



Towards "*universal*" energy density functionals of non-relativistic spin-1/2 Fermi gases

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Outline

- Introduction
- •Formalism
- •Results and discussion
- •Summary and future perspective

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Energy density of nonrelativistic spin-1/2 Fermi gases

<u>EDF</u>: E[n]

Application to DFT, TDDFT

However, its exact form is unknown except for free gases

$$E_{\rm FG}(n) = \frac{3k_{\rm F}^3}{10m} n \equiv \frac{3(3\pi^2)^{\frac{2}{3}}}{10m} n^{\frac{5}{3}}$$

Can we extend it to the interacting case?

$$f(n, V) \equiv \frac{E(n, V)}{E_{\rm FG}(n)}$$

Partial wave expansion of the bare interaction V

$$V = V_s(a_s, r_s, \dots) + V_p(v_p, k_p, \dots) + \cdots$$

 a_s : *s*-wave scattering length r_s : *s*-wave effective range

 v_p : *p*-wave scattering volume k_p : *p*-wave effective momentum <u>Approach from the dilute limit</u> Homogenous matter EOS $(k_F \rightarrow 0)$ $f(n, V) \equiv f(k_F a_s, k_F r_s, v_n k_F^3, ...)$

"Universal thermodynamics" and Bertsch parameter

Suppose the *s*-wave interaction is dominant and taking large scattering length limit, EDF does not depend on details of the interaction like a free gas.

Ya. B. Zel'dovich, JETP **38**, 1123 (1960).



A. Gezerlis, et al, arXiv: 1406.6109v2

$$k\cot\delta_k = -\frac{1}{a_s} + \frac{1}{2}k^2r_s + \cdots$$
$$a_s = -18.5 \text{ fm}, r_s = 2.8 \text{ fm}$$

Universal thermodynamics in a unitary Fermi gas

$$f(n, V) \to f(k_{\rm F}a_s \to \infty) \equiv \xi_{\rm B}$$

$$E(n, V) \to E(k_{\rm F}a \to \infty) \equiv \xi_{\rm B}E_{\rm FG}(n)$$

$\xi_{\rm B}$: Bertsch parameter



G. F. Bertsch, Challenge problem in many-body physics (1999)

Tunable scattering length in ultracold Fermi gases

"Academic problem" can be now tested in cold atoms



G. Zürn, et al., PRL 110, 135301 (2013).

C. Regal, et al., PRL 92, 040403 (2004).

BEC-BCS crossover

Y. Ohashi, HT, and P. van Wyk, Prog. Part. Nucl. Phys. 111, 103739 (2020).



Unitary Fermi gas and neutron matter

• The low-density neutron matter is also dominated by the *s*-wave scattering like an ultracold Fermi gas

M. Horikoshi, M. Koashi, HT, Y. Ohashi, and M. Kuwata-Gonokami, PRX, 7, 041004 (2017).





Density-induced BEC-BCS crossover

What happen when the effective range is not negligible?

(e.g., $k_F r \sim 1$ becomes non-negligible in neutron matter at subnuclear density)

Scattering phase shift

$$k \cot \delta_s(k) = -\frac{1}{a} + \frac{1}{2}rk^2 - Sr^3k^4 + O(k^5)$$

a: scattering length
r: effective range
S: shape parameter

Cold atoms (zero-range interaction, r/a = 0) Neutron matter (dineutron pairing) (r/a < 0) Nuclear matter (deuteron pairing) (r/a > 0)

*In this talk, we consider only the positive r



Dashed line: $\cot \delta_s (k = k_F) = 0$ HT, JPSJ **88**, 093001 (2019).

Mechanical instability in two-component Fermi gases with finite-range interaction



Interaction used in these work (in principle, nonzero shape parameter S...) \rightarrow unclear whether it is the effective-range correction or the effect beyond r_{eff}





Energy density and Tan's relation

How does the exact relation for the zero-range interaction can be modified?



