Correlation Energy of a Weakly–Interacting Fermi Gas

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Hamilton operator of N identical spinless particles on the (fixed size) 3D torus:

$$H_N := \sum_{i=1}^N (-\Delta_i) + \lambda \sum_{1 \le i < j \le N} V(x_i - x_j) \qquad ext{with } V : \mathbb{R}^3 o \mathbb{R} \;.$$

Acts on the L^2 -space of antisymmetric wave functions of 3N variables

$$\psi(x_{\sigma(1)}, x_{\sigma(2)}, \ldots, x_{\sigma(N)}) = \operatorname{sgn}(\sigma)\psi(x_1, x_2, \ldots, x_N) \qquad \forall \sigma \in S_N .$$

For reasonable potentials, the Hamiltonian is self-adjoint.

spec (H_N) is interpreted as excitation energies measurable in experiments.

Ground State Energy

The ground state energy is defined as

$$E_{N} := \inf \operatorname{spec} \left(H_{N} \right) = \inf_{\substack{\psi \in L_{a}^{2}(\mathbb{T}^{3N}) \\ \|\psi\|=1}} \langle \psi, H_{N}\psi \rangle .$$

How to compute E_N ? Define the reduced density matrices

$$\gamma^{(2)} := \frac{N!}{(N-2)!} \operatorname{tr}_{3,4,\dots,N} |\psi\rangle \langle\psi|, \qquad \gamma^{(1)} := \frac{1}{N-1} \operatorname{tr}_2 \gamma^{(2)}.$$

Then

$$\langle \psi, H_N \psi \rangle = \operatorname{tr} \left(-\Delta \gamma^{(1)} \right) + \frac{1}{2} \iint V(x_1 - x_2) \gamma^{(2)}(x_1, x_2; x_1, x_2) \, \mathrm{d}x_1 \mathrm{d}x_2 \; .$$

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So we simply minimize over $\gamma^{(2)}$?

The set of all 2-particle rdm is hard to characterize: N-representability problem.

This problem cannot be solved in full generality: H_N describes almost the entire variety of our daily lives, superconductors, neutron stars, our bodies...

Be more specific, look at well-defined physical situations!

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Simplest possibility: high density and with weak interaction.

 \sim We expect mean-field behavior: one particle moving through a continuous cloud generated by all the other particles.

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Mathematical Model: Mean-Field Scaling Regime

- high density: fixed volume (torus) and N particles, $N \to \infty$.
- weak interation: $\lambda = N^{-1/3}$ because

$$\left\langle \sum_{i=1}^N \left(-\Delta_i
ight)
ight
angle \sim N^{5/3} \quad (ext{antisymmetry!}) \;, \qquad \left\langle \lambda \sum_{1 \leq i < j \leq N} V(x_i - x_j)
ight
angle \sim \lambda N^2 \;.$$

Leading Order Approximation: Hartree–Fock Theory

Hartree–Fock Theory = Restriction to Slater Determinants

Multiply the entire Hamiltonian by $\times \hbar^2$, with $\hbar := N^{-1/3}$:

$$H_N = \sum_{i=1}^N \left(-\hbar^2 \Delta_i\right) + \frac{1}{N} \sum_{1 \leq i < j \leq N} V(x_i - x_j) .$$

Convergence to the Hartree–Fock energy [Bach '92, Graf–Solovej '94]:

$$|E_N - E_N^{\mathsf{HF}}| = o(N)$$
, where $E_N^{\mathsf{HF}} := \inf_{\substack{\psi \text{ is Slater} \\ \text{determinant}}} \langle \psi, H_N \psi \rangle$.

Achieved restriction to simplest fermionic states: antisymmetrized tensor products,

$$\psi_N = \text{Slater determinant} = \bigwedge_{j=1}^N f_j , \qquad f_j \in L^2(\mathbb{T}^3) .$$

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Moreover: Consider a Slater determinant and evolve it in time — it stays close to a Slater determinant, but with orbitals $f_{j,t}$ evolved under the time-dependent Hartree-Fock equation [B-Porta-Schlein '14]. This is optimal [B-Sok-Solovej '18].

