Discussion session on

New Challenges for Coulomb Gases

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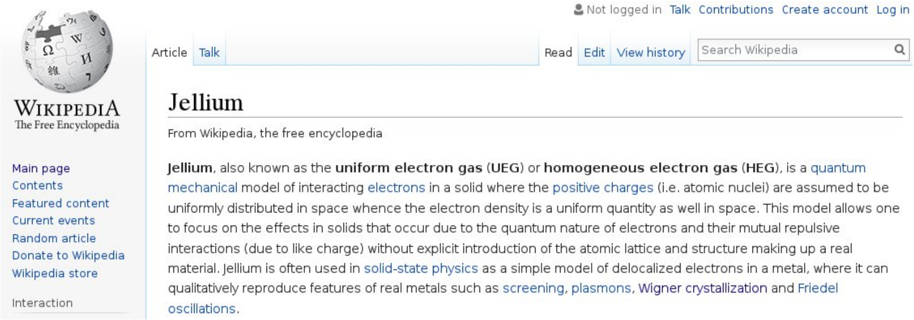
- Coulomb gas
- Jellium
- One-Component Plasma (OCP)
- Uniform Electron Gas (UEG)
- Homogeneous Electron Gas (HEG)
- Renormalized Energy
- Sine-β process, Brownian carousel



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Jellium

From Wikipedia, the free encyclopedia

Jellium, also known as the **uniform electron gas** (**UEG**) or **homogeneous electron gas** (**HEG**), is a quantum mechanical model of interacting electrons in a solid where the positive charges (i.e. atomic nuclei) are assumed to be uniformly distributed in space whence the electron density is a uniform quantity as well in space. This model allows one to focus on the effects in solids that occur due to the quantum nature of electrons and their mutual repulsive interactions (due to like charge) without explicit introduction of the atomic lattice and structure making up a real material. Jellium is often used in solid-state physics as a simple model of delocalized electrons in a metal, where it can qualitatively reproduce features of real metals such as screening, plasmons, Wigner crystallization and Friedel oscillations.

Instability of Coulomb Gas

- **Long range of Coulomb force $\Longrightarrow$ no simple thermodynamics**

$\Omega_N = N^{1/3}\Omega$ where Ω fixed domain with $|\Omega| = 1/\rho$

$$\min_{x_i\in\Omega_N}\left(\sum_{1\leq j<k\leq N}\frac{1}{|x_j-x_k|}\right)\underset{N\to\infty}{\sim}\frac{N^{5/3}}{2}\underbrace{\min_{\mu\ \text{proba}}\int_\Omega\int_\Omega\frac{d\mu(x)\,d\mu(y)}{|x-y|}}_{\text{Cap}(\Omega)}$$

Particles accumulate close to the boundary of Ω_N

One- & Two-Component Plasma

- **Jellium = OCP**: negatively charged particles in **uniform positive background**
  - good approx. to interiors of white dwarfs (fully ionized atoms)
  - electrons in a solid
  - Local Density Approximation of Density Functional Theory
  - classical OCP appears in many areas of Mathematics and Physics

- **TCP**: mixture of **positive** and **negative** charges
  - classical collapse: need short range regularization (or $T > T_c > 0$ in 2D)
  - quantum: stable only when one kind are fermions
    (Dyson '67, Conlon-Lieb-Yau '88, Lieb-Solovej '04, Dyson-Lenard '67, Lieb-Thirring '75)
  - functional integrals, Euclidean Field Theory, Sine-Gordon transformation
    (Siegert '60, Edwards-Lenard '62, Albeverio-Høegh Krohn '73, Fröhlich '76, Park '77, Fröhlich-Park '78,...)
  - 2D-TCP: Berezinski-Kosterlitz-Thouless (BKT) phase transition
    (Kosterlitz-Thouless '73, Fröhlich-Spencer '81)

