Marco Falconi
Università di Roma Tre

Ground State Energy of Interacting Fermions at Low Density

(Joint work with E.L. Giacomelli, C. Hainzl, M. Porta)

Seminario di Fisica Matematica
Università di Roma Tre, October 1st, 2020

Ground State Energy of Interacting Gases at Low Density

Let us consider a system of three dimensional interacting fermions of spin one-half in the thermodynamic limit.

- The pair interaction potential V is positive and short-range (more details later);
- Let us denote by ϱ_σ, $\sigma \in \{\uparrow, \downarrow\}$, the density of spin-up and spin-down fermions.
- In the dilute regime $\varrho_\sigma \ll 1$, it is well-known that the ground state energy density (energy per unit volume) of the system has the expansion

$$\boxed{e(\varrho_\uparrow, \varrho_\downarrow) = \frac{3}{5}(6\pi^2)^{\frac{2}{3}}(\varrho_\uparrow^{\frac{5}{3}} + \varrho_\downarrow^{\frac{5}{3}}) + 8\pi a \varrho_\uparrow \varrho_\downarrow + o(\varrho^2)\,.}$$

- The above expansion was firstly proved in a rigorous fashion by Lieb, Seiringer, and Solovej [*Phys. Rev.* 2005], and then extended by Seiringer [*CMP* 2006] to the computation of the thermodynamic pressure at positive temperature. For the related Hubbard model, an analogous result has been obtained combining the upper bound proved by Giuliani [*JMP* 2007] with the lower bound of Seiringer and Yin [*JSP* 2008].
- The interaction potential appears by means of the *scattering length* a. The scattering length is defined as follows: let f be the solution of

$$\left(-\Delta + \frac{V}{2}\right) f = 0$$

with boundary condition $f(x) \to 1$ as $|x| \to \infty$. Then

$$8\pi a_0 = \int_{\mathbb{R}^3} V(x) f(x) \mathrm{d}x \,.$$

- In the corresponding system of (spinless) bosons, the expansion is perfectly analogous:

$$e(\varrho) = 4\pi\varrho^2 + o(\varrho^2)\,.$$

This has been proved by Lieb and Yngvason [*PRL* 1998] (next order recently obtained by Fournais and Solovej [*arXiv* 2019], using the upper bound by Yau and Yin [*JSP* 2009]).

Fermi Gas Hamiltonian in Second Quantization

The Hamiltonian of a Fermi gas of N particles could be written in a standard fashion as

$$H_N = -\sum_{i=1}^{N} \Delta_{x_i} + \sum_{i<j} V(x_i - x_j) \, .$$

However, it is particularly convenient to recast its Hamiltonian in second quantized form.

- The *Fermionic Fock Space* $\mathcal{F} = \Gamma_{\mathrm{a}}(L^2(\Lambda, \mathbb{C}^2))$, where Λ is taken for convenience to be the torus of volume $|\Lambda| = L^3$, is defined as:

$$\mathcal{F} = \Gamma_{\mathrm{a}}(L^2(\Lambda, \mathbb{C}^2)) = \bigoplus_{n\in\mathbb{N}} \mathcal{F}_n \, ,$$

where $\mathcal{F}_0 = \mathbb{C}$, and for all $n \geq 1$

$$\mathcal{F}_n = \underbrace{L^2(\Lambda, \mathbb{C}^2) \wedge L^2(\Lambda, \mathbb{C}^2) \wedge \cdots \wedge L^2(\Lambda, \mathbb{C}^2)}_{n} \, .$$

- The *Creation and Annihilation Operators* $a^*_{x,\sigma}, a_{x,\sigma}$ respectively create and annihilate a fermionic particle with spin σ at position x. They satisfy the CAR:

$$\{a_{x,\sigma}, a^*_{y,\sigma'}\} = \delta_{\sigma\sigma'}\delta(x-y)\ ,\ \{a_{x,\sigma}, a_{y,\sigma'}\} = \{a^*_{x,\sigma}, a^*_{y,\sigma'}\} = 0\ .$$

- The number operator $\mathcal{N}_\sigma$ counts the (average) number of fermions with spin σ in a Fock state:

$$\mathcal{N}_\sigma = \int_\Lambda a^*_{x,\sigma} a_{x,\sigma} \mathrm{d}x\ .$$

- The Fock-sector $\mathcal{F}^{(N_\uparrow, N_\downarrow)} \subset \mathcal{F}$ is the one spanned by eigenstates of both $\mathcal{N}_\uparrow$ and $\mathcal{N}_\downarrow$, respectively with eigenvalues $N_\uparrow$ and $N_\downarrow$. In other words, these states have exactly $N = N_\uparrow + N_\downarrow$ particles.

