Exact relations for a strongly correlated Fermi gas

and a general method

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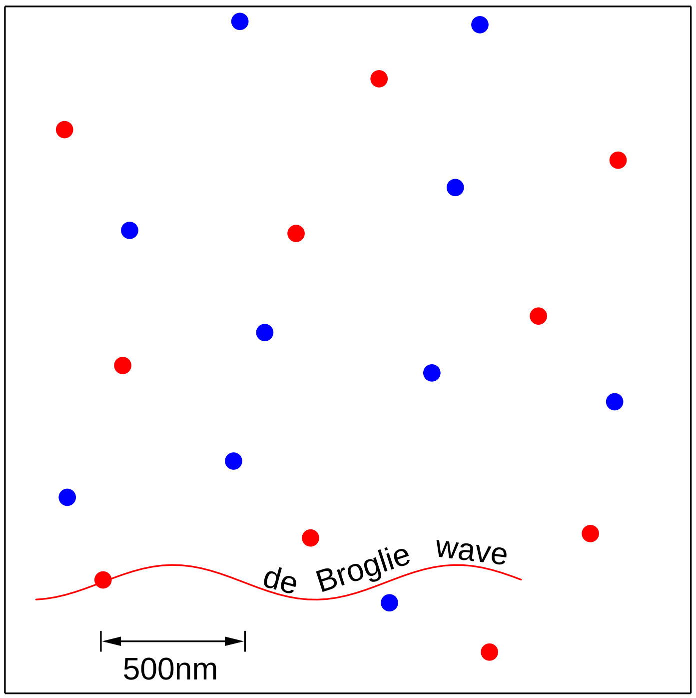
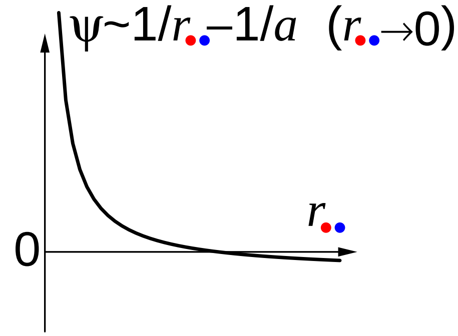
A dilute, ultracold atomic Fermi gas near a 2-body resonance





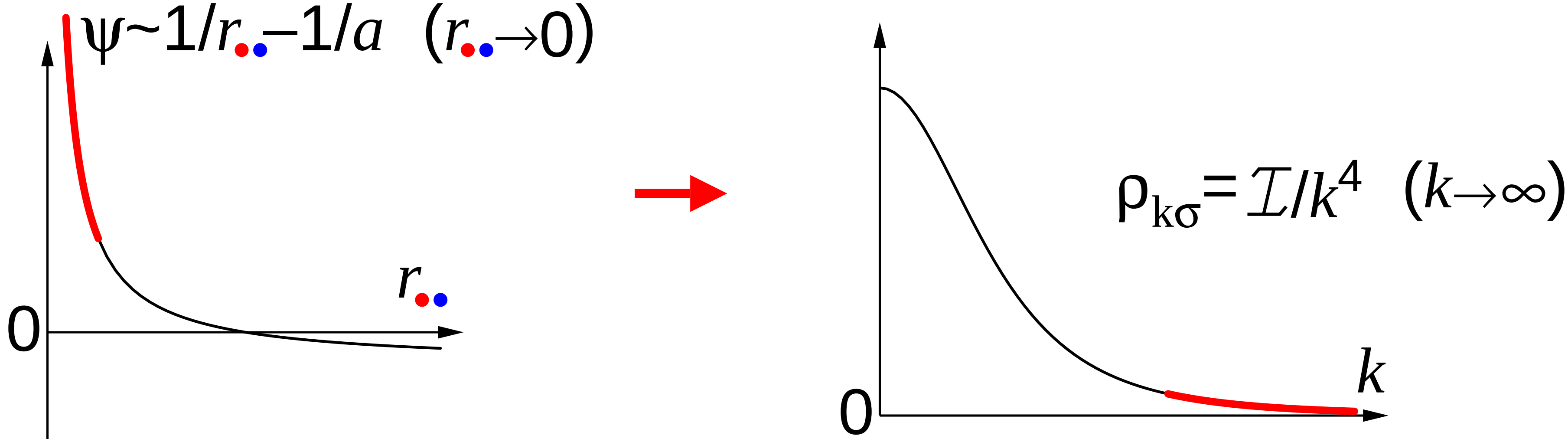
$$k_F^{-1}, \lambda_{dB}, |a| \gg \text{ range of the interaction } r_0 \sim 3\text{nm}$$

