Density Functional Theory for Dilute Fermions at Unitarity

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Density Functional Theory

The quantum many-body problem: Solve

$$H\psi(r_1, r_2, \ldots, r_N) = E\psi(r_1, r_2, \ldots, r_N)$$

Difficulty grows very quickly with N

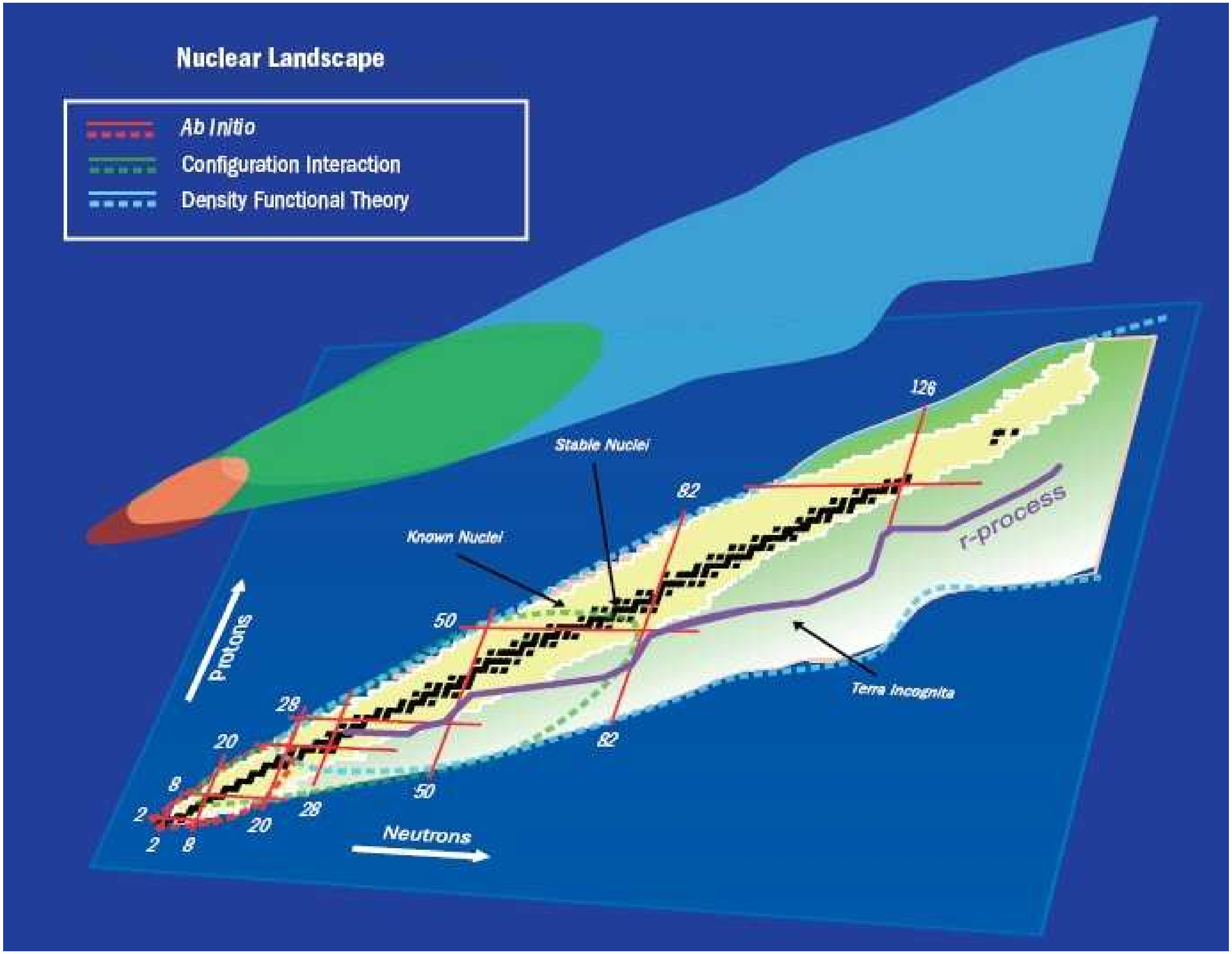
Energy Density Functional $\mathcal{E}[\rho(r)]$: Solve

$$\frac{\delta\mathcal{E}[\rho(r)]}{\delta\rho(r)} = 0 \qquad \int d^3r\, \rho(r) = N$$

Effective 1-body problem

Hohenberg-Kohn showed that $\mathcal{E}[\rho(r)]$ exists, but they did not provide a practical way to construct it.

