The interacting Fermi gas:
a step beyond Hartree-Fock
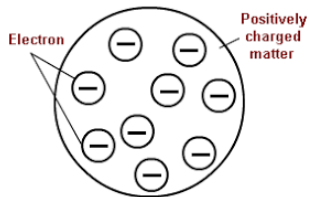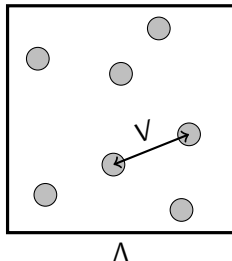
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joint work with M. Porta and F. Rexze
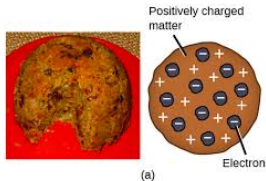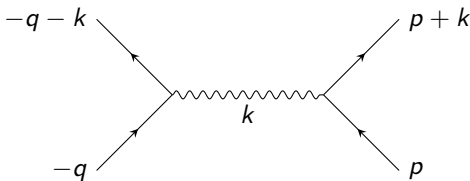
Heinzfest, Herrsching

Electrons in a metal

Hamiltonian

$$H = \sum_p (p^2 - \mu) \, a_p^\dagger a_p + \frac{1}{|\Lambda|} \sum_{k,p,q} \hat{V}(k) \, a_{p+k}^\dagger a_{-q-k}^\dagger a_{-q} a_p$$
$$+ H^{\mathrm{electron-background}} + H^{\mathrm{background-background}}$$

(a)

Jellium

The *electron-background* and *background-background* interaction is accounted for by omitting $k = 0$.

$$H = \sum_p (p^2 - \mu) \, a_p^\dagger a_p + \frac{1}{|\Lambda|} \sum_{k,p,q \, k \neq 0} \hat{V}(k) \, a_{p+k}^\dagger a_{-q-k}^\dagger a_{-q} a_p$$

For the Coulomb-gas one has

$$\hat{V}(k) = \frac{1}{|k|^2}.$$

In 1975 Lieb and Narnhofer showed existence of thermodynamic limit [LN].

Based on wonderful work of Volker Bach [B], Graf-Solovej [GS] showed that the Hartree-Fock energy is asymptotically exact (large μ).

$$E^{QM} = E^{HF} + \text{Error}$$

[LN] E. H. Lieb, H. Narnhofer, *The thermodynamic limit of Jellium*, JSP, **12** 291 (1975)
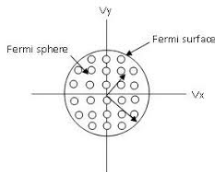[B] V. Bach, *Error bound for the Hartree-Fock energy of atoms and molecules*, CMP, **147**, 527-548 (1992)
[GS] J.-M. Graf, J. P. Solovej, *A correlation estimate with applications to Quantum systems*. Rev. Math. Phys. **6**, 977-997 (1994)

Hartree-Fock-energy

$$\langle \Omega | H | \Omega \rangle,$$

where Ω is given by the filled Fermi-sea with momenta smaller than $\sqrt{\mu}$.

$$\langle \Omega | \sum_p (p^2 - \mu) \, a_p^\dagger a_p | \Omega \rangle \simeq \int_{|p| \leq \sqrt{\mu}} (p^2 - \mu) dp = \mu^{5/2} \int_{|\bar{p}| \leq 1} (\bar{p}^2 - 1) d\bar{p},$$

$$\langle \Omega | \frac{1}{|\Lambda|} \sum_{k,p,q \, k \neq 0} \frac{1}{|k|^2} \, a_{p+k}^\dagger a_{-q-k}^\dagger a_{-q} a_p | \Omega \rangle \simeq \frac{1}{|\Lambda|} \sum_{p+k=-q \, k \neq 0} \frac{1}{|k|^2} \cdots$$

$$\simeq -\int_{|p|,|q| \leq \sqrt{\mu}} \frac{1}{|p+q|^2} = -\mu^2 \int_{|p|,|q| \leq 1} \frac{1}{|p+q|^2} \quad (1)$$

Correlation energy

Hence

$$E^{HF} = c_1(\sqrt{\mu})^5 - c_2(\sqrt{\mu})^4,$$

$$\sqrt{\mu} \sim \rho^{1/3}.$$

A big challenge is to recover the correlation energy

$$E_{corr} = E^{QM} - E^{HF}.$$

In the physics literature this was intensively studied in the fourties and fifties. People, e.g., Heisenberg [Hei], realized that second order perturbation theory does not work, logarithmic divergencies.

