Correlation Energy of the Mean-Field Fermi Gas by Collective Bosonization

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Quantum Many-Body Systems

General Hamiltonian of N identical spinless particles on the 3-dimensional torus

$$H_N := \sum_{i=1}^{N} (-\Delta_i) + \sum_{1 \leq i < j \leq N} V(x_i - x_j) \qquad \text{with } V : \mathbb{R}^3 \to \mathbb{R}$$

on the bosonic Hilbert space

$$L^2_{\text{symm}}(\mathbb{T}^{3N}) := \left\{ \psi \in L^2(\mathbb{T}^{3N}) \mid \psi(x_{\sigma(1)}, x_{\sigma(2)}, \ldots) = \psi(x_1, x_2, \ldots) \quad \forall \sigma \in S_N \right\}$$

or on the fermionic Hilbert space

$$L^2_{\text{antisymm}}(\mathbb{T}^{3N}) := \left\{ \psi \in L^2(\mathbb{T}^{3N}) \mid \psi(x_{\sigma(1)}, x_{\sigma(2)}, \ldots) = \text{sgn}(\sigma)\psi(x_1, x_2, \ldots) \quad \forall \sigma \in S_N \right\}.$$

Ground State Energy

What is the ground state energy

$$E_N := \inf_{\|\psi\|=1} \langle \psi, H_N \psi \rangle = \inf \operatorname{spec}(H_N) \,?$$

Defining the two- and one-particle reduced density matrices (r. d. m.)

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

we always have

$$\langle \psi, H_N \psi \rangle = \operatorname{tr}\left(-\Delta \gamma^{(1)}\right) + \frac{1}{2} \iint V(x_1 - x_2) \gamma^{(2)}(x_1, x_2; x_1, x_2) \, dx_1 dx_2 \,.$$

So we simply minimize over $\gamma^{(2)}$? Unfortunately not: the set of all two-particle reduced density matrices is hard to characterize: N-representability problem.

Bosons

Bosonic Mean-Field Limit

The way out: restrict to specific physical regimes.

Simplest: high density & weak interaction, s. th. we expect approximate mean-field behaviour:

$$H_N^{\mathrm{mf}} = \sum_{i=1}^{N} (-\Delta_i) + \frac{1}{N} \sum_{1 \leq i < j \leq N} V(x_i - x_j)\,, \quad \text{particle number } N \to \infty\,.$$

As $N \to \infty$, the set of two-particle r. d. m. is characterized by Quantum de-Finetti theorem:

$$\frac{(N-k)!}{N!} \gamma^{(k)} \quad \longrightarrow \quad \int |u^{\otimes k}\rangle\langle u^{\otimes k}| \mathrm{d}\mu(u) \qquad \text{factorized, no quantum correlations.}$$

Implies convergence to Hartree functional [Lewin–Nam–Rougerie '13, ...]

$$E_N^{\mathrm{mf}} \to N \inf_{\substack{u \in L^2(\mathbb{R}^3) \\ \|u\|=1}} \left[\int |\nabla u(x)|^2 \mathrm{d}x + \int |u(x)|^2 V(x-y) |u(y)|^2 \,\mathrm{d}x\mathrm{d}y \right] =: N\, E^{\mathrm{Hartree}}\,.$$

Correlation Corrections to the Hartree Functional

Next order correction: due to quantum correlations!

$$E_N^{\mathrm{mf}} \to N\, E^{\mathrm{Hartree}} + \mathcal{O}(1)\,.$$

Bogoliubov theory [Grech–Seiringer '13, Pizzo '15]:

$$E_N^{\mathrm{mf}} \to N\, E^{\mathrm{Hartree}} - \frac{1}{2} \sum_{p \in \mathbb{Z}^3} \left[p^2 + \hat{V}(p) - \sqrt{p^4 + 2p^2 \hat{V}(p)} \right] + \mathcal{O}(N^{-1/2})\,.$$

Remark: In the thermodynamic limit we expect the Lee-Huang-Yang formula

$$E(\rho) \to 4\pi\rho a \left[1 + \frac{128}{15\sqrt{\pi}} (\rho a^3)^{1/2} + \dots \right] \qquad a = \text{scattering length of } V\,, \quad \rho = \text{density}$$

- [Yau–Yin '09]: upper bound
- [Giuliani–Seiringer '09, Brietzke–Solovej '19]: lower bound for long-range potentials
- [Brietzke–Fournais–Solovej '19]: non-optimal lower bound
- [Boccato–Brennecke–Cenatiempo–Schlein '18]: lower bound for Gross-Pitaevskii limit
- lower bound for general case: open.