here, we focus mainly on Jellium

Jellium

$$\mathcal{E}_\rho(\Omega, x_1, ..., x_N) = \sum_{1\leq j<k\leq N} \frac{1}{|x_j - x_k|} - \rho \sum_{j=1}^N \int_\Omega \frac{1}{|x_j - y|}\, dy + \frac{\rho^2}{2} \int_\Omega \int_\Omega \frac{dx\, dy}{|x-y|}$$

$$e_{\rm Jell}^{\rm cl}(\rho) = \lim_{\substack{N\to\infty \\ \frac{N}{|\Omega_N|}\to\rho}} \frac{1}{|\Omega_N|} \min_{x_1,...,x_N\in\Omega_N} \mathcal{E}_\rho(\Omega_N, x_1, ..., x_N) = \rho^{4/3}\, e_{\rm Jell}^{\rm cl}(1)$$

$$f_{\rm Jell}^{\rm cl}(T,\rho) = -\lim_{\substack{N\to\infty \\ \frac{N}{|\Omega_N|}\to\rho}} \frac{T}{|\Omega_N|} \log \int_{(\Omega_N)^N} e^{-\frac{\mathcal{E}_\rho(\Omega_N,x_1,...,x_N)}{T}}\, dx_1\cdots dx_N$$

$$= \rho^{4/3}\, f_{\rm Jell}^{\rm cl}(T\rho^{-1/3}, 1)$$

Similar definition $f_{\rm Jell}(T,\rho)$ in quantum case, with $f_{\rm Jell}(T,\rho) \underset{\rho\to 0}{\sim} f_{\rm Jell}^{\rm cl}(T,\rho)$

(Lieb-Narnhofer '73)

Phase diagram of Jellium

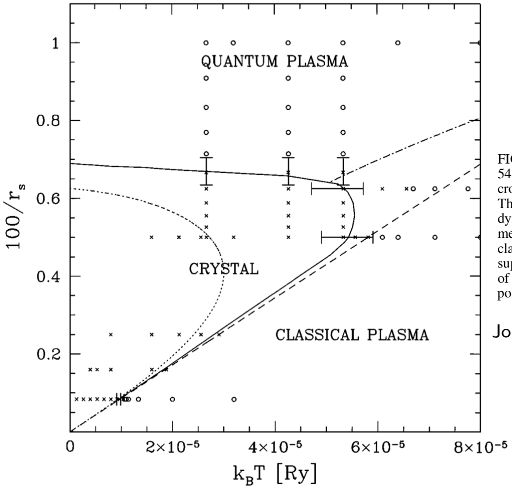


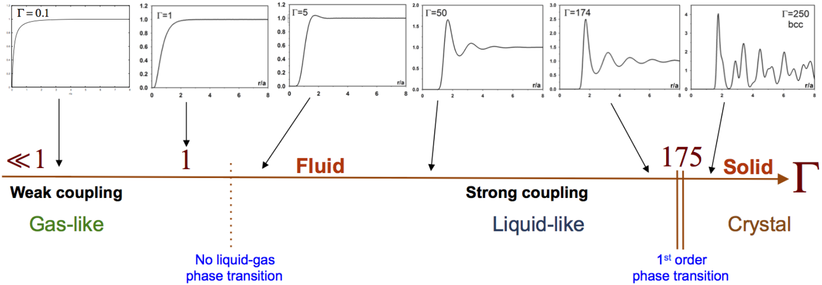
FIG. 1. The OCP phase diagram. The open circles are $N = 54$ simulations which remained in the liquid phase, while the crosses are simulations which remained in the crystal phase. The demarcation between these two sets of points marks the dynamical melting point. The dotted line is the predicted melting curve of Chabrier [16], and the dashed line is the classical melting point. The dash-dotted line is the projected super uid–normal uid transition temperature based upon that of ^{4}He [22]. Points with error bars are our PIMC melting points. The solid line is provided only to guide the eye.