$\Rightarrow$ we will mostly study the **zero-range interaction** problem (the interaction is solely described by a)

Despite the importance of this Fermi system (being studied in many labs), theoretical analysis is difficult, in particular in the most interesting cases of $N_\uparrow \neq N_\downarrow$
(Monte-Carlo simulations plagued by fermion sign problem)

$\Rightarrow$ EXACT RELATIONS ARE IMPORTANT

Tail of the momentum distribution



$$\int_{\mathbf{k}} \rho_{\mathbf{k}\sigma} \equiv N_\sigma \qquad \left[\hbar\mathbf{k} = \text{momentum}, \quad \sigma = \uparrow, \downarrow \qquad \int_{\mathbf{k}} \equiv \int \frac{d^3k}{(2\pi)^3}\right]$$

Summary of the relations

- Pair correlations: $\int \langle n_\uparrow(\mathbf{s}) n_\downarrow(\mathbf{s}+\mathbf{r})\rangle \mathrm{d}^3 s = \mathcal{I}/(4\pi r)^2 \quad (r \to 0)$
- Energy relation: $E_{\text{internal}} (= E - E_V) = \frac{\hbar^2 \mathcal{I}}{4\pi a m} + \int_{\mathbf{k}} \sum_\sigma \frac{\hbar^2 k^2}{2m} \Big(\rho_{\mathbf{k}\sigma} - \frac{\mathcal{I}}{k^4} \Big)$
- Adiabatic relation: $\frac{\mathrm{d}E}{\mathrm{d}(-1/a)}\Big|_{\text{adiabatic}} = \frac{\hbar^2 \mathcal{I}}{4\pi m}$
- Generalized virial theorem: $E - \frac{\beta+2}{2} E_V = -\frac{\hbar^2 \mathcal{I}}{8\pi a m}$
  $V(\mathbf{r}) = r^\beta f(\hat{\mathbf{r}})$ $(\beta > -2,\ \beta \neq 0)$
- Pressure relation: $P - \frac{2}{3}\rho_E = \frac{\hbar^2}{12\pi a m}(\mathcal{I}/volume)$
- Dynamic relation: $\frac{\mathrm{d}E}{\mathrm{d}t} = \frac{\hbar^2 \mathcal{I}(t)}{4\pi m} \frac{\mathrm{d}[-a(t)^{-1}]}{\mathrm{d}t} + \int \mathrm{d}^3 r\, n(\mathbf{r}t) \frac{\partial V(\mathbf{r}t)}{\partial t}$

I. Pair Correlations

$$\int \langle n_{\uparrow}(\mathbf{s}) n_{\downarrow}(\mathbf{s}+\mathbf{r})\rangle \mathrm{d}^3 s = \mathcal{I}/(4\pi r)^2 \quad (r \to 0)$$