Fermions

Fermionic Mean-Field Regime

Fermions have high kinetic energy (Fermi energy), to be tamed down in mean-field scaling

$$H_N^{\mathrm{mf}} = \sum_{i=1}^{N} \left(-\hbar^2 \Delta_i\right) + \frac{1}{N} \sum_{1 \leq i < j \leq N} V(x_i - x_j)\,, \qquad \hbar = N^{-1/3}\,.$$

No Quantum de-Finetti theorem — set of two-particle r. d. m. is complicated [Klyachko '06].

Special correlation estimate implies convergence to Hartree–Fock functional [Graf–Solovej '94]:

$$E_N^{\mathrm{mf}} \to \inf_{\substack{\omega^2 = \omega \text{ on } L^2(\mathbb{T}^3) \\ \operatorname{tr}\omega = N}} \left[\operatorname{tr}(-\Delta\omega) + \iint \omega(x,x) V(x-y) \omega(y,y) - \iint |\omega(x,y)|^2 V(x-y) \right] =: E_N^{\mathrm{HF}}\,.$$

[Wigner '34]: What is the next order term, due to quantum correlations?

The Gell-Mann–Brueckner Formula

Originally jellium model considered: no scaling of constants, thermodynamic limit, Coulomb interaction, and density $\rho \to \infty$.

The non-rigorous solution [Bohm–Pines '53, Gell-Mann–Brueckner '57, Sawada et al. '57] also explained screening and collective oscillations (the plasmon).

Random Phase Approximation

$$E^{\text{jellium}}(\rho) = \underbrace{C_{\text{TF}}\rho^{5/3} - C_{\text{D}}\rho^{4/3}}_{\substack{\text{Hartree-Fock energy} \\ \text{of Fermi ball}}} + \underbrace{C_{\text{BP}}\rho\log(\rho) + C_{\text{GB}}\rho}_{\text{correlation energy}} + o(\rho) \qquad \text{as } \rho \to \infty\,.$$

Mean-field scaling with regular interaction is slightly different:

$$E_N^{\text{mf}} = E_N^{\text{HF}} + \underbrace{E^{\text{BP}} + E^{\text{GB},1}}_{\sim N^{-1/3}} + \underbrace{E^{\text{GB},2}}_{\sim N^{-2/3}}\,.$$

How did Gell-Mann and Brueckner calculate the correlation energy?

The random phase approximation of Gell-Mann and Brueckner:

1. Notice: For Coulomb interaction, high orders are badly IR divergent,

$$\hat{V}(k)^n \sim |k|^{-2n} \quad \text{for } k \to 0\,.$$

2. Collect the most divergent term from each order of perturbation theory, finding

$$x - \frac{x^2}{2} + \frac{x^3}{3} + \ldots \qquad \text{with } x \sim \hat{V}(k)$$

Ignore divergence and resum it

$$= \log(1+x)\,.$$

$$\Rightarrow \quad \hbar \sum_{k\in\mathbb{Z}^3} |k| \left[\int_0^\infty \log\Big(1 + \hat{V}(k)\Big(1 - v\arctan v^{-1}\Big)\Big)\,\mathrm{d}v - \frac{1}{4}\hat{V}(k)\right] = E^{\text{BP}} + E^{\text{GB},1}\,.$$

Remark: $E^{\text{GB},2}$ is much simpler, just second-order perturbation of exchange type.