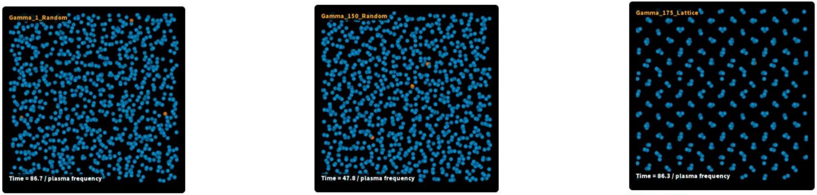
Jones-Ceperley, Phys. Rev. Lett. '96

Phase diagram of classical Jellium

$\Gamma = \left(\frac{4\pi}{3}\right)^{1/3} \frac{e^2\rho^{1/3}}{k_B T}$ www.lanl.gov/projects/dense-plasma-theory/

pair distribution function $g(r)$





$\Gamma = 1$ $\Gamma = 150$ $\Gamma = 175$

Brush-Salin-Teller '66, ...

With spin (electrons): Para/Ferromagnet transition

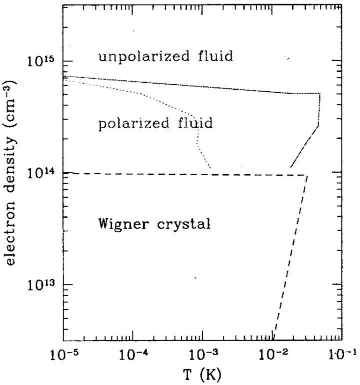


FIG. 8. The phase diagram of the electron gas. Conversion to units of cm and K was done using $a_0 = 1.3$ nm and Ry $= 250$ K using estimates [3] of the effective mass and the dielectric constant of SrB_6. The solid line is the mean- eld estimate of the magnetic transition temperature from the Stoner model, where the spin interaction is estimated from the zero temperature QMC data. The dotted line is the energy difference between the unpolarized and partially polarized system.

Zong-Lin-Ceperley, Phys. Rev. E. '02
Drummond *et al*, Phys. Rev. B. '04

Some rigorous results on 3D Jellium

- **Thermodynamics**
  - Existence (Lieb-Narnhofer '73)

- **States and screening**
  - BBGKY / KMS / KS / DLR (Gruber-Lugrin-Martin '79-80)
  - Cluster expansions & Debye screening (Brydges '78, Brydges-Federbush '80, Imbrie '83)
  - Clustering $\Longrightarrow$ Euclidean invariance (Gruber-Martin '80, Gruber-Martin-Oguey '82)
  - Sum rules, charge fluctuations (Gruber-Lebowitz-Martin '81, Gruber-Lugrin-Martin '80, Lebowitz-Martin '84)

- **Behavior at large density**
  - $e_{\rm Jell}(\rho) = c_{\rm TF}\rho^{5/3} - c_{\rm D}\rho^{4/3} + o(\rho^{4/3})_{\rho\to\infty}$ (Graf-Solovej '94)
  - $e_{\rm Jell}^{\rm bos}(\rho) = c_{\rm Foldy}\rho^{5/4} + o(\rho^{5/4})_{\rho\to\infty}$ (Lieb-Solovej '01–06)
  - $f_{\rm Jell}^{\rm bos/fer}(T,\rho) = f_{\rm free}^{\rm bos/fer}(T,\rho) \pm \frac{\rho}{2}\int_{\mathbb{R}^3}\frac{|\gamma_0(x)|^2}{|x|}\,dx + o(\rho^{4/3})_{\substack{\rho\to\infty\\ \beta\to 0}}$ (Seiringer '06)

Riesz gases

- Adding background $\equiv$ second-order Taylor expansion $\equiv$ screening
- Background works for any interaction potential $w(x) \sim_\infty |x|^{-s}$ for $d-2 \leq s < d$

Riesz gases

$$w_s(x) = \begin{cases} \dfrac{1}{s|x|^s} & \text{for } s \neq 0, \\ -\log|x| & \text{for } s = 0. \end{cases}$$