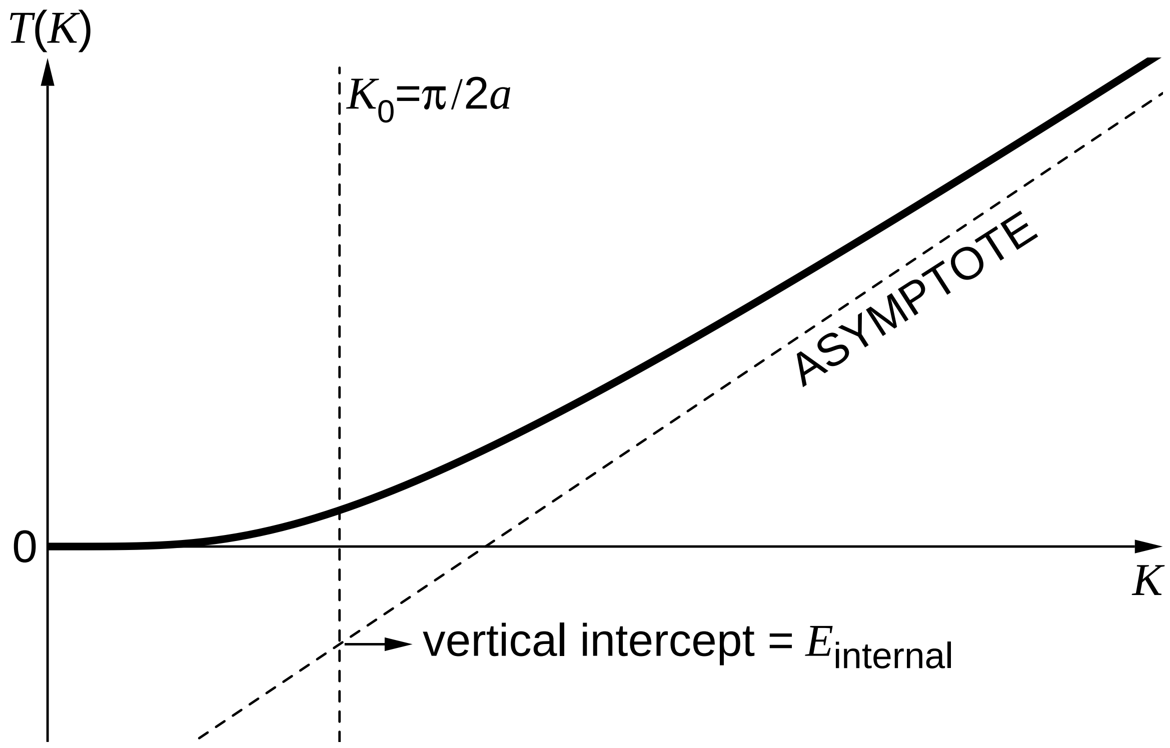
Implications for ultracold atoms:

- The event rate for 2-body inelastic decays: $\alpha_2 = c\mathcal{I}$
- If a is tuned near a broad Feshbach resonance, the average number of molecules in the closed channel is

$$N_{\text{closed}} = c'\mathcal{I} \quad (\ll N_\sigma)$$

$\Rightarrow$ one can infer $\mathcal{I}$ from measurements of α_2 or N_{closed}

II. Energy Relation



$$T(K) \equiv \int_{k<K} \sum_{\sigma} \frac{\hbar^2 k^2}{2m} \rho_{\mathbf{k}\sigma}$$