In this talk...

- We discuss the ground-state properties in non-relativistic spin-1/2 Fermi gases with the finite-range interaction.
- Specifically, we focus on the *pure* effective-range corrections by using the interaction potential exactly reproducing the phase shift without higher-order coefficients.

What can we say with only s-wave **scattering length** and **effective range** in spin-1/2 fermionic systems?

$$k \cot \delta_s(k) = -\frac{1}{a} + \frac{1}{2}rk^2$$

$$f(n, V) \equiv f(k_{\rm F}a, k_{\rm F}r) \rightarrow E(n, V) = f(k_{\rm F}a, k_{\rm F}r)E_{\rm FG}(n)$$

In particular, we address:

- 1. Is the formation of droplets found due to the effective range correction?
- 2. What about the relation between Tan's contact and nuclear contact?

$$\frac{\partial^2 (E/N)}{\partial n^2} \propto c_s^2 = 0? \qquad C = C_{\text{nucl.}}?$$

HT and H. Liang, PRA 106, 043308 (2022).

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Hamiltonian

 $H = H_0 + V$ $= \sum_{\boldsymbol{k},\sigma} \xi_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma}^{\dagger} c_{\boldsymbol{k},\sigma} + \sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{P}} U(\boldsymbol{k},\boldsymbol{k}') c_{\boldsymbol{k}+\boldsymbol{P}/2,\uparrow}^{\dagger} c_{-\boldsymbol{k}+\boldsymbol{P}/2,\downarrow}^{\dagger} c_{-\boldsymbol{k}'+\boldsymbol{P}/2,\downarrow}^{\dagger} c_{\boldsymbol{k}'+\boldsymbol{P}/2,\uparrow}^{\dagger}$ $\xi_{\boldsymbol{k},\sigma} = \frac{k^2}{2m} - \mu$: kinetic energy measured from the chemical potential μ $c_{\boldsymbol{k},\sigma}$: annihilation operator of a fermion with momentum \boldsymbol{k} and spin $\sigma = \uparrow,\downarrow$ $U(\boldsymbol{k},\boldsymbol{k}')$: non-local two-body interaction



k, **k**': relative momenta

P : c. o. m. momentum

Separable finite-range s-wave interaction

$$U(\boldsymbol{k},\boldsymbol{k}')=g\gamma_k\gamma_{k'}$$

Two-body T-matrix

$$T(\boldsymbol{k}, \boldsymbol{k}'; \omega) = U(\boldsymbol{k}, \boldsymbol{k}') + \sum_{\boldsymbol{p}} U(\boldsymbol{k}, \boldsymbol{p}) \frac{1}{\omega_{+} - 2\varepsilon_{\boldsymbol{p}}} T(\boldsymbol{p}, \boldsymbol{k}'; \omega)$$

Relation to the s-wave phase shift

$$-\frac{m}{4\pi}T(\mathbf{k},\mathbf{k}';2\varepsilon_{\mathbf{k}}) = \frac{1}{k\cot\delta_s(k) - ik} \qquad k\cot\delta_s(k) = -\frac{1}{a} + \frac{1}{2}rk^2$$

Form factor

$$\gamma_k = \frac{1}{\sqrt{1 + (k/\Lambda)^2}}$$

Two parameters can be expressed in terms of low-energy constants.

$$\Lambda = \frac{1}{r} \left[1 + \sqrt{1 - \frac{2r}{a}} \right]$$
$$g = \frac{4\pi a}{m} \frac{1}{1 - a\Lambda}.$$

*Non-separability is out of scope in this work because it cannot be characterized by the effective range theory