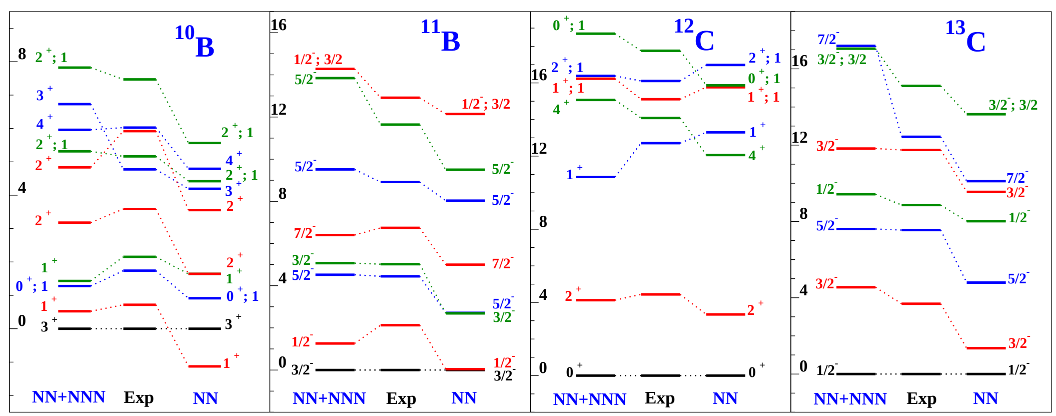
DFT and the nuclear landscape



Traditional Approach

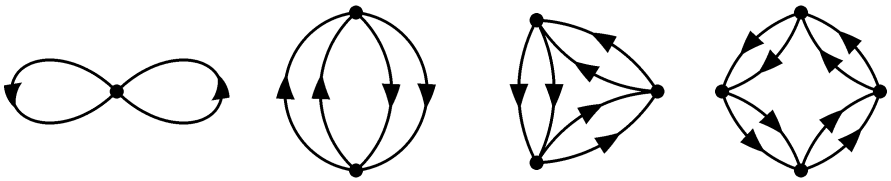
$$V_{NN}, V_{NNN}, \ldots$$

$$H\Psi = E\Psi$$

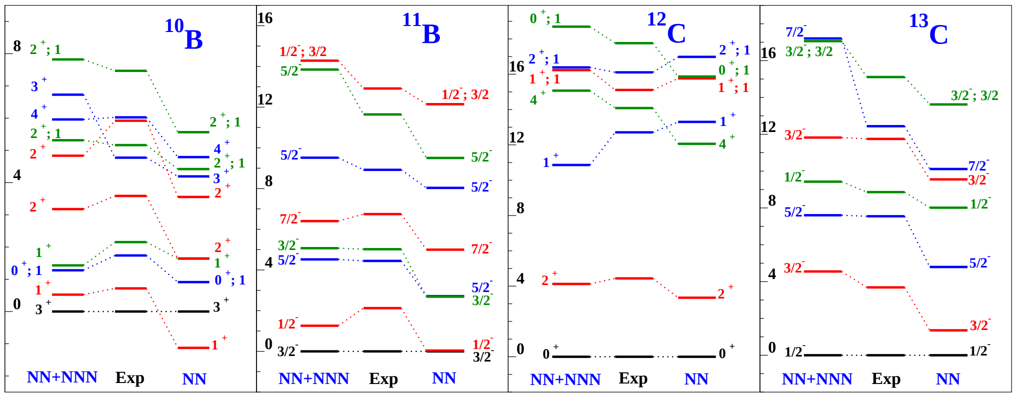


Modern Approach: From EFT to DFT

$$\mathcal{L}(\psi, \pi, \ldots)$$



$$\mathcal{E}(\rho)$$



DFT from a QFT perspective

Consider a non-relativistic field theory

$$S = \int \psi^\dagger(x)\Big(i\partial_0 + \frac{\nabla^2}{2M}\Big)\psi(x) + \int\int (\psi^\dagger\psi)(x_1)V(x_1 - x_2)(\psi^\dagger\psi)(x_2)$$