- The Hamiltonian H_N can thus be extended on the whole Fock space to (they coincide on $\mathcal{F}^{(N_\uparrow,N_\downarrow)}$):

$$\mathcal{H} = \sum_{\sigma\in\{\uparrow,\downarrow\}} \int_\Lambda \nabla_x a^*_{x,\sigma} \nabla_x a_{x,\sigma} \mathrm{d}x + \frac{1}{2} \sum_{\sigma,\sigma'\in\{\uparrow,\downarrow\}} \int_{\Lambda\times\Lambda} V(x-y) a^*_{x,\sigma} a^*_{y,\sigma'} a_{y,\sigma'} a_{x,\sigma} \mathrm{d}x\mathrm{d}y \,.$$

- The energy $E(N_\uparrow,N_\downarrow)$ and energy density $e(\varrho_\uparrow,\varrho_\downarrow)$ can thus be written as

$$E(N_\uparrow,N_\downarrow) = \inf_{\psi\in\mathcal{F}^{(N_\uparrow,N_\downarrow)}} \frac{\langle\psi,\mathcal{H}\psi\rangle_{\mathcal{F}}}{\langle\psi,\psi\rangle_{\mathcal{F}}} \;;$$

$$e(\varrho_\uparrow,\varrho_\downarrow) = \frac{E(N_\uparrow,N_\downarrow)}{|\Lambda|} \,.$$

Main Result

Theorem (F., Giacomelli, Hainzl, Porta [arXiv 2020])

Let $V \in L^1(\Lambda) \cap C^k(\Lambda)$, $V \geq 0$, and V "compactly supported"[a]. Then if $|\Lambda|$ is large enough, there exists $k_0 > 0$ such that, for all $k \geq k_0$:

$$e(\varrho_\uparrow, \varrho_\downarrow) = \frac{3}{5}(6\pi^2)^{\frac{2}{3}}(\varrho_\uparrow^{\frac{5}{3}} + \varrho_\downarrow^{\frac{5}{3}}) + 8\pi a \varrho_\uparrow \varrho_\downarrow + r(\varrho_\uparrow, \varrho_\downarrow) \, .$$

The remainder satisfies the following bound[b]*:*

$$-C_V \, \varrho^{2+\xi_2} \leq r(\varrho_\uparrow, \varrho_\downarrow) \leq C_V \, \varrho^{2+\xi_1} \, ,$$

with $\xi_1 = \frac{2}{9}$ and $\xi_2 = \frac{1}{9}$.

[a] V satisfies $V = \mathscr{F}_\Lambda^{-1}(\mathscr{F}_{\mathbb{R}^3}(V_\infty))$, with V_∞ compactly supported on $\mathbb{R}^3$.
[b] $\varrho = \varrho_\uparrow + \varrho_\downarrow$.

Remarks

- Some restrictions on V, in particular the regularity condition $V \in C^k$, although needed for our strategy, seem to be technical and could possibly be overcome. In fact, the original proof by Lieb, Seiringer, and Solovej even allows hard spheres' potentials.
- Compared to the original proof, however, we a better bound for the remainder, that is not so far from the optimal value ($\varrho^{\frac{7}{3}}$). In the original proof, $\xi_1 = \frac{2}{27}$ and $\xi_2 = \frac{1}{39}$.

Bosonic Bogoliubov Transformations

- To take into account correlations in Bose gases, and in particular to single out the scattering length a of the interaction potential V, *Bosonic Bogoliubov Transformations (BBTs) play a crucial role*. There is a large literature on the topic [BenDeOSch, BocBreCenSch, ...].
- A bosonic Bogoliubov transformation T_{b} is roughly speaking a canonical transformation for the canonical observables $a^*_{\mathrm{b}}, a_{\mathrm{b}}$ (satisfying CCR): it is a unitary operator such that the newly defined creation and annihilation operators

$$b^* := T^*_{\mathrm{b}} a^*_{\mathrm{b}} T_{\mathrm{b}} \ , \ b := T^*_{\mathrm{b}} a_{\mathrm{b}} T_{\mathrm{b}}$$

still satisfy the CCR.