Hartree-Fock-Bogoliubov theory

- Both density and pairing mean-fields are self-consistently treated
- Hartree-Fock term is NOT negligible in contrast to the zero-range interaction

$$\begin{split} H_{\rm HFB} &= \sum_{\boldsymbol{k},\sigma} \left[\xi_{\boldsymbol{k},\sigma} + \Sigma_{\sigma}(\boldsymbol{k}) \right] c_{\boldsymbol{k},\sigma}^{\dagger} c_{\boldsymbol{k},\sigma} \\ &- \sum_{\boldsymbol{k}} \left[\Delta^{*}(\boldsymbol{k}) c_{-\boldsymbol{k},\downarrow} c_{\boldsymbol{k},\uparrow} + \Delta(\boldsymbol{k}) c_{\boldsymbol{k},\uparrow}^{\dagger} c_{-\boldsymbol{k},\downarrow}^{\dagger} \right] \\ &- \sum_{\boldsymbol{k},\boldsymbol{k}'} U(\boldsymbol{k},\boldsymbol{k}') \langle c_{\boldsymbol{k},\uparrow}^{\dagger} c_{-\boldsymbol{k},\downarrow}^{\dagger} \rangle \langle c_{-\boldsymbol{k}',\downarrow} c_{\boldsymbol{k}',\uparrow} \rangle \\ &- \sum_{\boldsymbol{p},\boldsymbol{p}'} U \left(\frac{\boldsymbol{p} - \boldsymbol{p}'}{2}, \frac{\boldsymbol{p} - \boldsymbol{p}'}{2} \right) \langle c_{\boldsymbol{p},\uparrow}^{\dagger} c_{\boldsymbol{p},\uparrow} \rangle \langle c_{\boldsymbol{p}',\downarrow}^{\dagger} c_{\boldsymbol{p}',\downarrow} \rangle \\ \\ \frac{BCS \text{-type pairing field}}{\Delta(\boldsymbol{k}) = -\sum_{\boldsymbol{k}'} U(\boldsymbol{k},\boldsymbol{k}') \langle c_{-\boldsymbol{k}',\downarrow} c_{\boldsymbol{k}',\uparrow} \rangle \\ \end{array} \right] \frac{\text{Hartree-Fock-type self-energy}}{\Sigma_{\sigma}(\boldsymbol{p}) = \sum_{\boldsymbol{p}'} U \left(\frac{\boldsymbol{p} - \boldsymbol{p}'}{2}, \frac{\boldsymbol{p} - \boldsymbol{p}'}{2} \right) \langle c_{\boldsymbol{p}',\bar{\sigma}}^{\dagger} c_{\boldsymbol{p}',\bar{\sigma}} \rangle \end{split}$$

See also PRA 103, 063306 (2021).

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Superfluid order parameter



Effective-range dependence at $1/(k_F a) = 0$

*In the high-density regime, the value of $1/(k_F a)$ is not important



Sound velocity in the density-induced BEC-"BCS" crossover

No collapse in contrast to [PRA 95, 013633 (2017)] reporting the collapse ($c_s = 0$).



Sound velocity in the density-induced BEC-"BCS" crossover



High-momentum tails

More detailed investigations on the relation between Tan's contact and nuclear contact seem to be needed (e.g., repulsive core and so on).



The high momentum tails should be suppressed by the finite-range correction

Are they different?

Nuclear-contact-like parameter

Tan's contact and nuclear contact are slightly different in terms of relevant energy scales



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Summary

Paper: HT and H. Liang, PRA 106, 043308 (2022).

•We have discussed the ground-state properties of non-relativistic spin-1/2 Fermi gases with the finite range interaction.

What can we say with only two parameters (*a*, *r*)? Our answer is that the sound velocity exhibits a non-monotonic behavior but no collapse associated with the finite-range correction.
We elaborated the relation between Tan's contact and the nuclear contact. While Tan's contact characterizes short-range correlations beyond many-body scale, the nuclear contact captures the pair-correlations around the Fermi momentum.



Future work: Beyond the HFB calculation. Extension of Tan's energy relations to nuclear system and its applications to constructing true "*universal*" EDF.