Generating functional $W[j] = \log Z[j]$

$$Z[j(x)] = \int D\psi D\psi^\dagger \, \exp\left(iS + i\int \psi^\dagger\psi(x)j(x)\right)$$

$$\rho(x) = \langle\psi^\dagger\psi(x)\rangle = \frac{\delta W[j(x)]}{\delta j(x)}$$

Consider Legendre transform

$$\Gamma[\rho(x)] = W[j(x)] - \int j(x)\rho(x) \qquad\qquad j(x) = \frac{\delta\Gamma[\rho(x)]}{\delta\rho(x)}$$

Groundstate: Current vanishes and $\mathcal{E}[\rho(x)] = T\,\Gamma[\rho(x)]$

DFT and perturbative QFT

Consider a perturbative interaction

$$V(x-y) = \lambda\delta(x-y)$$

Zeroth order: Free field theory in the presence of a source

$$W[j(x)] = \log\det\left(i\partial_0 + \frac{\nabla^2}{2M} + j(x) + v_{ext}(x)\right)$$

Determinant can be computed in terms of Fermion orbitals

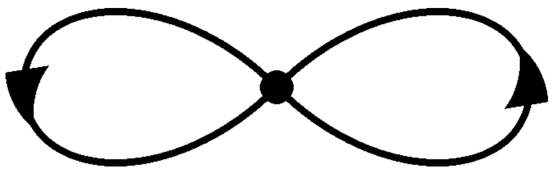
$$\left(\frac{\nabla^2}{2M} + v_{ext}(x)\right)\psi_i = \epsilon_i\psi_i$$

$$\mathcal{E} = \sum_{\epsilon_i<\epsilon_F}\epsilon_i \qquad \rho(x) = \sum_{\epsilon_i<\epsilon_F}\psi_i^\dagger\psi_i(x)$$