III. Adiabatic Relation

If we tune a adiabatically,

$$\frac{\mathrm{d}E}{\mathrm{d}(-1/a)} = \frac{\hbar^2 \mathcal{I}}{4\pi m}$$

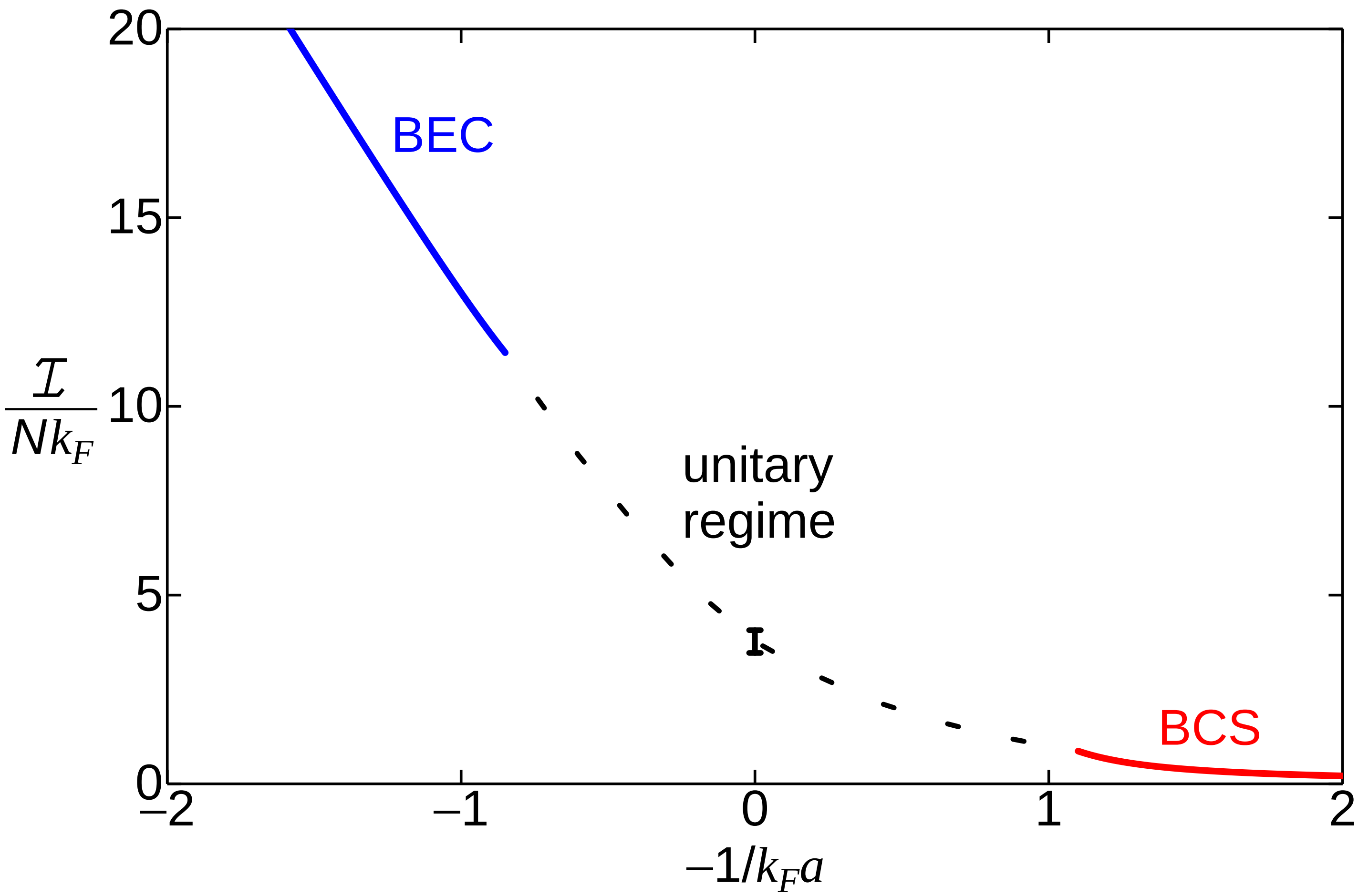
valid for

- any N-body energy levels, and
- any thermal equilibrium ensembles (microcanonical, canonical, grand canonical)

Physical meaning:

$\mathrm{d}E =$ the change of the interaction potential [$\propto \mathrm{d}(-1/a)$]
$\times$ the probablity that $\uparrow\downarrow$ fermions meet each other ($\propto \mathcal{I}$)

$\mathcal{I}$ in the BEC-BCS crossover



IV. Virial Theorem: The one previously known

For a harmonically trapped system in the unitarity limit ($a \to \infty$)

$$E = 2E_V$$

*J. E. Thomas, J. Kinast, and A. Turlapov, Phys.Rev.Lett.***95***, 120402 (2005);*

F. Chevy (unpublished);

*F. Werner and Y. Castin, Phys.Rev.A***74** *053604 (2006);*

D. T. Son, arXiv:0707.1851v1;

T. Mehen, arXiv:0712.0867v1.

IV. Virial Theorem: Generalization

away from unitarity

For a harmonically trapped system, for any a,

$$E - 2E_V = -\frac{\hbar^2 \mathcal{I}}{8\pi a m}$$

Proof of the Generalized Virial Theorem

Step 1. Adiabatic increase of the scatt. length

$a \rightarrow (1+\epsilon)a$

$E' - E = \frac{\hbar^2 \mathcal{I}}{4\pi a m}\epsilon + O(\epsilon^2)$

Step 2. Geometric compression (WITHOUT changing V)