Introduce the Slater determinant of N plane waves

$$\Psi_{\mathcal{N}} := \bigwedge_{k \in \mathcal{B}_{\mathcal{F}}} f_k \,, \qquad \mathcal{B}_{\mathcal{F}} = \text{Fermi ball} := \left\{ k \in \mathbb{Z}^3 \mid |k| \le N^{1/3} \left(\frac{3}{4\pi} \right)^{1/3} \right\}.$$

For the translation-invariant situation on the torus [Gontier-Hainzl-Lewin '18]:

$$E_N^{\mathrm{pw}} := \langle \Psi_N, H_N \Psi_N \rangle = E_N^{\mathsf{HF}} + \mathcal{O}(e^{-N^{1/3}})$$

To summarize:

$$E_N < E_N^{\sf HF} \simeq E_N^{\sf pw}$$
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[Wigner '34]: How to compute the correlation energy $E_N - E_N^{HF}$ (or $E_N - E_N^{pw}$)?

Do better than antisymm. tensor products, include non-trivial quantum correlations!

Describing Correlations by Bosonization

Separating the Slater Determinant

Hamiltonian in momentum representation, written with anti-commuting operators:

$$H_{N} := \hbar^{2} \sum_{k \in \mathbb{Z}^{3}} |k|^{2} a_{k}^{*} a_{k} + \frac{1}{N} \sum_{q,s,k \in \mathbb{Z}^{3}} \hat{V}(k) a_{q+k}^{*} a_{s-k}^{*} a_{s} a_{q}, \qquad \hbar = N^{-1/3}$$

Define the unitary map R ("particle-hole transformation") on fermionic Fock space by

$$egin{array}{ll} R \ket{0} := \Psi_N \;, & R \: a_k^* \: R^* := \left\{ egin{array}{ll} a_k^* & k \in \mathcal{B}_F^c \ a_k & k \in \mathcal{B}_F \end{array}
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Write $\tilde{\Psi}_N = R\xi$, expand R^*H_NR , normal-order: with $e(p) := |\hbar^2|p|^2 - (3/4\pi)^{2/3}|$ get

$$\langle \tilde{\Psi}_{N}, H_{N}\tilde{\Psi}_{N} \rangle = E_{N}^{\mathsf{HF}} + \langle \xi, \left[\underbrace{\sum_{p \in \mathcal{B}_{F}^{c}} e(p)a_{p}^{*}a_{p} + \sum_{h \in \mathcal{B}_{F}} e(h)a_{h}^{*}a_{h}}_{=: H_{\mathsf{kin}}} + \underbrace{Q}_{\mathsf{operators}\ a^{*}, a} \right] \xi \rangle$$

Slater determinant corresponds to $\xi = |\Omega\rangle$: in particular $(H_{\rm kin} + Q) |0\rangle = 0$.

Collective Particle–Hole Pairs

Key observation: if we introduce collective pair creation operators

$$b_k^* := \sum_{\substack{p \in \mathcal{B}_F^c \\ h \in \mathcal{B}_F}} \delta_{p-h,k} a_p^* a_h^* \qquad \qquad p \quad \text{``particle'' outside the Fermi ball} \\ h \quad \text{``hole'' inside the Fermi ball}$$

then

$$Q=rac{1}{N}\sum_{k\in\mathbb{Z}^3}\hat{V}(k)ig(2b_k^*b_k+b_k^*b_{-k}^*+b_{-k}b_kig)+Q_{ ext{non-paired}}$$

This is convenient because the b_k^* and b_k have approximately bosonic commutators:

$$[b_k^*, b_l^*] = 0$$
, $[b_l, b_k^*] = \delta_{k,l} n_k^2 + \mathcal{E}(k,l)$.

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But how to express H_{kin} through pair operators?