DFT with auxiliary Fermion orbitals: Kohn-Sham theory

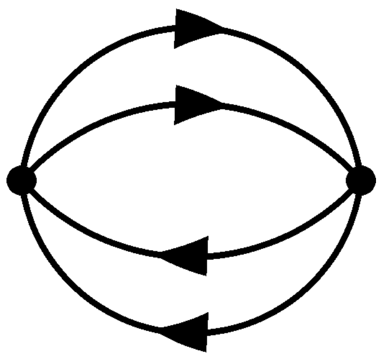
DFT and perturbative QFT

First order correction



$$\Gamma_1[\rho] = \frac{C_0}{4} \int d^3x\, |\rho(x)|^2$$

Second order correction



Non-local

Density matrix expansion

DFT in Nuclear Physics: Problems

Interactions are non-perturbative

Scattering length large, strong tensor force

Interactions are not local

pion exchanges

Broken Symmetries

Translations, rotations, particle number

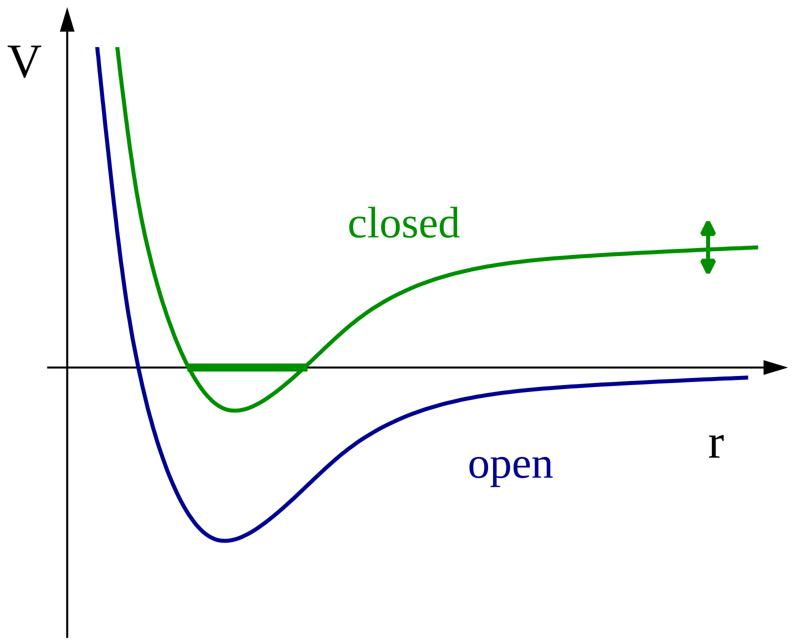
Nuclei are self-bound

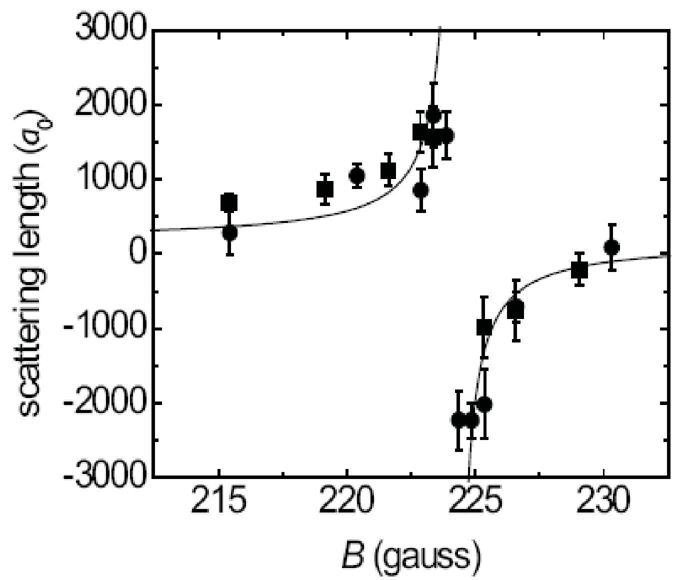
No external potential, intrinsic density needed

Here: Study role of large scattering length

Designer Fluids

Atomic gas with two spin states: "↑" and "↓"