Important results by Bohm-Pines, Macke, Gell-Mann-Bruckner, Sawada, ... Using a specific subset of Feynman diagrams Gell-Mann and Bruckner derived

$$E_{corr} = (\sqrt{\mu})^3(c_3 \log \mu + c_4) + O(\mu),$$

with explicit constants c_3 and c_4.

But from a mathematical point of view there is no proof.

[Hei] W. Heisenberg *Zur Theorie der Supraleitung* Z. f. Naturforschung **2**, 185 (1947)

Mean-field scaling

We replace

$$\frac{1}{k^2} \to \frac{1}{\sqrt{\mu}} \hat{V}(k),$$

Coulomb by a mean-field interaction.

$$H = \sum_p (p^2 - \mu) \, a_p^\dagger a_p + \frac{1}{\sqrt{\mu}} \sum_{k,p,q} \hat{V}(k) \, a_{p+k}^\dagger a_{-q-k}^\dagger a_{-q} a_p.$$

Then the exchange energy is of the order

$$-\frac{1}{\sqrt{\mu}} \sum_{|p|,|q| \le \sqrt{\mu}} \hat{V}(p+q) dp dq \simeq -(\sqrt{\mu})^2,$$

hence we expect the correlation energy to be of the order of $\sqrt{\mu}$.

Correlation energy

Theorem

There exist constants $V_0, C > 0$, independent of μ, such that for $\|\hat{V}\|_1 \leq V_0$ the following is true:

$$-C\|\hat{V}\|_1 \mu^{1/4} + \frac{1}{(1-C\|\hat{V}\|_1)}E^{(2)} \leq E_{corr} \leq (1-C\|\hat{V}\|_1)E^{(2)} + C\|\hat{V}\|_1 \mu^{1/4},$$

with

$$E^{(2)} = -\frac{1}{\mu} \sum_{\substack{|p|,|q| \leq \sqrt{\mu} \\ |p+k|,|q+k| > \sqrt{\mu}}} \frac{|\hat{V}(k)|^2}{e(p+k) + e(-q-k) + e(p) + e(q)}$$

$$= -\frac{1}{\mu} \sum_{\substack{|p|,|q| \leq \sqrt{\mu} \\ |p+k|,|q+k| > \sqrt{\mu}}} \frac{|\hat{V}(k)|^2}{2k \cdot (k+p+q)} = -a_1\sqrt{\mu} + o(\sqrt{\mu}),$$

$$e(p) = |p^2 - \mu|.$$

Second order perturbation

Take $\frac{\lambda}{\sqrt{\mu}} V$ as potential.

Corollary

Let $\hat{V} \in L^1$, $\hat{V} \geq 0$, then there is an explicit constant a_1 such that, for μ large, and λ small enough,

$$E_{corr} = -\lambda^2 a_1 \sqrt{\mu} + O(\lambda^3)\sqrt{\mu} + o(\mu),$$

or equivalently

$$\lim_{\mu \to \infty} \frac{E_{corr}}{\sqrt{\mu}} = -\lambda^2 a_1 + O(\lambda^3).$$

We recover the correlation energy to second order and estimate all the error terms uniformly in μ, using a rigorous perturbation scheme developed in [H], refined in [CH], see also [HHS, HS, HVV].

[H] C. HAINZL, One non-relativistic particle coupled to a photon field. Ann. Henri Poincare 4, 217-237 (2003)
[HS] C. HAINZL, R. SEIRINGER, Mass renormalization and energy level shift in non-relativistic QED. Adv. Theor. Math. Phys. 6, 847 (2002)
[CH] I. CATTO, C. HAINZL, Self-energy of one electron in non-relativistic QED. J. Funct. Anal. 207, 1, 68-110 (2004)
[HVV] C. HAINZL, V. VOUGALTER, S.A. VUGALTER, Enhanced binding in non-relativistic QED. Commun. Math. Phys. 233, 13-26 (2003)
[HSS] C. HAINZL, M. HIROKAWA, H. SPOHN, Binding energy for hydrogen-like atoms in the Nelson model. J. Funct. Anal 220, 2, 424-459 (2005)