Linearizing the Kinetic Energy Locally in Patches

Localize to M = M(N) patches near the Fermi surface,

Fermi ball \mathcal{B}_F



[Benfatto–Gallavotti '90] [Haldane '94]

$$\begin{split} b^*_{\alpha,k} &:= \frac{1}{n_{\alpha,k}} \sum_{\substack{p \in \mathcal{B}_F^c \cap B_\alpha \\ h \in \mathcal{B}_F \cap B_\alpha \\ k \in \mathcal{B}_F \cap B_\alpha }} \delta_{p-h,k} a_p^* a_h^* \end{split}$$
with $n_{\alpha,k}$ such that $\|b^*_{\alpha,k}|0\rangle\| = 1.$

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Linearize kinetic energy around patch center ω_{α} :

 $|H_{
m kin}b^*_{lpha,k}|0
angle\simeq 2\hbar|k\cdot\hat{\omega}_lpha|b^*_{lpha,k}|0
angle$

Approximate as if $b^*_{\alpha,k}$ was a harmonic oscillator mode:

 $egin{aligned} \mathcal{H}_{\mathsf{kin}} &\simeq \sum_{k \in \mathbb{Z}^3} \sum_{lpha = 1}^M 2 \hbar u_lpha(k)^2 b^*_{lpha,k} b_{lpha,k}\,, \quad u_lpha(k)^2 := |k \cdot \hat{\omega}_lpha| \end{aligned}$

(c. f., [Lieb–Mattis '65] for the 1D Luttinger model).

Quadratic Effective Hamiltonian

Recall

$$Q = \frac{1}{N} \sum_{k \in \mathbb{Z}^3} \hat{V}(k) \left(2b_k^* b_k + b_k^* b_{-k}^* + b_{-k} b_k \right) + Q_{\text{non-paired}}$$
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Normalization:

$$n_{lpha,k}^2 = \#$$
p-h pairs in patch B_lpha with momentum $\simeq rac{4\pi N^{2/3}}{M} |k \cdot \hat{\omega}_lpha| = rac{4\pi N^{2/3}}{M} u_lpha(k)^2 \;.$



k

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Effective Bosonic Hamiltonian

$$H^{\text{eff}} = \hbar \sum_{k \in \mathbb{Z}^3} \left[\sum_{\alpha} u_{\alpha}(k)^2 b_{\alpha,k}^* b_{\alpha,k} + \frac{\hat{V}(k)}{M} \sum_{\alpha,\beta} \left(u_{\alpha}(k) u_{\beta}(k) b_{\alpha,k}^* b_{\beta,k} + u_{\alpha}(k) u_{\beta}(k) b_{\alpha,k}^* b_{\beta,-k}^* + \text{h.c.} \right) \right]$$

k



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Diagonalization of the Bosonic Hamiltonian

 $H^{\text{eff}} = \hbar \sum_{k, e^{\pi/2}} \left[h^{\text{eff}}(k) - \frac{1}{2} \operatorname{tr}(D(k) + W(k)) \right]$ We can write where $h^{\text{eff}} = \frac{1}{2} \begin{pmatrix} (b^*)^T & b^T \end{pmatrix} \begin{pmatrix} D+W & \widetilde{W} \\ \widetilde{W} & D+W \end{pmatrix} \begin{pmatrix} b \\ b^* \end{pmatrix}, \qquad b = \begin{pmatrix} \vdots \\ b_{\alpha} \\ \vdots \end{pmatrix},$ $D = \begin{pmatrix} \operatorname{diag}(u_{\alpha}^2) & 0\\ 0 & \operatorname{diag}(u^2) \end{pmatrix}, \quad W = \hat{V} \begin{pmatrix} |u\rangle\langle u| & 0\\ 0 & |u\rangle\langle u| \end{pmatrix}, \quad \widetilde{W} = \hat{V} \begin{pmatrix} 0 & |u\rangle\langle u| \\ |u\rangle\langle u| & 0 \end{pmatrix}.$

The model is solved (spectrum computed) if we can find linear combinations of b- and b^* -operators, called \tilde{b} , with the same CCR such that

$$h^{ ext{eff}} = \sum_{\gamma=1}^M e_\gamma \left(ilde{b}^*_\gamma \, ilde{b}_\gamma + rac{1}{2}
ight) \;, \quad e_\gamma \in \mathbb{R} \;.$$

These are Bogoliubov transformations (or complexified symplectic transformations).