Our Result:
Optimal Upper Bound

Upper Bound on Correlation Energy

Theorem: [B-Nam-Porta-Schlein-Seiringer, arXiv:1809.01902]

Let $\hat{V}(k)$ be non-negative, bounded, and compactly supported. Then

$$E_N^{\mathrm{mf}} \leq E_N^{\mathrm{HF}} + E^{\mathrm{BP}} + E^{\mathrm{GB},1} + \mathcal{O}(\hbar N^{-1/27})\,.$$

Remarks:

- [Hainzl-Porta-Rexze '18] obtained a perturbative upper and lower bound to second order in $\hat{V}$.
- We use a trial state which in principle also captures $E^{\mathrm{GB},2}$, but in the mean-field scaling this contribution is too small to be seen.

Preparation: Extracting the Hartree–Fock Energy

Extracting the Hartree–Fock Energy

Hamiltonian in momentum representation, written with fermionic canonical operators:

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

Introduce the simplest fermionic state (Slater determinant) of N plane waves in the Fermi ball

$$\Psi_N := \bigwedge_{k\in\mathcal{B}_F} f_k \,, \qquad \mathcal{B}_F := \left\{ k \in \mathbb{Z}^3 \mid |k| \leq N^{1/3} (3/4\pi)^{1/3} \right\} .$$

Then, following [Gontier–Hainzl–Lewin '18],

$$\langle \Psi_N, H_N^{\mathrm{mf}} \Psi_N \rangle = E_N^{\mathrm{HF}} + \mathcal{O}(e^{-N^{1/6}}) .$$

Goal: find $\tilde{\Psi}_N$ s. th. $\langle \tilde{\Psi}_N, H_N^{\mathrm{mf}} \tilde{\Psi}_N \rangle = E_N^{\mathrm{HF}} + E^{\mathrm{BP}} + E^{\mathrm{GB},1} + o(N^{-1/3})$.

Adding Correlations:
The Method of Collective Bosonization

Particle-Hole Transformation

Define the unitary map R on fermionic Fock space by

$$R\Omega := \Psi_N = \bigwedge_{k\in\mathcal{B}_F} f_k\,, \qquad\qquad Ra_k^* R^* := \begin{cases} a_k & k\in\mathcal{B}_F \\ a_k^* & k\in\mathcal{B}_F^c \end{cases}$$

Write $\tilde{\Psi}_N = R\xi$. Calculate $R^* H_N^{\mathrm{mf}} R$ to get

$$\langle\tilde{\Psi}_N, H_N^{\mathrm{mf}}\tilde{\Psi}_N\rangle = E_N^{\mathrm{HF}} + \langle\xi, \Big(\underbrace{\hbar^2\sum_{p\in\mathcal{B}_F^c} p^2 a_p^* a_p - \hbar^2\sum_{h\in\mathcal{B}_F} h^2 a_h^* a_h}_{=:\; H^{\mathrm{kin}}} + Q\Big)\xi\rangle + \mathcal{O}(N^{-1})$$

where Q is quartic in fermionic operators. (Notice: $Q\Omega = 0$.)

Our task: construct a non-perturbatively correlated trial state ξ.

Collective Particle-Hole Pairs

The dominant part Q of the interaction can be expressed through collective pair operators

$$b^*_k := \sum_{\substack{p \in \mathcal{B}_F^c \\ h \in \mathcal{B}_F}} \delta_{p-h,k} a^*_p a^*_h$$

as

$$Q = \frac{1}{N} \sum_{k \in \mathbb{Z}^3} \hat{V}(k) \left(2 b^*_k b_k + b^*_k b^*_{-k} + b_{-k} b_k \right) .$$

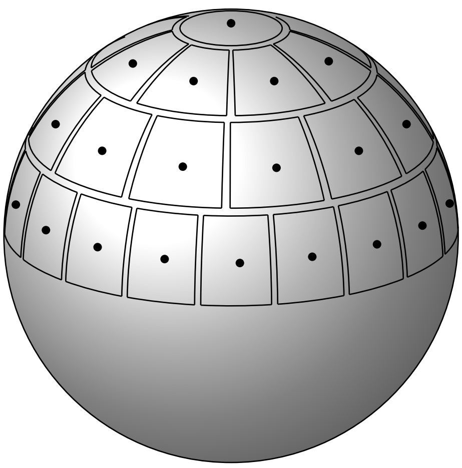
This is convenient because

- The b^* and b have approximately bosonic commutators:
  a^* odd $\rightsquigarrow$ $a^* a^*$ even, and summation over many modes relaxes the Pauli principle!
- ground state of quadratic Hamiltonians is explicitly given by a Bogoliubov transformation.