BBT for Pairs of Fermions

- The intuition at the core of our proof strategy is the following:

  Pairs of fermions almost behave as bosons.

- Therefore, *we will mimic the BBT, using suitable couples of fermionic creation and annihilation operators in place of each bosonic one*. Since the generator of any (unitary) BBT is quadratic in bosonic creation and annihilation operators, the generator of the fermionic implementation of the BBT will be quartic in fermionic creation and annihilation operators.

The Free Fermi Gas: Slater Determinants

- A simple upper bound for the energy density $e(\varrho_\uparrow, \varrho_\downarrow)$ (correctly describing the lowest order contribution) is obtained considering the so-called *Free Fermi Gas State*, or *Slater Determinant* as a trial state.
- In order to define the Slater Determinant, it is convenient to pass to momentum representation. Let us define plane waves f_k, $k \in \left(\frac{2\pi}{|\Lambda|^{\frac{1}{3}}}\right)\mathbb{Z}^3$, as

$$f_k(x) = \frac{1}{\sqrt{|\Lambda|}} e^{ik\cdot x} \ .$$

Then the creation and annihilation operators in momentum space are given by

$$\hat{a}^*_{k,\sigma} = \frac{1}{\sqrt{|\Lambda|}} \int_\Lambda a^*_{x,\sigma} f_k(x) \mathrm{d}x \ , \ \hat{a}_{k,\sigma} = \frac{1}{\sqrt{|\Lambda|}} \int_\Lambda a_{x,\sigma} \bar{f}_k(x) \mathrm{d}x \ .$$

- Let us also define the Fermi Momenta k_{F}^{σ} and Fermi Balls $\mathcal{B}_{\mathrm{F}}^{\sigma}$ as

$$\mathcal{B}_{\mathrm{F}}^{\sigma} = \{k \in (\frac{2\pi}{|\Lambda|^{\frac{1}{3}}})\mathbb{Z}^3 \, , \, |k| \leq k_F^{\sigma}\} \, ;$$

with k_{F}^{σ} chosen in such a way that $N_{\sigma} = |\mathcal{B}_{\mathrm{F}}^{\sigma}|$.

Remark

Depending on N_{σ}, there may be no possible choice of k_{F}^{σ} such that $N_{\sigma} = |\mathcal{B}_{\mathrm{F}}^{\sigma}|$. However, since we are interested in the thermodynamic regime $N_{\sigma} \to \infty$, we can restrict to (increasing) values of N_{σ} such that equality is possible.

- We are now able to define the *Slater Determinant* (SD) as

$$\Phi_{\mathrm{FFG}} = \prod_{\sigma\in\{\uparrow,\downarrow\}} \prod_{k\in\mathcal{B}_{\mathrm{F}}^{\sigma}} \hat{a}^*_{k,\sigma}\Omega \,,$$

where Ω is the Fock vacuum.

- Let us additionally define the 1-particle reduced density matrix $\omega_{\sigma,\sigma'}$ of the SD as the operator on $L^2(\Lambda;\mathbb{C}^2)$ with integral kernel

$$\omega_{\sigma,\sigma'}(x,y) = \delta_{\sigma,\sigma'} \sum_{k\in\mathcal{B}_{\mathrm{F}}^{\sigma}} \bar{f}_k(y) f_k(x) \,,$$

and the operators $u_{\sigma,\sigma'}, v_{\sigma,\sigma'}$ with kernels

$$u_{\sigma,\sigma'}(x,y) = \delta_{\sigma,\sigma'}\delta(x-y) - \omega_{\sigma,\sigma'}(x,y) \,,\ v_{\sigma,\sigma'}(x,y) = \delta_{\sigma,\sigma'}\bar{f}_k(y)\bar{f}_k(x) \,.$$