- $s > d$ (short range): well defined thermodynamics without background
- $d-2 \leq s < d$ (long range): background necessary
- $s < d-2$: background does not screen enough, unstable

$\Longrightarrow$ natural family in statistical mechanics, even includes hard spheres ($s \to \infty$)

parameters: $\begin{cases} s, \Gamma = \rho^{\frac{s}{d}}/T & \textit{(classical)} \\ s, T, \rho & \textit{(quantum)} \end{cases}$

Crystallization conjecture & analytic number theory

Crystallization conjecture $T = 0$ in classical case (Blanc-Lewin, EMS Rev. '15)

2D: Riesz gas crystallized on hexagonal lattice $\forall s \geq 0$
3D: on BCC lattice for $1 \leq s \leq 3/2$ and FCC lattice for $s \geq 3/2$

If particles on lattice $\mathcal{L}$ and $s > d$, then

$$s \times \text{energy} = \frac{1}{2} \sum_{\ell \in \mathcal{L} \setminus \{0\}} \frac{1}{|\ell|^s} = \zeta_{\mathcal{L}}(s) = \text{Epstein Zeta Function}$$

which admits analytic extension on $\mathbb{C} \setminus \{d\}$, with pole at d independent of $\mathcal{L}$

2D: Epstein is minimal for hexagonal lattice $\forall s \geq 0$

(Rankin '53, Cassels '59, Ennola '64, Diandana '64, Montgomery '88)

3D: BCC-FCC conjectured, FCC known for $s \gg 1$

Theorem (Analytic extension)

If crystallization on lattice $\mathcal{L}$, then $e_{Jel}(s) = \zeta_{\mathcal{L}}(s)/s$.
At $T = 0$, classical Jellium = analytic extension in s of long range case!

(Borwein-Borwein-Shail '89, Borwein-Borwein-Straub '14, Lewin-Lieb '15)

1D Riesz gases

- $s = -1$: Crystallization at all $T \geq 0$ and all $\rho > 0$, classical and quantum

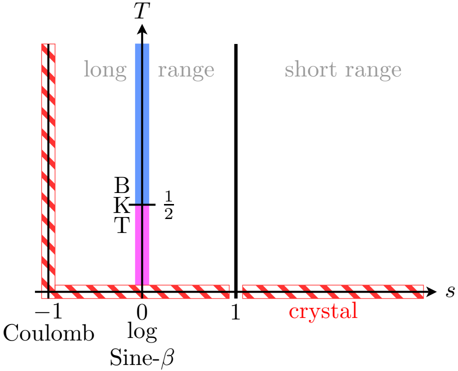
(Kunz '74, Aizenman-Martin '80, Brascamp-Lieb '75, Jansen-Jung '14)

- $T = \hbar = 0$: Crystallization for all $1 \neq s \geq 0$

(Nijboer-Ventevogel '79, Borodin-Serfaty '13, Sandier-Serfaty '14, Brauchart-Hardin-Saff '12, Leblé '16)

- $\hbar = 0$: No breaking of translations for $T > 0$ and $s \geq 0$

(Fröhlich-Pfister '81, Baus '80, Alastuey-Jancovici '81, Chakravarty-Dasgupta '81, Martinelli-Merlini '84, Requardt-Wagner '90)



1D classical Riesz gas at $s = 0$

N-particle classical probability density on $\mathbb{S}^1$ at $\beta = 1/T$
$\equiv$ exact quantum ground state[2] of N bosons with $\sim g\pi^2/r^2$ interactions,
$\beta = 1 + \sqrt{1+2g}$ (Sutherland '72, Forrester '84)

Haldane's formula

$$\rho_2^T(r) = -\frac{T}{\pi^2 r^2} + \sum_{m\geq 1} \frac{a_m}{r^{4Tm^2}} \cos(2\pi m r) + o(r^{-2})_{r\to\infty}$$

