now the Hamiltonian

$$H \approx J\frac{q}{2}N\langle s\rangle^2 - (B^{\mathrm{mf}} + B)\sum_i s_i$$

is a pure one-body Hamiltonian! The single spin variable s_i sees an external field B and an effective field B^{mf} created by all the spins in the system.

But H alone is not enough, we still do not know $\langle s\rangle$! One way to determine $\langle s\rangle$ comes from the two definitions of magnetization (average magnetic dipole moment)

$$D = N\langle s\rangle \quad \text{and} \quad D = -\frac{\partial}{\partial B}F(N, B, T, \langle s\rangle)\,\Big|_{N,T,\langle s\rangle}$$

with

$$F(N, B, T, \langle s\rangle) = -kT \ln Z_N(B, T)$$

This leads to

$$\langle s \rangle = \tanh\left\{\beta(qJ\langle s \rangle + B)\right\},$$

an implicit equation for $\langle s \rangle$.

- **Instead of one linear many-body Hamiltonian with a huge complex state space we now have a set of nonlinear equations, effective one-body Hamiltonian, in a simple state space.**
- Here we can solve the MF equations "analytically", but in most systems we need numerical methods.
- Nonlinear equations $\leftrightarrow$ linear algebra + iterations.

Electronic structure of matter

How do we approach the equation of motion

$$\left[\sum_{i=1}^{N}\left\{\frac{1}{2m^*}\left(\mathbf{p}_i+\mathbf{A}(\mathbf{r}_i)\right)^2+V_{ext}(\mathbf{r}_i)\right\}+\frac{1}{2}\sum_{i\neq j}^{N}\frac{e^2}{\kappa|\mathbf{r}_i-\mathbf{r}_j|}-E\right]\Psi=0$$

with the time-independent many-electron antisymmetrized wave function $\Psi(\mathbf{r}_1,\mathbf{r}_2,\cdots,\mathbf{r}_N)$.

If Ψ is constructed from single-electron wave functions then it is a sum over **all** possible Slater determinants of them!

If $N=100$ then we have equivalent to a minimization problem in $3^{300}\approx 10^{150}$ dimensions! (W. Kohn RMP, **71**, 1253 (1998))

Daniela Pfannkuche will talk about the systems with low N where exact numerical methods can be used.

Walter Kohn has stated in a provocative manner:

In general the many-electron wave function Ψ for a system of N electrons is not a legitimate scientific concept, when $N \leq N_0$, where $N_0 \approx 10^3$.

There are 3+ solutions (finite $\leftrightarrow$ extended systems)

- Monte Carlo methods for Ψ.
- Second quantization, $\rightarrow$ Nonlinear operator eq,'s, Greens functions, occupation space...
- Mean field methods.

Facts from many-body calculations

One of the largest triumphs of the 20th century

We check homogeneous 3D electron system (3DEG) with density n_0 and constant background charge density en_b

small parameter for perturbation calc. $r_s(n_0)$:

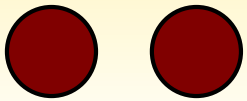
$$n_0 = \frac{3}{4\pi r_0^3} = \frac{3}{4\pi r_s^3 a_B^3}$$

$$r_s = \frac{r_0}{a_B}, \quad a_B = \frac{\hbar^2}{me^2} = 0.529 \text{ Å}$$

Electron interaction

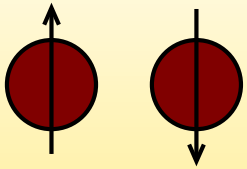
Electrons are indistinguishable!

Direct Coulomb (classic)

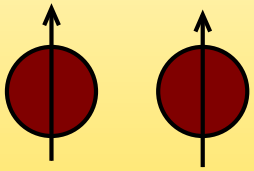


Repulsion

Exchange force (quantum phen.)



No force



Attraction

Mean total energy per electron (in $E_{Ryd} = me^4/(2\hbar^2) = 13.6$ eV):

$$E = \underbrace{\frac{2.21}{r_s^2}}_{\text{kinetic}} - \underbrace{\frac{0.916}{r_s}}_{\text{exchange}} - \overbrace{0.094 + 0.0622 \ln(r_s) + O(r_s)}^{\text{correlation}}$$

Direct Coulomb-energy $= 0$, due to background

$E_{kin} >> E_{int}$ when $r_s \to 0$, high density

Metals: $1.8 < r_s < 5$

Interaction is important for low density

n_0 is variable in 2DEG

Inhomogeneous - finite system

The Direct Coulomb term is not canceled

Numerically exact methods

Many-electron Hamilton operator

$$H = \sum_{i=1}^{N} \left\{ \frac{1}{2m^*} \left(\mathbf{p}_i + \mathbf{A}(\mathbf{r}_i) \right)^2 + V_{conf}(\mathbf{r}_i) \right\} + \frac{1}{2} \sum_{i \neq j}^{N} \frac{e^2}{\kappa |\mathbf{r}_i - \mathbf{r}_j|}$$

is diagonalized in a truncated many-electron state space

Works for 2-12 electrons

Mean field methods

$$\underbrace{\text{Many-electron operator } H}_{\text{linear equation of motion}} \rightarrow \underbrace{\text{one-electron in} V_{eff}}_{\text{nonlin. eq. of motion}}$$

For example, Hartree or Hartree-Fock approximation constructed as:

- An infinite perturbation series, Feynman diagrams, many-body theory. (A. Fetter and J.D. Walecka, Quantum Theory of Many-Particle Systems, McGraw-Hill, (1971).
- Variational approach to H with the condition that the wave function is a single Slater determinant. E.K.U. Gross, E. Runge and O. Heinonen, Many-particle Theory, Adam Hilger (1991).

HF-equations of motion

$$\{H_0 \quad + \quad V_{\text{ext}}(\mathbf{r}) + V_H(\mathbf{r})\}\psi_\alpha(\mathbf{r})$$
$$- \quad \int d\mathbf{r}'\Delta(\mathbf{r},\mathbf{r}')\psi_\alpha(\mathbf{r}') = \epsilon_\alpha\psi_\alpha(\mathbf{r})$$

$$V_H(r) = \frac{e^2}{\kappa}\int d\mathbf{r}'\,\frac{n(\mathbf{r}') - n_b(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$$

$$\Delta(\mathbf{r},\mathbf{r}') = \frac{e^2}{\kappa}\sum_\beta f(\epsilon_\beta - \mu)\frac{\psi^*_\beta(\mathbf{r}')\psi_\beta(\mathbf{r})}{|\mathbf{r}-\mathbf{r}'|}$$

$$n(\mathbf{r}) = \sum_\alpha |\psi_\alpha(\mathbf{r})|^2 f(\epsilon_\alpha - \mu)$$

$$\int d\mathbf{r}'\, n(\mathbf{r}',\mu) = N, \text{ number of electrons}$$

- Exchange force $\rightarrow$ nonlocal, not a functional of n
- Nonlinear equations, solved in one-electron state space with iterations, we will go through this later.
- The exchange can be expensive if the density n is a primary variable in a program. To be discussed later.
- Exact solutions to the nonlinear equations...
- Lack of correlations...
- Higher order approximations...