- Then, since $uv^* = 0$ and $v^*v = \omega$, by Shale–Stinespring's theorem there exists a unitary operator R on the Fock space such that:
  - $$\Phi_{\mathrm{FFG}} = R\Omega\,;$$
  - $$R^* a_{x,\sigma} R = \int_\Lambda (\bar{u}_{\sigma,\sigma}(x,y) a_{y,\sigma} + \bar{v}_{\sigma,\sigma}(y,x) a^*_{y,\sigma}) \mathrm{d}y =: a_\sigma(u_x) + a^*_\sigma(\bar{v}_x)\,;$$
  - $$R^* \hat{a}_{k,\sigma} R = \begin{cases} \hat{a}_{k,\sigma} & \text{if } k \notin \mathcal{B}^\sigma_{\mathrm{F}} \\ \hat{a}^*_{k,\sigma} & \text{if } k \in \mathcal{B}^\sigma_{\mathrm{F}} \end{cases}.$$
- As previously mentioned,

$$\tfrac{1}{|\Lambda|}\langle R\Omega, \mathcal{H} R\Omega\rangle_{\mathcal{F}} \leq \frac{E_{\mathrm{HF}}(\omega)}{|\Lambda|} = \tfrac{3}{5}(6\pi^2)^{\frac{2}{3}}(\varrho_\uparrow^{\frac{5}{3}} + \varrho_\downarrow^{\frac{5}{3}}) + \hat{V}(0)\varrho_\uparrow\varrho_\downarrow + \mathrm{O}(\varrho^{\frac{7}{3}})\,,$$

and thus the SD is a good trial state to capture the kinetic order of the ground state expansion, but not correlations.

The Correlation Fermionic BBT

- Let us consider the solution $1-\varphi_\infty$ of the scattering equation for the "unperiodized" potential:

$$\left(-\Delta + \frac{V_\infty}{2}\right)(1-\varphi_\infty) = (1-\varphi_\infty)\,.$$

  And define its "periodization" $\varphi = \mathscr{F}_\Lambda^{-1}(\mathscr{F}_{\mathbb{R}^3}(\varphi_\infty))$.

- In addition define the *pseudo-bosonic* creation and annihilation operators $\hat{b}^*_{p,\sigma}, \hat{b}_{p,\sigma}$ defined by

$$\hat{b}_{p,\sigma} = \int_\Lambda e^{ip\cdot x} a_\sigma(u_x) a_\sigma(\bar{v}_x) \mathrm{d}x = \sum_{k\in\mathcal{B}_F^\sigma\,:\,k+p\notin\mathcal{B}_F^\sigma} \hat{a}_{k+p,\sigma}\hat{a}_{k,\sigma}\,.$$

Remark

$$[\hat{b}_{p,\sigma}, \hat{b}^*_{q,\sigma'}] = \underbrace{|\mathcal{B}_{\mathrm{F}}^{\sigma}|\delta_{\sigma,\sigma'}\delta_{p,q}}_{\text{CCR}} + \underbrace{\delta_{\sigma,\sigma'} \sum_{\substack{k,k' \in \mathcal{B}_{\mathrm{F}}^{\sigma} \\ k+p, k'+q \notin \mathcal{B}_{\mathrm{F}}^{\sigma}}} \left(\delta_{k,k'} \hat{a}^*_{k'+q,\sigma} \hat{a}_{k+p,\sigma} + \delta_{k+p,k'+q} \hat{a}^*_{k',\sigma'} \hat{a}_{k,\sigma}\right)}_{\text{Error - Subdominant Contribution}}$$

Definition (Correlation Fermionic BBT)

$$T_\lambda = e^{\lambda(B-B^*)}\ ;$$

where $\lambda \in [0,1]$, and

$$B = \int_{\Lambda\times\Lambda} \varphi(z-z')a_\uparrow(u_z)a_\uparrow(\bar{v}_z)a_\downarrow(u_{z'})a_\downarrow(\bar{v}_{z'})\mathrm{d}z\mathrm{d}z' = \sum_p \hat{\varphi}(p)\hat{b}_{p,\uparrow}\hat{b}_{-p,\downarrow}\ .$$

Definition (Correlation Fermionic BBT)

$$T_\lambda = e^{\lambda(B - B^*)} \; ;$$

where $\lambda \in [0,1]$, and

$$B = \int_{\Lambda \times \Lambda} \varphi_\varrho(z - z') a_\uparrow(u_z^{r_\varrho}) a_\uparrow(\overline{v}_z^{r_\varrho}) a_\downarrow(u_{z'}^{r_\varrho}) a_\downarrow(\overline{v}_{z'}^{r_\varrho}) \mathrm{d}z \mathrm{d}z' = \sum_p \hat{\varphi}_\varrho(p) \hat{b}_{p,\uparrow}^{r_\varrho} \hat{b}_{-p,\downarrow}^{r_\varrho} \, .$$