(Haldane, Phys. Rev. Lett. '81)

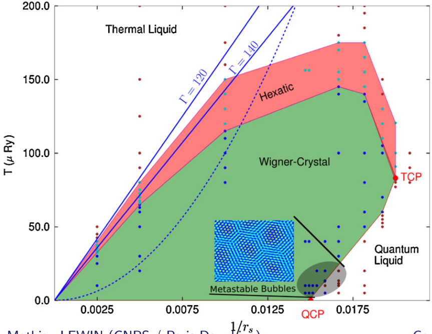
BKT-type transition

$$\rho_2^T(r) \underset{r\to\infty}{\sim} \begin{cases} -\dfrac{T}{\pi^2 r^2} & T > 1/2 \\ \dfrac{a_1}{r^{4T}} \cos(2\pi r) & T < 1/2 \end{cases}$$

(Forrester '84)

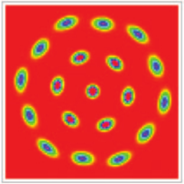
2D Riesz gas ($s = 0, 1$)

- Mermin-Wagner does not apply, but seems valid (Baus '80, Alastuey-Jancovici '81, Martinelli-Merlini '84, Requardt-Wagner '90). Common belief:
  - **"solid" phase** with (algebraic) quasi-long-range positional order and long range orientational order
  - **intermediate hexatic phase** (Kosterlitz-Thouless-Halperin-Nelson-Young) (Muto-Aoki '99, He-Cui-Ma-Liu-Zou '03)
- For many years, computer simulations indicated a 1st order solid-fluid transition (Gann-Chakravarti-Chester '78, de Leeuw-Perram '82, Caillol-Levesque-Weis-Hansen '82)



2D boltzons with $1/r$ interaction ($s = 1$)
Clark-Casula-Ceperley, Phys. Rev. Lett '09

Mean-field limit for confined Riesz gases



Bonitz et al, Phys. Plasma '08

Forget background and put external confining potential

$$\mathcal{E}_{V_{\rm ext}}(x_1,\ldots,x_N)=\sum_{j=1}^N V_{\rm ext}(x_j)+\frac{1}{N}\sum_{1\leq j<k\leq N} w(x_j-x_k)$$

Theorem (Mean-field limit)

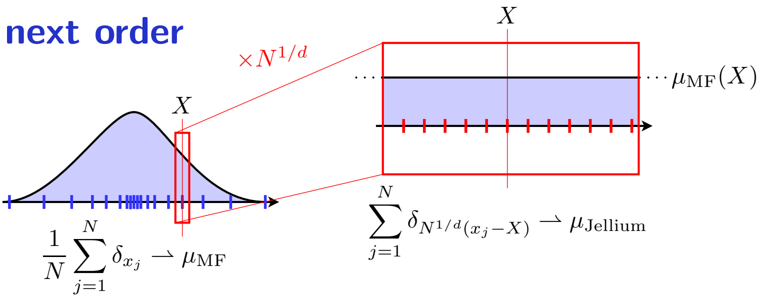
$$\frac{\min_{x_j}\mathcal{E}_{V_{ext}}(x_1,\ldots,x_N)}{N}\underset{N\to\infty}{\longrightarrow}\min_{\mu\ proba}\left\{\int_{\mathbb{R}^d}V_{ext}\,d\mu+\frac12\iint_{\mathbb{R}^{2d}}w(x-y)d\mu(x)\,d\mu(y)\right\}$$

$$-T\frac{\log\int_{\mathbb{R}^{dN}}\exp\left(-\frac{\mathcal{E}_{V_{ext}}}{T}\right)}{N}\underset{N\to\infty}{\longrightarrow}\min_{\mu\ proba}\left\{\int_{\mathbb{R}^d}V_{ext}\,d\mu+\frac12\iint_{\mathbb{R}^{2d}}w(x-y)d\mu(x)\,d\mu(y)+T\int_{\mathbb{R}^d}\mu\log\mu\right\}$$