We achieve diagonalization up to a one-particle unitary [B '19] (which is sufficient):

$$h^{ ext{eff}} = \sum_{\gamma,\delta=1}^{M} E_{\gamma,\delta} \, ilde{b}_{\gamma}^{*} \, ilde{b}_{\delta} + rac{1}{2} \, ext{tr} \, E \;, \qquad E \simeq \sqrt{ ext{diag}(u_{lpha}^{2}) + \hat{V} |u
angle \langle u|} \geq 0 \;.$$

In the limit of large number of patches, $M
ightarrow \infty$, the correlation energy becomes

$$\begin{split} \hbar \sum_{k \in \mathbb{Z}^3} \frac{1}{2} \operatorname{tr} \left(E(k) - D(k) - W(k) \right) \\ \to E_N^{\mathsf{RPA}} := \hbar \sum_{k \in \mathbb{Z}^3} |k| \left[\int_0^\infty \log \left(1 + \hat{V}(k) \left(1 - \lambda \arctan \lambda^{-1} \right) \right) \mathsf{d}\lambda - \frac{1}{4} \hat{V}(k) \right] \; . \end{split}$$

Predicted by partial resumm. of pert. theory [Macke '50, Gell-Mann-Brueckner '57].

Rigorous Result: Correlation Energy

Theorem: [B-Nam-Porta-Schlein-Seiringer '19, '20]

Let $\hat{V}(k)$ be non-negative and compactly supported with sufficiently small $\|\hat{V}\|_{\ell^{\infty}}$. Then as number of particles $N \to \infty$ we have

$$E_N = E_N^{HF} + E_N^{RPA} + \mathcal{O}(\hbar^{1+\frac{1}{48}}) \qquad (\hbar = N^{-1/3}) \; .$$

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The upper bound follows from a computation with a trial state (variational principle). Proof of the lower bound is the rest of the talk.

Remarks: [Hainzl–Porta–Rexze '19] obtained a rigorous lower bound to second order in \hat{V} ,

$$E_N \geq E^{\mathsf{HF}} - \hbar rac{\pi}{2} (1 - \log 2) \sum_{k \in \mathbb{Z}^3} |k| \hat{V}(k)^2 + \mathcal{O}(\hat{V}^3) \; .$$

Proof of the Lower Bound

Explicit Diagonalization of the Hamiltonian

The previously introduced Bogoliubov transformation has an explicit formula:

$$T = \exp\left(\sum_{k \in \mathbb{Z}^3} \sum_{\alpha,\beta=1}^M K(k)_{\alpha,\beta} b^*_{\alpha,k} b^*_{\beta,-k} - \mathsf{h.c.}\right), \quad K(k) = \log|S_1|$$

and thus, in the exactly bosonic picture,

$$\mathcal{T} \ h^{ ext{eff}} \mathcal{T}^* = \sum_{\gamma,\delta=1}^M \mathcal{E}_{\gamma,\delta} \ b_\gamma^* \ b_\delta + rac{1}{2} \operatorname{tr} \mathcal{E} \quad \geq rac{1}{2} \operatorname{tr} \mathcal{E} \ .$$

Makes sense even if the b^* -operators are actually pairs of fermionic operators.

To control: gapless excitations, non-bosonizable terms, errors in approximate CCR.

Strategy (1/2)

- 1. A-priori estimate: $\|b(k)\psi\| \le CN^{1/2} \|H_{kin}^{1/2}\psi\|$ [Hainzl-Porta-Rexze '19]. Thus $H_{kin} \le C(H_{kin} + Q) \le \hbar$.
- 2. Bound on the number operator: $|\{| attice points on the sphere \}| \leq C_{\epsilon} N^{1/3+\epsilon}$, thus

$$\mathcal{N} := \sum_{i \in \mathbb{Z}^3} a_i^* a_i \le \sum_{e(i) \le N^{-\theta}} 1 + \sum_{e(i) > N^{-\theta}} a_i^* a_i^* \stackrel{\theta = 2/3}{\le} CN^{1/3 + \epsilon} + N^{2/3} H_{\mathsf{kin}} = \mathcal{O}(N^{1/3}) \; .$$

- 3. IMS localization in Fock space to control also powers of $\ensuremath{\mathcal{N}}.$
- Removing gapless pair excitations (momentum approximately parallel to Fermi surface) and corridors from Hamiltonian using H_{kin}-, N-bounds.
- 5. Approximate CCR:

$$[b_{\alpha,k}, b_{\beta,l}^*] = \delta_{\alpha,\beta} \left(\delta_{k,l} + \mathcal{E}_{\alpha}(k,l) \right) , \qquad \mathcal{E}_{\alpha}(k,l) \text{ bounded by } \mathcal{N}$$

6. $Tb_{\alpha,k}T^* = \sum_{\gamma} \cosh(K)_{\alpha,\gamma}b_{\gamma,k} + \sum_{\gamma} \sinh(K)_{\alpha,\gamma}b_{\gamma,k}^* + \mathfrak{E}_{\alpha,k}$ (almost bosonic BT).