Feshbach resonance

$$a(B) = a_0\left(1 + \frac{\Delta}{B - B_0}\right)$$

"Unitarity" limit $a \to \infty$

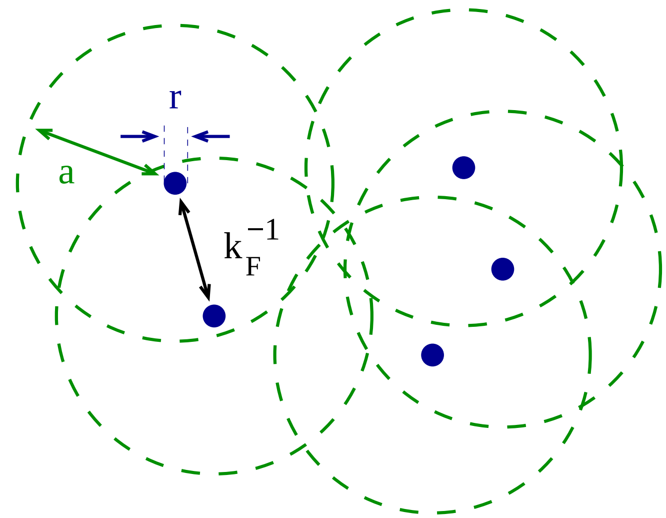
$$\sigma = \frac{4\pi}{k^2}$$

Universality

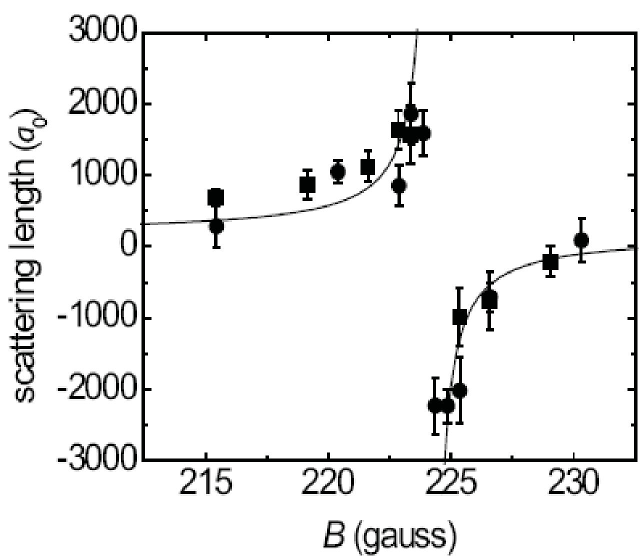
What does this system have in common with nuclear matter?

dilute: $r\rho^{1/3} \ll 1$

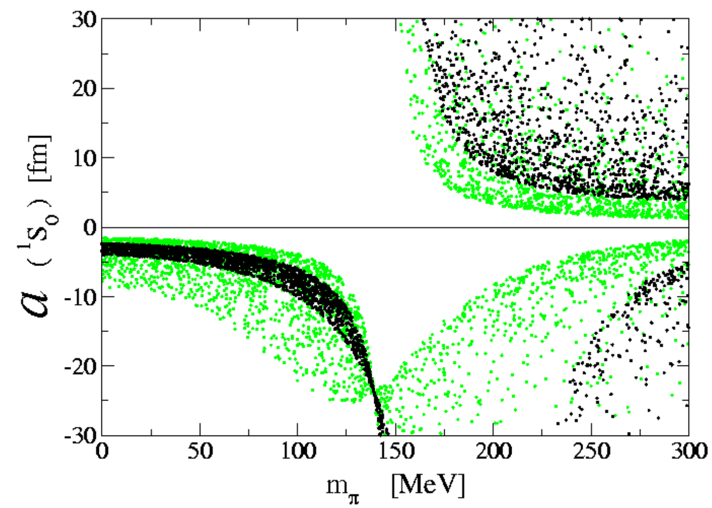
strongly correlated: $a\rho^{1/3} \gg 1$



Feshbach Resonance in ^{6}Li



Neutron Matter



Effective Field Theory

Effective field theory for pointlike, non-relativistic neutrons

$$\mathcal{L}_{\text{eff}} = \psi^\dagger \left(i\partial_0 + \frac{\nabla^2}{2M} \right) \psi - \frac{C_0}{2} (\psi^\dagger \psi)^2 + \frac{C_2}{16} \left[(\psi\psi)^\dagger (\psi \overleftrightarrow{\nabla}^2 \psi) + h.c. \right] + \ldots$$

Match to effective range expansion

$$C_0 = \frac{4\pi a}{M} \qquad a = -18\,\text{fm}$$

$$C_2 = \frac{4\pi a^2}{M} \frac{r}{2} \qquad r = 2.8\,\text{fm}$$

Unitarity limit: $C_0 \to \infty$, $C_2 \to 0$

Effective Low Energy Lagrangian

Superfluid phase: Response governed by Goldstone boson

$$\psi\psi = e^{2i\varphi}\langle\psi\psi\rangle$$

Effective Lagrangian

$$\mathcal{L} = f^2\left((\partial_0\varphi)^2 - c_s^2(\nabla\varphi)^2\right) + \ldots$$

Higher orders? Need to incorporate symmetry constraints:

$U(1)$ symmetry, Gallilean invariance, conformal symmetry

Strategy: Promote $U(1)$ and Galilean invariane to local symmetries

Effective Lagrangian

Leading order

$$\mathcal{L}_1 = c_0 m^{3/2} X^{5/2} \qquad\qquad X = \mu - A_0 - \dot{\varphi} - \frac{(\vec{\nabla}\varphi)^2}{2m}$$

$$\text{Check}:\ \mathcal{L}_1 = \frac{15 c_0 m^{3/2} \mu^{1/2}}{8} \left(const + (\partial_0 \varphi)^2 - \frac{2\mu}{3m} (\nabla \varphi)^2 + \ldots \right)$$