(Messer-Spohn '82, Kiessling '89, ..., Pecot lectures by Rougerie '14)

Rmk. with other convention $\mathcal{E}_{V_{\rm ext}}\rightsquigarrow N\mathcal{E}_{V_{\rm ext}}$, effective temperature $T/N\to 0$

The next order



Theorem (2nd order)

Assume w =Riesz with $\max(0,d-2)\leq s<d$. If $N^{1-\frac{s}{d}}T\to T_0\in[0,\infty)$ then

$$-T\log\int_{\mathbb{R}^{dN}}\exp\left(-\frac{\mathcal{E}_{V_{\rm ext}}}{T}\right)=N\,e_{\rm MF}-\frac{\delta_0(s)}{d}\log N$$

$$+N^{\frac{s}{d}}\left\{\int_{\mathbb{R}^d}f^{\rm cl}_{\rm Jell}\big(s,T_0,\mu_{\rm MF}(x)\big)\,dx+\left(T_0-\frac{\delta_0(s)}{d}\right)\int_{\mathbb{R}^d}\mu_{\rm MF}\log\mu_{\rm MF}\right\}+o(N^{\frac{s}{d}})$$

[Weak CV of states holds as well]

Sandier-Serfaty '14, Borodin-Serfaty '13, Petrache-Serfaty '15, Rougerie-Serfaty '14, Leblé-Serfaty '17, Bauerschmidt-Bourgade-Nikula-Yau '17,...

Rmk. Also true for $s>d$! Should not matter that V confining and w =Riesz

Random Matrices

$$\begin{cases} V(x) = |x|^2 \\ w(x) = -\log|x| \quad (s=0) \\ NT = T_0 > 0 \end{cases}$$

Random matrices with Gaussian iid entries

- $d = 1$, $\mu_{\rm MF} = \sqrt{(4-x^2)_+}$ *(Wigner-Dyson semi-circle law)*

  GOE: $T = \frac{1}{N}$ **Quaternions:** $T = \frac{1}{4N}$

  GUE: $T = \frac{1}{2N}$

- $d = 2$, $\mu_{\rm MF} = \mathbb{1}_{B(0,R)}$

  Ginibre: $T = \frac{1}{2N}$

Jellium describes the local behavior of eigenvalues of Gaussian random matrices, with interaction $w = -\log$ in 1D or 2D.

Rmk. In 2D, $\equiv$ Laughlin wavefunction[2] *(Fractional Quantum Hall Effect)*

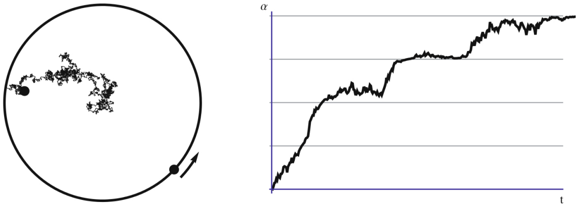
Invent math (2009) 177: 463–508
DOI 10.1007/s00222-009-0180-z

Continuum limits of random matrices and the Brownian carousel

Benedek Valkó · Bálint Virág

Abstract We show that at any location away from the spectral edge, the eigenvalues of the Gaussian unitary ensemble and its general β siblings converge to Sine_β, a translation invariant point process. This process has a geometric description in term of the Brownian carousel, a deterministic function of Brownian motion in the hyperbolic plane.

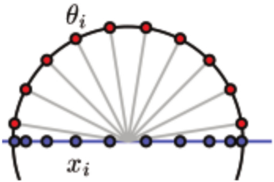
The Brownian carousel, a description of the a continuum limit of random matrices, provides a convenient way to analyze the limiting point processes. We show that the gap probability of Sine_β is continuous in the gap size and β, and compute its asymptotics for large gaps. Moreover, the stochastic differential equation version of the Brownian carousel exhibits a phase transition at $\beta = 2$.