Strategy (2/2)

- 7. Major improvement I: boson bounds avoiding the uncontrollable energy gap $\|b_{\alpha,k}\psi\| \leq \|\mathcal{N}_{\delta}^{1/2}\psi\| \qquad \text{where } \mathcal{N}_{\delta} := \sum_{e(i) > \frac{1}{4}N^{-1/3-\delta}} a_i^*a_i \ , \quad \delta \text{ to be optimized.}$
- 8. Major improvement II: strong control on the Bogoliubov kernel K(k)

$$|\mathcal{K}(k)_{\alpha,\beta}| \leq \frac{C}{M} \min\left\{\frac{u_{\alpha}(k)}{u_{\beta}(k)}, \frac{u_{\beta}(k)}{u_{\alpha}(k)}\right\}$$
(1)

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- 9. Major improvement III: strong bound on linearization of kinetic energy permits $M \gg N^{2\delta}$ instead of $M \gg N^{1/3}$.
- 10. Major improvement IV: non-bosonizable terms

partial transformation & completing the square $\Rightarrow Q_{\text{non-pair}} \ge -\|\hat{V}\|_{\ell^{\infty}}H_{\text{kin}}$. 11. $H_{\text{kin}} + Q = H_{\text{kin}} - H_{\text{kin}}^{\text{B}} + H_{\text{kin}}^{\text{B}} + Q$. We have $T\left(H_{\text{kin}} - H_{\text{kin}}^{\text{B}}\right)T^* \simeq \left(H_{\text{kin}} - H_{\text{kin}}^{\text{B}}\right)$, $H_{\text{kin}}^{\text{B}} + Q = \sum_{\gamma,\delta=1}^{M} E_{\gamma,\delta} \tilde{b}_{\gamma}^* \tilde{b}_{\delta} + \frac{1}{2} \operatorname{tr} E \ge H_{\text{kin}}^{\text{B}} - \|\hat{V}\|_{\ell^{\infty}}H_{\text{kin}} + \frac{1}{2} \operatorname{tr} E$ using (1).

Kinetic bound [Hainzl-Porta-Rexze '19]

Proof of the kinetic bound.

$$\begin{split} \|b(k)\psi\| &\leq \sum_{\substack{p \in B_{\mathsf{F}}^{c} \\ h \in B_{\mathsf{F}}}} \delta_{p-h,k} \|a_{h}a_{p}\psi\| = \sum_{\substack{p \in B_{\mathsf{F}}^{c} \\ h \in B_{\mathsf{F}}}} \delta_{p-h,k} \frac{1}{\sqrt{e(p) + e(h)}} \sqrt{e(p) + e(h)} \|a_{h}a_{p}\psi\| \\ &\leq \left[\sum_{\substack{p \in B_{\mathsf{F}}^{c} \\ h \in B_{\mathsf{F}}}} \delta_{p-h,k} \frac{1}{e(p) + e(h)}\right]^{1/2} \left[\sum_{\substack{p \in B_{\mathsf{F}}^{c} \\ h \in B_{\mathsf{F}}}} \delta_{p-h,k} (e(p) + e(h)) \|a_{h}a_{p}\psi\|^{2}\right]^{1/2} \\ &\leq \left[\sum_{\substack{p \in B_{\mathsf{F}}^{c} \\ h \in B_{\mathsf{F}}}} \delta_{p-h,k} \frac{1}{e(p) + e(h)}\right]^{1/2} \left[\sum_{\substack{p \in B_{\mathsf{F}}^{c} \\ h \in B_{\mathsf{F}}}} \delta_{p-h,k} \left(e(p) \|a_{p}\psi\|^{2} + e(h) \|a_{h}\psi\|^{2}\right)\right]^{1/2} \\ &\leq CN^{1/2} \|H_{\mathsf{kin}}^{1/2}\psi\| \;. \end{split}$$

The sum is singular near the Fermi surface – estimate by $CN^{1/2}$ requires use of number theoretic results about counting of lattice points!