Appendix

Large effective-range limit

$$U(\mathbf{k}, \mathbf{k}) = g \frac{1}{1 + (k/\Lambda)^2} \qquad \Lambda = \frac{2}{r} \quad (a^{-1} = 0) \quad \text{``Lorentzian form''}$$

$$U(\mathbf{k}, \mathbf{k}) \to -\frac{4\pi^2}{m}\delta(k) \quad (r \to \infty)$$

Vanishing HF self-energy

$$\Sigma_{r \to \infty}(\boldsymbol{k}) = g \sum_{\boldsymbol{k}'} \gamma_{\frac{|\boldsymbol{k} - \boldsymbol{k}'|}{2}}^2 \theta \left(-\frac{k'^2}{2m} + \mu - \Sigma(\boldsymbol{k}') \right) = \boldsymbol{0}$$



Equations for physical quantities



Ground-state energy

$$E = \sum_{\boldsymbol{k}} \left[\xi_{\boldsymbol{k}} + \Sigma(\boldsymbol{k}) - E_{\boldsymbol{k}} \right] - \frac{|\Delta|^2}{g} - \sum_{\boldsymbol{k}} \Sigma(\boldsymbol{k}) n_{\boldsymbol{k}}$$

 $\frac{\partial \rho}{\partial \mu}$

Sound velocity Compressibility
$$c_s = \sqrt{\frac{1}{m\rho\kappa}} \qquad \kappa = \frac{1}{\rho^2} \left(\frac{\partial}{\partial r}\right)$$

Beyond effective-range theory?

Yamaguchi interaction



Screened Coulomb interaction



Do we encounter the mechanical collapse?

-No, at least within the effective-range corrections.

Comparison with zero-momentum Hartree approximation



*However, the collapse occurs in PRA 95, 013633 (2017) at $k_{\rm F}r \simeq 2$ because of higher coefficients in $\delta_s(k)$.

Optical control of the effective range in cold atoms



PRL 116, 075301 (2016), PRL 121, 163404 (2018), PRL 122, 040405 (2019).



Rabi-frequency dependence of controllable effective range PRA **86**, 063625 (2012).

➡ A system with both large scattering length and effective range (compared to higher order coefficients) can be realized in future experiments.

BEC-BCS crossover in condensed matter systems

Scattering length (interaction) CANNOT be tuned → Density can be tuned

BEC-BCS crossover in Li_x ZrNCl (lithium-intercalated layered nitride)



Y. Nakagawa, et al., Science 372, 6538 (2021).

Others: FeSe [PNAS **111**, 16309 (2014).], Organic SC [PRX **12**, 011016 (2022).], Excitons in bilayer graphene [Science **375**, 6577 (2022).], etc...

Sound velocity throughout the BCS-BEC crossover in "*ultracold Fermi gases*"

• Smooth change from the Anderson-Bogoliubov (AB) mode of Fermi superfluids to the Bogoliubov phonon of molecular bosons



Cold atom expr.: M. Horikoshi, et al., PRX, 7, 041004 (2017).

S. Hoinka, et al., Nat. Phys. 13, 943 (2017).

Large effective range limit is really BCS? (high density)



Mechanical collapse to the droplet phase?

rla

-0.5

0.5

1.5 BEC

0

 $1/(k_{\rm F}a)$

k_Fr

0.5

-1.5 BCS (note that these are four-component mixtures)