The Brownian carousel and the winding angle α_λ

Fekete points & the Thomson problem

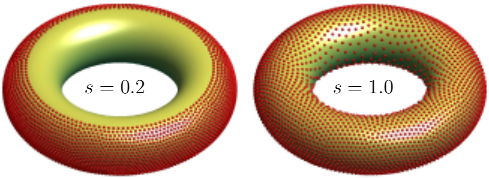
Hardin & Saff, Discretizing Manifolds via Minimum Energy Points, *Notices of the AMS*, 2004

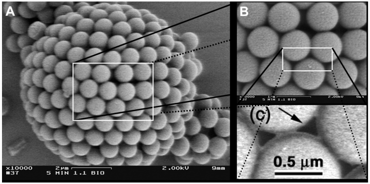


Runge: interpolating a smooth function on $[0,1]$ by regularly-spaced points can be disastrous. Much better to follow arcsin distribution.

Fekete: discretization of 2D manifolds by minimizing $-\sum_{j<k}\log|x_j-x_k|$, with $x_j\in\mathcal{M}$

Thomson: proposed to minimize $\sum_{j<k}|x_j-x_k|^{-1}$ with $x_j\in\mathbb{S}^2$ (Smale 18th pb)





Dinsmore et al, Science, 2002

Fekete points & the Thomson problem II

Exactly the same limit as with a confining potential

Theorem (Hardin-Saff-... '04–17)

Let $\mathcal{M} \subset \mathbb{R}^k$ be a compact manifold of dimension d. Assume that $d-2 \leq s < d$, then

$$\frac{1}{N} \min_{x_j \in \mathcal{M}} \sum_{j<k} \frac{1}{s|x_j - x_k|^s} = \frac{N}{2} \iint_{\mathcal{M}\times\mathcal{M}} \frac{d\mu_{\rm MF}(x)\, d\mu_{\rm MF}(y)}{s|x-y|^s} + N^{\frac{s}{d}} e^{\rm cl}_{\rm Jell}(s,\rho=1) \int_{\mathbb{R}^d} \mu_{\rm MF}(x)^{1+\frac{s}{d}}\, dx + o(N^{\frac{s}{d}})$$

Rmk. Similar for $s=0$ and for $s \geq d$.

The Local Density Approximation of DFT

Levy-Lieb functional in Density Functional Theory (DFT)

$$\mathcal{E}_{\rm LL}(\rho) = \min_{\substack{\Psi \text{ antisym.} \\ \rho_\Psi = \rho}} \left\langle \Psi, \left(\sum_{j=1}^N -\Delta_{x_j} + \sum_{1 \le j < k \le N} \frac{1}{|x_j - x_k|} \right) \Psi \right\rangle$$

$$\mathcal{E}_{\rm LL}^{\rm cl}(\rho) = \min_{\substack{\mathbb{P} \text{ sym.} \\ \rho_{\mathbb{P}} = \rho}} \int_{(\mathbb{R}^3)^N} \sum_{1 \le j < k \le N} \frac{1}{|x_j - x_k|} d\mathbb{P}$$

(multi-marginal optimal transport problem)

(Levy '79, Lieb '83, Cotar-Friesecke-Klüppelberg '13, Seidl-Di Marino-Gerolin-Nenna-Giesbertz-GoriGiorgi '17)

Local Density Approximation

For ρ slowly varying

$$\mathcal{E}_{\rm LL}(\rho) \simeq \frac{1}{2} \iint_{\mathbb{R}^6} \frac{\rho(x)\rho(y)}{|x-y|} \, dx \, dy + \int_{\mathbb{R}^3} e_{\rm UEG}\big(\rho(x)\big) \, dx$$

$e_{\rm UEG}(\rho)$=indirect energy per unit vol. of infinite gaz with cst density ρ in $\mathbb{R}^3$.