Next-to-leading order

$$\mathcal{L}_2 = c_1 m^{1/2} \frac{(\vec{\nabla} X)^2}{\sqrt{X}} + \frac{c_2}{\sqrt{m}} \left[\left(\nabla^2 \varphi \right)^2 - 9m \nabla^2 A_0 \right] \sqrt{X}$$

Density Functional

Construct energy functional $\mathcal{E}[n(x)] = \mu n(x) - P[\mu - A_0(x)]$

$$\mathcal{E}(x) = n(x)A_0(x) + \frac{3 \cdot 2^{2/3}}{5^{5/3} m c_0^{2/3}} n(x)^{5/3}$$

$$- \frac{4}{45} \frac{2c_1 + 9c_2}{mc_0} \frac{\left(\nabla n(x)\right)^2}{n(x)} - \frac{12}{5} \frac{c_2}{mc_0} \nabla^2 n(x) + \ldots$$

Non-perturbative physics in $c_0, c_1, c_2, \ldots$

c_0 Equation of state, $c_{1,2}$ phonon dispersion relation

Many body physics: Use epsilon ($\epsilon = d - 4$) expansion

Upper and lower critical dimension

Zero energy bound state for arbitrary d

$$\psi''(r) + \frac{d-1}{r}\psi'(r) = 0 \qquad (r > r_0)$$

d=2: Arbitrarily weak attractive potential has a bound state

$$\xi = \frac{\mu}{E_F^0} = 1$$

d=4: Bound state wave function $\psi \sim 1/r^{d-2}$. Pairs do not overlap

$$\xi = \frac{\mu}{E_F^0} = 0$$

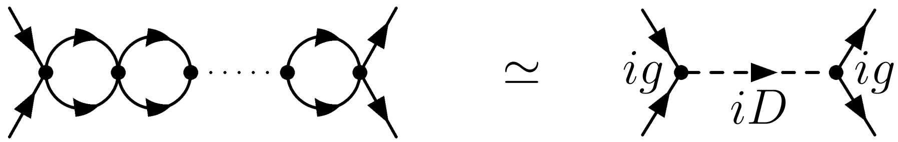
Conclude $\xi(d=3) \sim 1/2$?

Try expansion around $d = 4$ or $d = 2$?

Nussinov & Nussinov (2004)

Epsilon Expansion

EFT version: Compute scattering amplitude ($d = 4 - \epsilon$)



$$T = \frac{1}{\Gamma\left(1 - \frac{d}{2}\right)} \left(\frac{m}{4\pi}\right)^{-d/2} \left(-p_0 + \frac{\epsilon_p}{2}\right)^{1-d/2} \simeq \frac{8\pi^2\epsilon}{m^2} \frac{i}{p_0 + \frac{\epsilon_p}{2} + i\delta}$$

$$g^2 \equiv \frac{8\pi^2\epsilon}{m^2} \qquad D(p_0, p) = \frac{i}{p_0 + \frac{\epsilon_p}{2} + i\delta}$$

Weakly interacting bosons and fermions

Epsilon Expansion

Effective lagrangian for atoms $\Psi = (\psi_\uparrow, \psi_\downarrow^\dagger)$ and dimers ϕ

$$\mathcal{L} = \Psi^\dagger \left(i\partial_0 + \frac{\sigma_3 \nabla^2}{2m} \right) \Psi + \mu \Psi^\dagger \sigma_3 \Psi + \Psi^\dagger \sigma_+ \Psi \phi + h.c.$$

Perturbative expansion: $\phi = \phi_0 + g\varphi$. Free part

$$\mathcal{L}_0 = \Psi^\dagger \left[i\partial_0 + \sigma_3 \frac{\vec{\nabla}^2}{2m} + \phi_0(\sigma_+ + \sigma_-) \right] \Psi + \varphi^\dagger \left(i\partial_0 + \frac{\vec{\nabla}^2}{4m} \right) \varphi \, .$$