$$E^{QM} := \inf_{\substack{\psi \in \mathcal{H} \\ ||\psi||=1}} \langle \psi | H | \psi \rangle = \inf_{\substack{\psi \in \mathcal{H} \\ ||\psi||=1}} \langle R^\dagger R \psi | H | R^\dagger R \psi \rangle = \inf_{\substack{\psi \in \mathcal{H} \\ ||\psi||=1}} \langle R\psi | RHR^\dagger | R\psi \rangle$$

with [BPS]

$$R|0\rangle = |\Omega\rangle.$$

$$RHR^\dagger = E^{HF} + \sum_{p \in \mathbb{Z}^3} |p^2 - \mu| \, (c_p^\dagger c_p + b_p^\dagger b_p) + \frac{1}{2\sqrt{\mu}} \sum_{k,p,q \in \mathbb{Z}^3} \hat{V}(k) \times$$

$$\times \left(b_{p+k} c_p b_{-q-k} c_{-q} + c_{-q}^\dagger b_{-q-k}^\dagger c_p^\dagger b_{p+k}^\dagger + 2 c_{p+k}^\dagger b_p^\dagger b_{-q-k} c_{-q} \right) + \dots$$

$$= E^{HF} + H_0 + F + F^\dagger + V_2 + \dots$$

Hence

$$E_{corr} = \inf_{\substack{\psi \in \mathcal{H} \\ ||\psi||=1}} \langle \psi | (H_0 + F + F^\dagger + V_2 + \dots) | \psi \rangle.$$

[BPS] N. Benedikter, M. Porta, B. Schlein, Mean field evolution of fermionic systems, *CMP* **331** 1087-1131 (2014)

Lower bound

$$\langle\varphi|H_0|\varphi\rangle + 2\Re\langle\varphi|F^\dagger|\varphi\rangle = \delta\langle\varphi|H_0|\varphi\rangle + (1-\delta)\langle\varphi|H_0|\varphi\rangle + 2\Re\langle\varphi|F^\dagger|\varphi\rangle,$$

with

$$\alpha\langle\varphi|H_0|\varphi\rangle + 2\Re\langle\varphi|F^\dagger|\varphi\rangle = \alpha\langle\varphi|H_0|\varphi\rangle + 2\Re\langle\varphi|H_0^{1/2}H_0^{-1/2}F^\dagger|\varphi\rangle =$$

$$\|\alpha^{1/2}H_0^{1/2}\varphi + \alpha^{-1/2}H_0^{-1/2}F^\dagger\varphi\|^2 - \alpha^{-1}\|H_0^{-1/2}F^\dagger\varphi\|^2 \geq -\langle\varphi|F\frac{1}{\alpha H_0}F^\dagger|\varphi\rangle.$$

Lemma

$$\langle\varphi|F\frac{1}{H_0}F^\dagger|\varphi\rangle \leq \langle 0|F\frac{1}{H_0}F^\dagger|0\rangle\|\varphi\|^2 + C\|\hat{V}\|_1^2\langle\varphi|H_0|\varphi\rangle + C\|\hat{V}\|_1^2\|\varphi\|^2\,\mu^{1/4}$$

$$\langle 0|F\frac{1}{H_0}F^\dagger|0\rangle = \frac{\lambda^2}{\sqrt{\mu}}\sum_{\substack{|p|,|q|\leq\sqrt{\mu}\\|p+k|,|q+k|>\sqrt{\mu}}}\frac{|\hat{V}(k)|^2}{2k\cdot(k+p+q)} = \lambda^2 a_1\sqrt{\mu} + o(\sqrt{\mu})$$

Upper bound

Recall

$$E_{corr} = \inf_{\|\varphi\|=1} \langle \varphi, (H_0 + F + F^\dagger + V_2 + \dots)\varphi \rangle$$

As trial state one uses

$$\varphi = \frac{1}{No}(1 - \frac{1}{H_0}F^*)|0\rangle,$$

where No is the norm of $(1 - \frac{1}{H_0}F^*)|0\rangle$.
So,

$$E_{corr} \le \frac{1}{(No)^2}\langle 0|(1 - F\frac{1}{H_0})(H_0 + F + F^\dagger + V_2 + \dots)(1 - \frac{1}{H_0}F^*)|0\rangle$$

Heinz

Thanks for your past contribution to MATHEMATICAL PHYSICS

May there be more in the future

You are YOUNG