But: How to express H^{kin} through pair operators?

Localization to Patches

Fermi ball $\mathcal{B}_F$



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

$$b^*_{\alpha,k} := \frac{1}{n_{\alpha,k}} \sum_{\substack{h \in \mathcal{B}_F \cap B_\alpha \\ p \in \mathcal{B}_F^c \cap B_\alpha}} \delta_{p-h,k} a^*_p a^*_h$$

where $n_{\alpha,k} = \sqrt{\#\text{p-h pairs in } \alpha \text{ with momentum } k}$.

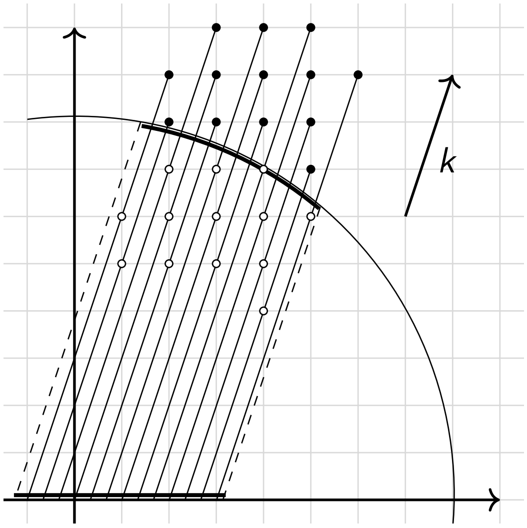
Linearize kinetic energy around centers ω_α:

$$H^{\text{kin}} b^*_{\alpha,k} \Omega \simeq 2\hbar \underbrace{|k \cdot \hat{\omega}_\alpha|}_{=: u_\alpha(k)^2} b^*_{\alpha,k} \Omega .$$

By comparison to the harmonic oscillator:

$$H^{\text{kin}} \simeq \sum_{k \in \mathbb{Z}^3} \sum_\alpha 2\hbar u_\alpha(k)^2 b^*_{\alpha,k} b_{\alpha,k} .$$

Quadratic Effective Hamiltonian



$$n_{\alpha,k}^2 = \#\text{p-h pairs in patch } B_\alpha \text{ with momentum } k$$
$$\simeq \frac{4\pi N^{2/3}}{M} |k \cdot \hat{\omega}_\alpha| = \frac{4\pi N^{2/3}}{M} u_\alpha(k)^2$$

Decompose

$$b_k^* = \sum_\alpha n_{\alpha,k} b_{\alpha,k}^* + \text{lower order}$$

in

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

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

Heuristics: Bosonic Approximation

For this slide only: Assume $b_{\alpha,k}^*$, $b_{\alpha,k}$ are *exactly bosonic* operators.

Then the ground state of H^{eff} is given by a Bogoliubov transformation:

$$\xi_{\text{gs}} = T\Omega, \quad T = \exp\left(\sum_{k \in \mathbb{Z}^3} \sum_{\alpha,\beta} K(k)_{\alpha,\beta} b_{\alpha,k}^* b_{\beta,-k}^* - \text{h.c.} \right) \tag{1}$$

$K(k)$ is an almost explicit $M \times M$-matrix

and

$$\langle \xi_{\text{gs}}, H^{\text{eff}} \xi_{\text{gs}} \rangle \to E^{\text{BP}} + E^{\text{GB},1} \qquad \text{as } M \to \infty .$$

To get a rigorous upper bound for the fermionic system:
Use (1) to define a trial state in fermionic Fock space.