$\phi'(\mathbf{R}) \rightarrow \phi'((1+\epsilon)\mathbf{R})$

$E'_{\text{internal}} \rightarrow E'_{\text{internal}}(1+\epsilon)^2$

$E'_V \rightarrow E'_V/(1+\epsilon)^2$

$(1+\epsilon)a \rightarrow a$

$E'' - E' = 2\epsilon E'_{\text{internal}} - 2\epsilon E'_V + O(\epsilon^2) = 2\epsilon E_{\text{internal}} - 2\epsilon E_V + O(\epsilon^2).$

Result. Variational stability of energy levels implies that $E'' - E = O(\epsilon^2)$, or $-\frac{\hbar^2 \mathcal{I}}{8\pi a m} = E - 2E_V$.

V. Pressure Relation

$V = 0$

$$P - \frac{2}{3}\rho_E = \frac{\hbar^2}{12\pi a m}\frac{\mathcal{I}}{\Omega}$$

Ω=volume

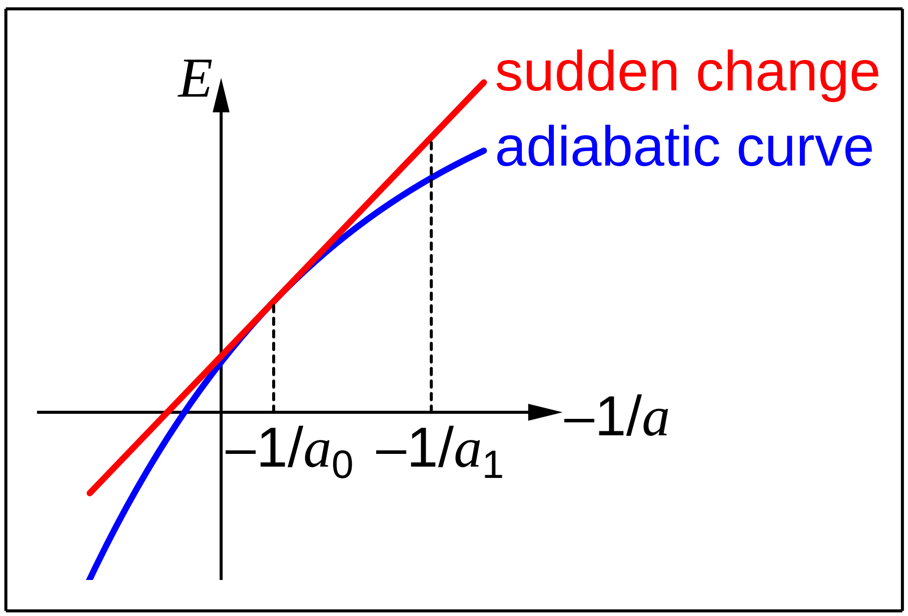
$\rho_E = E/\Omega$: energy density

VI. Dynamic Relation

$a = a(t)$

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \frac{\hbar^2 \mathcal{I}(t)}{4\pi m} \frac{\mathrm{d}[-a(t)^{-1}]}{\mathrm{d}t} + \int \mathrm{d}^3 r\, n(\mathbf{r}t) \frac{\partial V(\mathbf{r}t)}{\partial t}$$

$\mathcal{I}(t) \equiv \lim_{k\to\infty} k^4 \rho_{\mathbf{k}\sigma}(t)$ *[$\mathcal{I}(t)$ is always continuous]*



Tangent law for a sudden change of a

Summary

Quantum Short-Range Interaction $\Rightarrow$ Universal Exact Relations

MANY MORE exact relations ...

- Local relations, eg, local conservation laws
- Other physical quantities, perhaps entropy and viscosities?
- Other quantum systems
  - 2D and 1D quantum gases
  - Mixed-Dimensional quantum gases
    Nishida and Tan, arXiv:0806.2668
  - Quantum gases with both two- and three-body resonances
    Nishida, Son, and Tan, PRL **100**, *090405 (2008)*
  - ......