Matrix Green's function

$$\widehat{G}(\boldsymbol{p},\tau) = -\left\langle T_{\tau} \left[\Psi_{\boldsymbol{p}}(\tau) \Psi_{\boldsymbol{p}}^{\dagger}(0) \right] \right\rangle$$

$$= -\left(\left\langle T_{\tau} \left[c_{\boldsymbol{p},\uparrow}(\tau) c_{\boldsymbol{p},\uparrow}^{\dagger}(0) \right] \right\rangle \quad \left\langle T_{\tau} \left[c_{\boldsymbol{p},\uparrow}(\tau) c_{-\boldsymbol{p},\downarrow}(0) \right] \right\rangle \\ \left\langle T_{\tau} \left[c_{-\boldsymbol{p},\downarrow}^{\dagger}(\tau) c_{\boldsymbol{p},\uparrow}^{\dagger}(0) \right] \right\rangle \quad \left\langle T_{\tau} \left[c_{-\boldsymbol{p},\downarrow}^{\dagger}(\tau) c_{-\boldsymbol{p},\downarrow}(0) \right] \right\rangle \right) \left\langle \mathbf{T}_{\tau} \left[c_{-\boldsymbol{p},\downarrow}^{\dagger}(\tau) c_{-\boldsymbol{p},\downarrow}(0) \right] \right\rangle$$
Scalar representation Scalar representation
$$\mathbf{F}_{\boldsymbol{p},\uparrow}(\tau) = -\left\langle T_{\tau} \left[c_{\boldsymbol{p},\uparrow}(\tau) c_{\boldsymbol{p},\uparrow}^{\dagger}(0) \right] \right\rangle \quad \left\langle T_{\tau} \left[c_{-\boldsymbol{p},\downarrow}(\tau) c_{-\boldsymbol{p},\downarrow}(0) \right] \right\rangle$$
Dyson's equation with the matrix self-energy $\widehat{\boldsymbol{\Sigma}}(\boldsymbol{p})$

$$\begin{split} \hat{G}(p) &= \hat{G}^0(p) + \hat{G}^0(p)\hat{\Sigma}(p)\hat{G}^0(p) + \hat{G}^0(p)\hat{\Sigma}(p)\hat{G}^0(p)\hat{\Sigma}(p)\hat{G}^0(p) + \cdots \\ &= \hat{G}^0(p) + \hat{G}^0(p)\hat{\Sigma}(p)\hat{G}(p) \end{split}$$



BCS-Gor'kov Green's function

 $\hat{G}^{0}(p) = \left[i\omega_{n} - \left(\varepsilon_{p} - \mu\right)\tau_{3} + \Delta\tau_{1} + h\right]^{-1} \qquad \hat{G}_{\sigma}(p) = \int_{0}^{\beta} d\tau \hat{G}_{\sigma}(\boldsymbol{p}, \tau) e^{i\omega_{n}\tau} \quad \stackrel{}{\times} p = (\boldsymbol{p}, i\omega_{m})$

Extended *T*-matrix approximation

ETMA self-energy $\widehat{\Sigma}(p)$

$$\widehat{\Sigma}(p) = -T \sum_{q} \sum_{i,j=\pm} \Gamma^{ij}(q) \tau_i \widehat{G}(p+q) \tau_j \quad -\underbrace{\sum}_{q \in I} = \underbrace{f^{ij}(q)}_{\text{*Ordinary TMA uses } G^0 \text{ (non-interacting one) here}}$$

Particle-Particle scattering matrix $\widehat{\Gamma}(q)$



Diagonal Green's function

 $G_{11} = G_{11}^0 + G_{11}^0 \Sigma_{11} G_{11}$



Diagonal scattering matrix





Diagonal Green's function

 $G_{11} = G_{11}^{0} + G_{11}^{0} \Sigma_{11} G_{11} + G_{12}^{0} \Sigma_{21} G_{11}$ $+ G_{11}^{0} \Sigma_{12} G_{21} + G_{12}^{0} \Sigma_{22} G_{21}$

Anomalous Green's function

 $G_{21} = G_{21}^{0} + G_{21}^{0} \Sigma_{11} G_{11} + G_{22}^{0} \Sigma_{21} G_{11}$ $+ G_{21}^{0} \Sigma_{12} G_{21} + G_{22}^{0} \Sigma_{22} G_{21}$