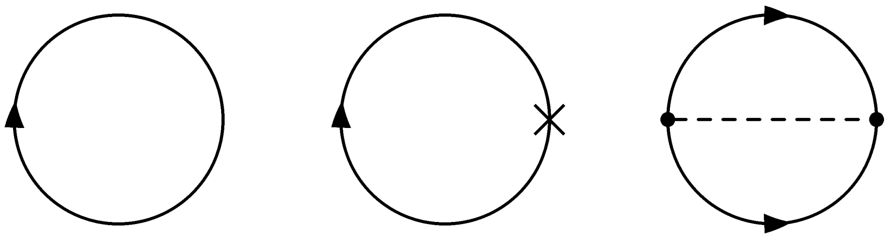
Interacting part $(g^2, \mu = O(\epsilon))$

$$\mathcal{L}_I = g\left(\Psi^\dagger \sigma_+ \Psi \varphi + h.c \right) + \mu \Psi^\dagger \sigma_3 \Psi - \varphi^\dagger \left(i\partial_0 + \frac{\vec{\nabla}^2}{4m} \right) \varphi \, .$$

Nishida & Son (2006)

Matching Calculations

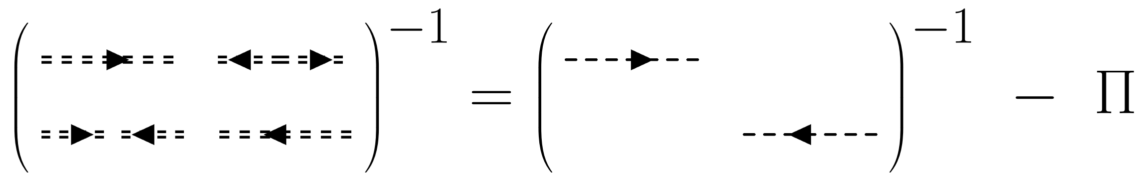
Effective potential

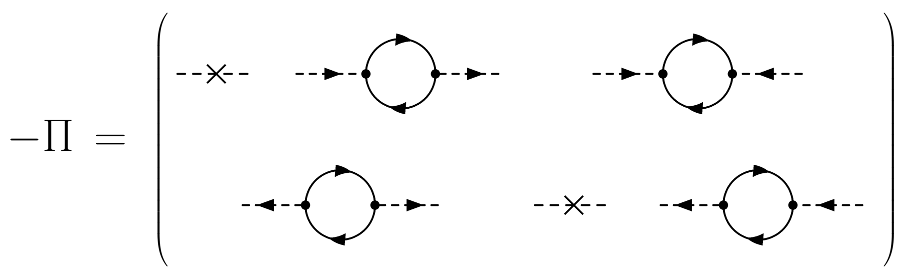


$O(1)$ $O(1)$ $O(\epsilon)$

$$P = \#(2m)^{d/2}\mu^{d/2+1}$$

Phonon Propagator

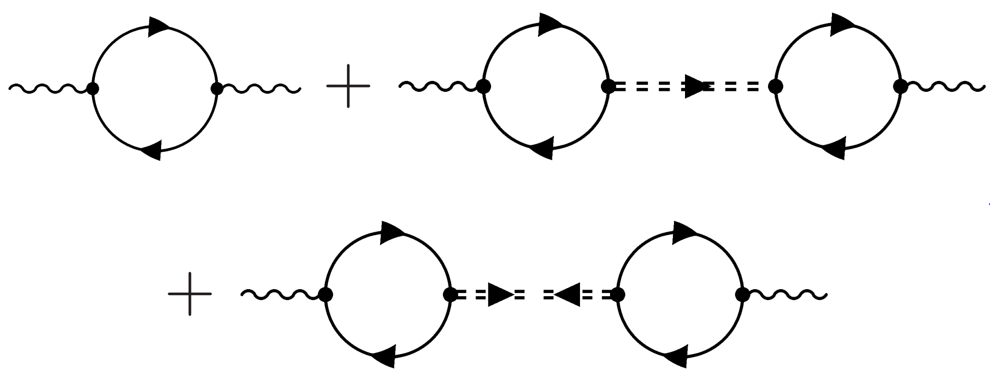




$$\omega = c_s p \left\{ 1 + \# \left(\frac{p^2}{m\mu} \right) + \ldots \right\}$$

Matching (continued)