References

ST, cond-mat/0505200
ST, cond-mat/0508320
ST, arXiv:0803.0841
ST, cond-mat/0505615

For alternative derivations, see
Braaten and Platter, arXiv:0803.1125;
Zhang and Leggett, arXiv:0809.1892

For a similar study of the generalized virial theorem, see
Werner, arXiv:0803.3277

For the number of closed channel molecules, see
Werner, Tarruell, and Castin, arXiv:0807.0078

Part II: a mathematical method

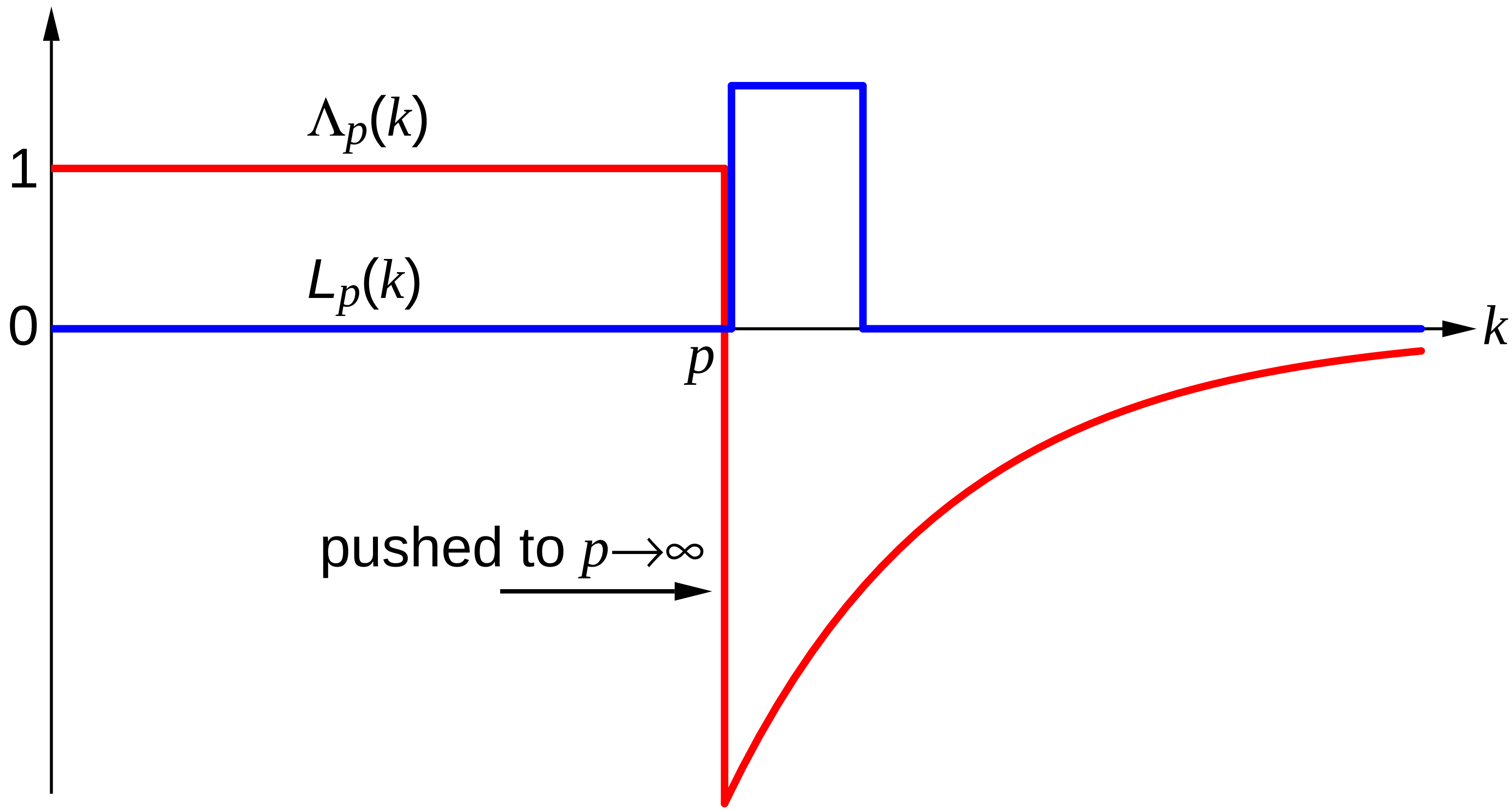
Generalized Functions

$$\Lambda(\mathbf{k}) = 1 \ (\text{if } k < \infty), \ \int \frac{d^3k}{(2\pi)^3} \frac{\Lambda(\mathbf{k})}{k^2} = 0, \ \Lambda(-\mathbf{k}) = \Lambda(\mathbf{k}).$$