Rigorous Analysis

Convergence to Bosonic Approximation

Lemma: We have approximately bosonic commutators:

$$[b^*_{\alpha,k}, b^*_{\beta,l}] = 0 = [b_{\alpha,k}, b_{\beta,l}] \qquad \text{and} \qquad [b_{\alpha,k}, b^*_{\beta,l}] = \delta_{\alpha,\beta}\Big(\delta_{k,l} + \mathcal{E}_\alpha(k,l)\Big)\,,$$

where for all ξ in fermionic Fock space the deviation operator $\mathcal{E}_\alpha(k,l)$ is bounded by

$$\|\mathcal{E}_\alpha(k,l)\xi\| \leq \frac{2}{n_{\alpha,k}n_{\alpha,l}}\|\mathcal{N}\xi\| \qquad (\mathcal{N} = \text{fermionic number operator})\,.$$

Approximate Bogoliubov Transformations

Proposition: With $K(k)$ from the bosonic approximation, let in fermionic Fock space

$$T_\lambda := \exp(\lambda B), \qquad B := \sum_{k\in\mathbb{Z}^3}\sum_{\alpha,\beta} K(k)_{\alpha,\beta} b^*_{\alpha,k} b^*_{\beta,-k} - \text{h.c.}$$

Then T_λ acts as an approximate Bogoliubov transformation on $b^*_{\alpha,k}$ and $b_{\alpha,k}$, i. e.,

$$T^*_\lambda b_{\alpha,k} T_\lambda = \sum_{\beta=1}^{M} \cosh(\lambda K(k))_{\alpha,\beta} b_{\beta,k} + \sum_{\beta=1}^{M} \sinh(\lambda K(k))_{\alpha,\beta} b^*_{\beta,-k} + \mathfrak{E}_{\alpha,k}$$

where the error is bounded by

$$\left[\sum_\alpha \|\mathfrak{E}_{\alpha,k}\psi\|^2\right]^{1/2} \leq \frac{C}{\min_\alpha n^2_{\alpha,k}} \|(\mathcal{N}+2)^{3/2} T_\lambda \psi\| \quad \text{for all } \psi \text{ in fermionic Fock space}.$$

Bound on $\mathcal{N}$

Lemma: The particle number on our trial state

$$\xi_{\text{trial}} := T_{\lambda=1}\Omega$$

is bounded by

$$\langle \xi_{\text{trial}}, (\mathcal{N}+1)^3 \xi_{\text{trial}} \rangle \leq C \quad \text{independent of } N.$$

Conclusion: We introduce a cutoff excluding patches with $u_\alpha(k)^2 \leq N^{-\delta}$; thus the error terms are small,

$$\text{errors} \sim \frac{\langle \xi_{\text{trial}}, (\mathcal{N}+2)^3 \xi_{\text{trial}} \rangle}{\min_\alpha n^2_{\alpha,k}} \leq \frac{C}{\frac{N^{2/3}}{M} u_\alpha(k)^2} \leq C \frac{M}{N^{2/3} N^{-\delta}},$$

$\rightsquigarrow$ bosonic approximation is self-consistent for $M(N) \ll N^{2/3-\delta}$.

Dealing with the Kinetic Energy

Lemma: The kinetic energy can be linearized as $H^{\text{kin}} = H^{\text{linear}} + \mathfrak{E}$, where

$$H^{\text{linear}} = \hbar \sum_{\alpha=1}^{M} \Bigg[\sum_{p \in \mathcal{B}_F^c \cap B_\alpha} |p \cdot \hat{\omega}_\alpha| a_p^* a_p - \sum_{h \in \mathcal{B}_F \cap B_\alpha} |h \cdot \hat{\omega}_\alpha| a_h^* a_h \Bigg]$$

and the error operator $\mathfrak{E}$ is small compared to $\hbar = N^{-1/3}$ if $M(N) \gg N^{1/3}$; namely

$$|\langle \xi, \mathfrak{E} \xi \rangle| \leq \frac{C}{M} \langle \xi, \mathcal{N} \xi \rangle \qquad \text{for all } \xi \text{ in fermionic Fock space}.$$

Lemma: We have

$$[H^{\text{linear}}, b^*_{\alpha,k}] = 2\hbar |k \cdot \hat{\omega}_\alpha| b^*_{\alpha,k} \,;$$

in this (and only this) sense we have $H^{\text{linear}} \simeq \sum_{k \in \mathbb{Z}^3} \sum_\alpha 2\hbar u_\alpha(k)^2 b^*_{\alpha,k} b_{\alpha,k}$.