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Removing Gapless Excitations



Removing Gapless Excitations



Introduce a cut-off: instead of $b_k^* = \sum_{\alpha = 1^M} n_{\alpha,k} b_{\alpha,k}^*$ consider

$$b_k^*\simeq \sum_{lpha\in \mathcal{I}_k^+} n_{lpha,k} b_{lpha,k}^* \; ,$$

where

$$\mathcal{I}_k^+ := \left\{ lpha \in \{1, 2, \dots, M\} : \ k \cdot \hat{\omega}_lpha > N^{-\delta}
ight\}$$

Difference can be controlled by

$$(\ldots) \leq C N^{1/2 - \delta/2} \| H_{kin}^{1/2} \psi \| .$$

Boson bounds avoiding the uncontrollable energy gap

Proof of $\|b_{\alpha,k}\psi\| \le \|\mathcal{N}_{\delta}^{1/2}\psi\|$. Recall $\mathcal{N}_{\delta} := \sum_{e(i) > \frac{1}{4}N^{-1/3-\delta}} a_i^*a_i, \delta$ as in the cut-off. $\|b_{\alpha,k}\psi\| \leq \frac{1}{n_{\alpha}(k)} \sum_{p \in B^{\underline{c}}} \delta_{p-h,k} \|a_h a_p \psi\|$ h∈B $\leq \frac{1}{n_{\alpha}(k)} \sum_{p \in B^{c}} \delta_{p-h,k} \min\{\|a_{p}\psi\|, \|a_{h}\psi\|\}.$ $h \in \mathbb{R}_{\mathbb{P}}$ Due to $\alpha \in \mathcal{I}_{L}^{+}$ we have $k \cdot \hat{\omega}_{\alpha} > N^{-\delta}$, thus $e(p) + e(h) = \hbar^2 p^2 - \hbar^2 h^2 = \hbar^2 \left(p^2 - (p-k)^2 \right) = \hbar^2 \left(2p \cdot k - k^2 \right)$ $\simeq \hbar^2 2 \omega_lpha \cdot k = 2 (rac{3}{4\pi})^{1/3} \hbar k \cdot \hat{\omega}_lpha \geq rac{1}{2} \mathcal{N}^{-1/3-\delta} \; .$

Thus $e(p) > \frac{1}{4}N^{-1/3-\delta}$ or $e(h) > \frac{1}{4}N^{-1/3-\delta}$. "Lower bound on excitation energy".

Linearization of the Kinetic Energy



Error bounded by $\hbar N_{\delta}^{1/2} M^{-1/2} \ll \hbar$. Major improvement: $M \gg N^{\delta}$ is sufficient.

Non–Bosonizable Terms

Non–bosonizable terms. Positive non–pair term + coupling to pairs

$$Q_{ ext{non-pair}} = rac{1}{N} \sum_{k \in \mathbb{Z}^3} \hat{V}(k) \left(D^*(k) D(k) + D^*(k) b(k) + b(k) D^*(k)
ight) \; .$$

Of course

$$D^*(k)b(k) \geq -rac{1}{2}D^*(k)D(k) - rac{1}{2}b^*(k)b(k) \geq -rac{1}{2}D^*(k)D(k) - rac{1}{2}H_{ ext{kin}} \; .$$

To use this bound we need to first transform the b-operators with the Bogoliubov transformation, and afterward use a similar bound. Only possible because

$$|K(k)_{\alpha,\beta}| \leq \frac{C}{M} \min\left\{\frac{u_{\alpha}(k)}{u_{\beta}(k)}, \frac{u_{\beta}(k)}{u_{\alpha}(k)}\right\} \quad \Rightarrow \quad \sum_{\alpha} K_{\alpha,\beta} n_{\alpha} \leq C n_{\beta} .$$

allows us to remove the cosh(K) and sinh(K) from the transformed expression.

QED