$$L(\mathbf{k}) = 0 \ (\text{if } k < \infty), \ \int \frac{d^3k}{(2\pi)^3} \frac{L(\mathbf{k})}{k^2} = 1, \ L(-\mathbf{k}) = L(\mathbf{k}).$$

$$\lambda(\mathbf{r}) = 0 \ (\text{if } r > 0), \ \int d^3r \lambda(\mathbf{r}) = 1, \ \int d^3r \lambda(\mathbf{r})/4\pi r = 0, \ \lambda(-\mathbf{r}) = \lambda(\mathbf{r}).$$

$$l(\mathbf{r}) = 0 \ (\text{if } r > 0), \ \int d^3r l(\mathbf{r}) = 0, \ \int d^3r l(\mathbf{r})/4\pi r = 1, \ l(-\mathbf{r}) = l(\mathbf{r}).$$



$$\int \frac{\mathrm{d}^3 k}{(2\pi)^3} \frac{\Lambda_p(\mathbf{k})}{k^2} = 0 \qquad \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \frac{L_p(\mathbf{k})}{k^2} = 1$$

η function

$$\eta(\mathbf{k}) \equiv \Lambda(\mathbf{k}) + L(\mathbf{k})/4\pi a$$
$$\tilde{\eta}(\mathbf{r}) \equiv \lambda(\mathbf{r}) + l(\mathbf{r})/4\pi a.$$

$$\int \mathrm{d}^3 r \tilde{\eta}(\mathbf{r})(1/r - 1/a) = \int \mathrm{d}^3 r [\lambda(\mathbf{r}) + l(\mathbf{r})/4\pi a](1/r - 1/a)$$
$$= \int \mathrm{d}^3 r \lambda(\mathbf{r})/r - (1/a)\int \mathrm{d}^3 r \lambda(\mathbf{r}) + \int \mathrm{d}^3 r l(\mathbf{r})/4\pi a r - (1/4\pi a^2)\int \mathrm{d}^3 r l(\mathbf{r})$$
$$= 0 \qquad - 1/a \qquad + 1/a \qquad - 0 \qquad = 0$$

$$\int \frac{\mathrm{d}^3 k}{(2\pi)^3} \eta(\mathbf{k}) S_{\mathbf{k}} = \frac{u}{4\pi a} + \lim_{K\to\infty} \int_{|\mathbf{k}|<K} \frac{\mathrm{d}^3 k}{(2\pi)^3}\left[S_{\mathbf{k}} - \frac{u}{k^2}\right], \quad u \equiv \lim_{k\to\infty} k^2 S_{\mathbf{k}}.$$

IF $\sum_{\mathbf{k}} S_{\mathbf{k}}$ is convergent, $u = 0$ and $\sum_{\mathbf{k}} \eta(\mathbf{k}) S_{\mathbf{k}} = \sum_{\mathbf{k}} S_{\mathbf{k}}$

Formulation of the physical problem

1) Hamiltonian:

$$H_{\text{internal}} = \sum_{\mathbf{k}\sigma} \frac{k^2}{2m} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \frac{4\pi a}{m\Omega} \sum_{\mathbf{q}\mathbf{k}\mathbf{k}'} \Lambda(\mathbf{k}') c^\dagger_{\mathbf{q}/2+\mathbf{k}\uparrow} c^\dagger_{\mathbf{q}/2-\mathbf{k}\downarrow} c_{\mathbf{q}/2-\mathbf{k}'\downarrow} c_{\mathbf{q}/2+\mathbf{k}'\uparrow}$$

$$H_{\text{ext}} = \sum_\sigma \int \mathrm{d}^3 r V_{\text{ext}}(\mathbf{r}) \psi^\dagger_\sigma(\mathbf{r}) \psi_\sigma(\mathbf{r})$$