Basis for most DFT fns (Perdew-Wang '92, Becke '93, Parr-Yang '94, Perdew-Burke-Ernzerhof '96,...)

Uniform Electron Gas

Theorem: Definition of the UEG (Lewin-Lieb-Seiringer '17)

Let $\Omega \subset \mathbb{R}^3$ be a convex set with $|\Omega| = 1/\rho$ and $\Omega_N = N^{1/3}\Omega$. The following limits exist and are independent of Ω:

$$e_{\rm UEG}^{\rm cl}(\rho) = \rho^{4/3} e_{\rm UEG}^{\rm cl}, \quad e_{\rm UEG}^{\rm cl} = \lim_{N\to\infty} \frac{\mathcal{E}_{\rm LL}^{\rm cl}(\mathbb{1}_{\Omega_N}) - D(\mathbb{1}_{\Omega_N}, \mathbb{1}_{\Omega_N})}{|\Omega_N|}$$

$$e_{\rm UEG}(\rho) = \lim_{N\to\infty} \min_{\rho\mathbb{1}_{\Omega_{N-1}} \leq \nu \leq \rho\mathbb{1}_{\Omega_{N+1}}} \frac{\mathcal{E}_{\rm LL,GC}(\nu) - D(\nu,\nu)}{|\Omega_N|}$$

Rmk. Clear that $e_{\rm UEG}(\rho) \geq e_{\rm Jel}(\rho)$ (using ρ as a background)

Theorem: LDA, classical case (Lewin-Lieb-Seiringer '17)

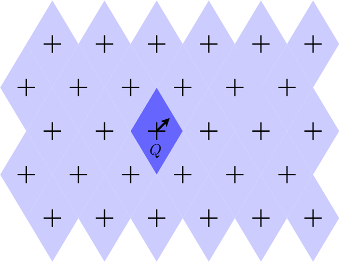
Let $\rho \in C^1_c(\mathbb{R}^3)$ with $\int \rho \in \mathbb{N}$, and $\rho_N(x) = \rho(x/N^{1/3})$. Then

$$\lim_{N\to\infty} \frac{\mathcal{E}_{\rm LL}^{\rm cl}(\rho_N) - D(\rho_N, \rho_N)}{N} = e_{\rm UEG}^{\rm cl} \int_{\mathbb{R}^3} \rho^{4/3}$$

Rmk. Equivalent of 2nd order mean-field with fixed ρ_N instead of fixed $NV_{\rm ext}$

(Cotar-Petrache '17: extension to Riesz)

Uniform Electron Gas controversy



In Physics & Chemistry, UEG $\equiv$ Jellium

For $x_1, ..., x_N$, N distincts points of a lattice $\mathcal{L}$, define the Monge state (floating crystal)

$$\mathbb{P} = \int_Q \delta_{x_1+\tau} \otimes_s \delta_{x_2+\tau} \cdots \otimes_s \delta_{x_N+\tau}\, \mathrm{d}\tau$$

which has $\rho_{\mathbb{P}} = \mathbb{1}_\Omega$ with $\Omega = \cup_{j=1}^N (x_j + Q)$

Theorem: An unexpected shift (Lewin-Lieb '15)

For a Riesz potential with $d-2 \le s < d$ and $s > 0$,

$$\frac{\text{indirect - Jellium energy of } \mathcal{L}}{N} \underset{N\to\infty}{\longrightarrow} \begin{cases} 0 & d-2 < s < d \\ \dfrac{d-2}{d} \dfrac{\pi^{d/2}}{\Gamma(d/2)} \displaystyle\int_Q |x|^2\, dx & s = d-2 \end{cases}$$

Choquard-Favre-Gruber '80, Borwein^2-Shail '89, Borwein^2-Straub '14, Colombo-De Pascale-Di Marino '13 (1D)
Cotar-Petrache '17: Jellium $\equiv$ UEG for $d-2 < s < d$