Definition (Correlation Fermionic BBT)

$$T_\lambda = e^{\lambda(B-B^*)}\ ;$$

where $\lambda \in [0,1]$, and

$$B = \int_{\Lambda\times\Lambda} \varphi_\varrho(z-z')a_\uparrow(u_z^{\mathrm{r}\varrho})a_\uparrow(\overline{v}_z^{\mathrm{r}\varrho})a_\downarrow(u_{z'}^{\mathrm{r}\varrho})a_\downarrow(\overline{v}_{z'}^{\mathrm{r}\varrho})\mathrm{d}z\mathrm{d}z' = \sum_p \hat{\varphi}_\varrho(p)\hat{b}_{p,\uparrow}^{\mathrm{r}\varrho}\hat{b}_{-p,\downarrow}^{\mathrm{r}\varrho}\ .$$

Definition (Trial State for ϱ^2)

$$\psi_{\mathtt{trial}} = T_1 R\Omega\ .$$

Proposition (Upper Bound)

$$\frac{1}{|\Lambda|}\langle\psi_{\mathtt{trial}},\mathcal{H}\psi_{\mathtt{trial}}\rangle_{\mathcal{F}} \leq \frac{3}{5}(6\pi^2)^{\frac{2}{3}}(\varrho_\uparrow^{\frac{5}{3}}+\varrho_\downarrow^{\frac{5}{3}}) + 8\pi a\varrho_\uparrow\varrho_\downarrow + r(\varrho_\uparrow,\varrho_\downarrow)\,.$$

Remarks

- The right φ was not guessed. If one computes the above expectation with an arbitrary φ, $8\pi a\varrho_\uparrow\varrho_\downarrow$ is obtained only if $(1-\varphi)$ is the solution of the scattering equation.
- $\langle\psi_{\mathtt{trial}},\mathcal{H}\psi_{\mathtt{trial}}\rangle_{\mathcal{F}} = \langle\Omega, R^*T_1^*\mathcal{H}T_1R_1\Omega\rangle_{\mathcal{F}}$. $R^*T_1^*\mathcal{H}T_1R_1$ is explicitly computable, and the second order correlation energy is extracted from it.

Lower Bound

- The lower bound requires some additional work. The basic idea is to start from an *approximate ground state* ψ, *i.e.* a state satisfying
$$\left|\langle\psi,\mathscr{H}\psi\rangle_{\mathcal{F}} - \sum_{\sigma\in\{\uparrow,\downarrow\}}\sum_{k\in\mathcal{B}_{\mathrm{F}}^{\sigma}}|k|^2\right| \leq C|\Lambda|\varrho^2\,.$$
- From ψ, we extract the kinetic energy:

$$\langle\psi,\mathscr{H}\psi\rangle \geq E_{\mathrm{HF}}(\omega) + \langle\xi_0,(\diamond+\sharp+\star)\xi_0\rangle + \text{controllable error}\,,$$

where
$$\xi_\lambda = T_\lambda^* R^* \psi\,.$$

- Now, in order to extract the correlation energy from $\langle \xi_0, (\dots)\xi_0 \rangle$, we "interpolate": for all

$$\langle \xi_0, (\cdots)\xi_0 \rangle = \langle \xi_1, (\cdots)\xi_1 \rangle - \int_0^1 \frac{\mathrm{d}}{\mathrm{d}\lambda} \langle \xi_\lambda, (\cdots)\xi_\lambda \rangle = -\rho_\uparrow \varrho_\downarrow \int_{\Lambda\times\Lambda} V(x-y)\varphi_\varrho(x-y)\mathrm{d}x\mathrm{d}y$$

+controllable error.

- Now using the scattering equation (again up to some controllable error), we finally obtain the lower bound

$$\frac{1}{|\Lambda|}\langle \psi, \mathscr{H}\psi \rangle \geq \frac{3}{5}(6\pi^2)^{\frac{2}{3}}(\varrho_\uparrow^{\frac{5}{3}} + \varrho_\downarrow^{\frac{5}{3}}) + 8\pi a \varrho_\uparrow \varrho_\downarrow + r(\varrho_\uparrow, \varrho_\downarrow)\,.$$

- To control the errors we make crucial use of some *a priori* bounds, valid for any ξ_λ constructed from approximate ground states.

Thank you for the attention