NOTE: $\Lambda(\mathbf{k}')$ *annihilates* $1/k'^2 \Leftrightarrow \frac{\partial}{\partial r} r$ *annihilates* $1/r$, *in Fermi pseudopotential*

2) Short-range boundary condition:

$$\sum_{\mathbf{k}} \eta(\mathbf{k}) c_{\mathbf{q}/2-\mathbf{k}\downarrow} c_{\mathbf{q}/2+\mathbf{k}\uparrow} |\phi\rangle = 0 \quad \text{(any } \mathbf{q}\text{)}$$

Derivation of the Energy Relation

$$E_{\text{internal}} = \langle\phi|H_{\text{internal}}|\phi\rangle = \sum_{\mathbf{k}} S_{\mathbf{k}},$$
$$S_{\mathbf{k}} = \langle\phi|\left(\frac{k^2}{2m}c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + \frac{4\pi a}{m\Omega}\sum_{\mathbf{q}\mathbf{k}'}\Lambda(\mathbf{k}')c^\dagger_{\mathbf{q}/2+\mathbf{k}\uparrow}c^\dagger_{\mathbf{q}/2-\mathbf{k}\downarrow}c_{\mathbf{q}/2-\mathbf{k}'\downarrow}c_{\mathbf{q}/2+\mathbf{k}'\uparrow}\right)|\phi\rangle.$$

E_{internal} is finite $\Rightarrow$ $\sum_{\mathbf{k}} S_{\mathbf{k}}$ is convergent $\Rightarrow$

$$\begin{aligned}
E_{\text{internal}} &= \sum_{\mathbf{k}} \eta(\mathbf{k}) S_{\mathbf{k}} \\
&= \sum_{\mathbf{k}\sigma} \eta(\mathbf{k})\frac{k^2}{2m}\langle\phi|c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}|\phi\rangle \\
&\quad + \frac{4\pi a}{m\Omega}\sum_{\mathbf{q}\mathbf{k}'} \underbrace{\sum_{\mathbf{k}}\langle\phi|\eta(\mathbf{k})c^\dagger_{\mathbf{q}/2+\mathbf{k}\uparrow}c^\dagger_{\mathbf{q}/2-\mathbf{k}\downarrow}}_{=0 \text{ (short-range bd condition)}} c_{\mathbf{q}/2-\mathbf{k}'\downarrow}c_{\mathbf{q}/2+\mathbf{k}'\uparrow}\Lambda(\mathbf{k}')|\phi\rangle \\
&= \sum_{\mathbf{k}\sigma} \eta(\mathbf{k})\frac{k^2}{2m}\langle\phi|c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}|\phi\rangle = \int_{\mathbf{k}}\sum_{\sigma}\eta(\mathbf{k})\frac{k^2}{2m}\rho_{\mathbf{k}\sigma}
\end{aligned}$$

Energy relation: $E_{\text{internal}} \leftrightarrow \rho_{\mathbf{k}\sigma}$

$$E_{\text{internal}} = \int_{\mathbf{k}} \sum_{\sigma} \eta(\mathbf{k}) \frac{\hbar^2 k^2}{2m} \rho_{\mathbf{k}\sigma}$$

$$E_{\text{internal}} = \frac{\hbar^2 \mathcal{I}}{4\pi a m} + \int_{\mathbf{k}} \sum_{\sigma} \frac{\hbar^2 k^2}{2m} \Big(\rho_{\mathbf{k}\sigma} - \frac{\mathcal{I}}{k^4} \Big)$$

The General Method

We can "assign" finite values to any divergent integral.

- *by changing the integrand to generalized functions which are exactly the same as the original integrand, except at the divergence point(s).*

I believe this method will be useful in dealing with UV and IR divergences,
and other divergences in many fields of physics.

Application to IR divergences

ST, Phys. Rev. A **78**, 013636 (2008),
where the low-energy scattering of 3 bosons (and some basic properties of dilute Bose-Einstein condensates) are studied.