Proof of Main Theorem: Variational Principle

Proof: We just have to calculate $\langle R\xi_{\text{trial}}, H_N^{\text{mf}} R\xi_{\text{trial}} \rangle \simeq \langle \Omega, T^*_{\lambda=1} \left(H^{\text{linear}} + Q \right) T_{\lambda=1} \Omega \rangle$.

- The interaction part Q is quadratic in b^* and b —
  just calculate the action of the approximate Bogoliubov transformation.
- The linearized kinetic energy H^{linear} is not quadratic in b^* and b —
  expand into commutators by applying once the Duhamel formula

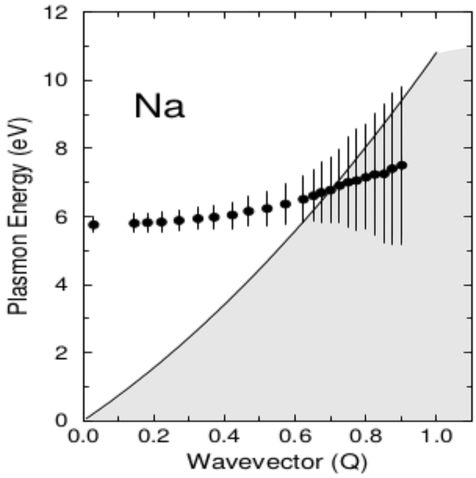
$$\begin{aligned}
\langle \xi_{\text{trial}}, H^{\text{linear}} \xi_{\text{trial}} \rangle &= \int_0^1 \langle \Omega, T^*_\lambda [H^{\text{linear}}, B] T_\lambda \Omega \rangle \, \mathrm{d}\lambda \\
&= \int_0^1 \langle \Omega, T^*_\lambda \sum_{k \in \mathbb{Z}^3} \sum_{\alpha,\beta} K(k)_{\alpha,\beta} [H^{\text{linear}}, b^*_{\alpha,k} b^*_{\beta,-k} - \text{h.c.}] T_\lambda \Omega \rangle \, \mathrm{d}\lambda \\
&= \int_0^1 \langle \Omega, T^*_\lambda \sum_{k \in \mathbb{Z}^3} \sum_{\alpha,\beta} K(k)_{\alpha,\beta} 2\hbar \Big(|k \cdot \hat{\omega}_\alpha| + |k \cdot \hat{\omega}_\beta| \Big) b^*_{\alpha,k} b^*_{\beta,-k} T_\lambda \Omega \rangle + \text{c.c.}
\end{aligned}$$

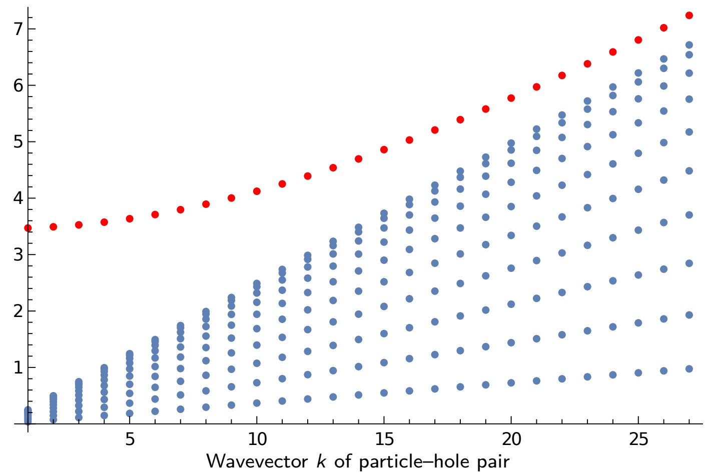
and $T^*_\lambda b^*_{\alpha,k} T_\lambda$ is given by the approximate Bogoliubov transformation. □

QED

Work in Progress

- Corresponding lower bound – notice that we are dealing with a gapless system!
- Coulomb interaction and the plasmon:





Thank you!