Static susceptibility $\quad \chi(q) = \int d^3x\, e^{iqx} \langle \psi^\dagger\psi(x)\psi^\dagger\psi(0)\rangle$



$$\chi(q) = \chi(0)\left\{1 - \#\left(\frac{q^2}{m\mu}\right) + \ldots\right\}$$

Nishida, Son (2007)

Rupak, Schaefer (2008)

Density Functional

Unitarity Limit

$$\mathcal{E}(x) = n(x)A_0(x) + 1.364\,\frac{n(x)^{5/3}}{m} + 0.032\,\frac{\left(\nabla n(x)\right)^2}{mn(x)} + O(\nabla^4 n)$$

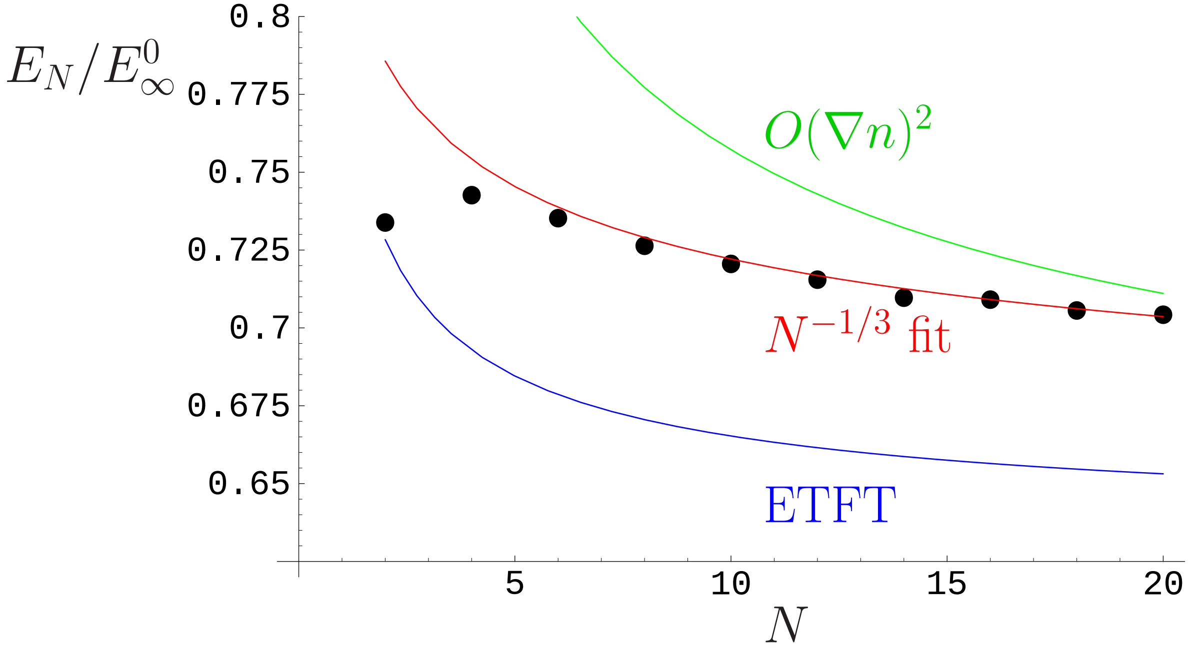
$$E_{trap} = \frac{\sqrt{0.475}}{4}\omega(3N)^{4/3}\left(1 + \frac{2.4}{(3N)^{2/3}} + \ldots\right)$$

Free Fermions

$$\mathcal{E}(x) = n(x)A_0(x) + 2.871\,\frac{n(x)^{5/3}}{m} + 0.014\,\frac{\left(\nabla n(x)\right)^2}{mn(x)} + 0.167\,\frac{\nabla^2 n(x)}{m}$$

$$E_{trap} = \frac{1}{4}\omega(3N)^{4/3}\left(1 + \frac{0.5}{(3N)^{2/3}} + \ldots\right)$$

Comparison to Data



Outlook

Kohn Sham theory at unitarity?

Asymptotic behavior ($N^{-1/3}$?)

Superfluid density functional?

Perturbative pions, range corrections?