Isospin-Asymmetry Dependence of the <u>Thermody</u>namic Nuclear Equation of State

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The Nuclear EoS: Interplay of Nuclear Physics and Astrophysics

Neutron Stars: $T \sim 0$



www2.astro.puc.cl

Binary Mergers: $T \lesssim 50$ MeV



Rosswog: Phil. Trans. R. Soc. A 371 (2013)

- astrophysical constraints on the EoS from (e.g.,) neutron-star masses and radii, moments of intertia, ...
- task of nuclear theory: computation of the EoS from microphysics
 - \rightarrow EoS numerical input for simulations of supernovae and neutron-star mergers

Novel developments in theoretical nuclear physics: chiral EFT, renormalization group

- \rightarrow low-momentum interactions (no "hard core")
- ightarrow enables the use of Many-Body Perturbation Theory to compute the EoS

Modern Theory of Nuclear Interactions

- chiral EFT: general low-energy effective field theory consistent with symmetries of QCD, degrees of freedom: nucleons & pions
- systematic hierarchy of nuclear interactions controlled by expansion parameter $Q/\Lambda_{\chi} =$ soft scale/hard scale, where $\Lambda_{\chi} \sim 1~{\rm GeV}$



- restrict resolution via UV cutoff $\Lambda < \Lambda_{\chi}$ in momentum space
- LECs $c_i(\Lambda)$ fixed by high-precision fits to few-nucleon observables

 \rightarrow NN and 3N nuclear potentials for many-body calculations Nuclear potentials are not unique! \rightarrow uncertainty estimations (but: artifacts possible)

Low-momentum potentials $\Lambda \lesssim$ 450 MeV: MBPT becomes valid approach!

Many-Body Perturbation Theory (MBPT)

- linked-cluster expansion ("Goldstone expansion") for ground state energy (T = 0)
- textbook approach at finite T: expansion of grand-canonical potential $\Omega(T, \mu) = \Omega_0(T, \mu) + \Omega_1(T, \mu) + \Omega_2(T, \mu) + \mathcal{K}_{anom}(T, \mu) + \dots$ But: not consistent with Goldstone expansion, cannot describe spinodal instability

Proper finite-temperature MBPT: canonical ensemble, expansion for free energy

- "naive" approach: linked-cluster expansion of free energy; does not work because canonical-ensemble averages are constrained (fixed N)
- instead: evaluate ensemble averages via Legendre transform of cumulants; gives $F(T, \tilde{\mu}) = F_0(T, \tilde{\mu}) + A_1(T, \tilde{\mu}) + A_2(T, \tilde{\mu}) + \mathcal{K}_{anom}(T, \tilde{\mu}) + \mathcal{K}_{corr}(T, \tilde{\mu}) + \dots$
 - $\tilde{\mu}$ fixed by $\rho(T, \tilde{\mu}) = \partial F_0 / \partial \tilde{\mu} \rightarrow \text{consistent with Goldstone expansion}!$
 - additional contributions from unlinked diagrams \mathcal{K}_{corr} , renormalize $\tilde{\mu}$
- canonical series can be also derived via reorganization of grand-canonical series (Kohn-Luttinger method), but equivalence is only formal (asymptotic series!)

Mean-field benchmark

- fully renormalized MBPT: SCHF
- large \mathcal{K}_{anom} (ε renormalization), but $\mathcal{K}_{anom} + \mathcal{K}_{corr}$ (ε and $\tilde{\mu}$ renormalization) is small
- spinodal region only from canonical and fully renormalized MBPT



Chiral Nuclear EoS: Order-By-Order Results for various NN+3N Potentials





- $n_{3}^{10414} \& n_{3}^{10450}$: good perturbative behavior $F_{1} > F_{2} \gg F_{3}$ (third order: Holt & Kaiser: 1612.04309 (2016))
- n3lo500: less perturbative (F_{1,NN} & F_{2,NN} similar magnitude)
- VLK21 & VLK23: NN perturbative, but large contributions from 3N potential

Chiral Nuclear EoS: Effective-Mass Improved Results



- empirical saturation point: n3lo414, n3lo450, n3lo500, VLK21, VLK23
- VLK21 & VLK23 ruled out by thermodynamics (pressure isotherm crossing)



Need Chiral Nuclear EoS for Astrophysics Applications



Direct computation expensive; \rightsquigarrow explicit parametrizations of the nuclear EoS? \rightsquigarrow parabolic approximation of δ dependence: $\overline{F}(\delta) \simeq \overline{F}(\delta = 0) + F_{sym} \delta^2$ Question: is this really appropriate?



Steiner: PRC 74 (2006)

Sensitivity to δ dependence of threshold density for direct URCA process:

• Quartic parametrization of EoS $F(\delta) = F(0) + A_2 \delta^2 + A_4 \delta^4$

• Change
$$A_{2,4}$$
 with $A_2 + A_4$ fixed
 $(\eta = 1/2, A_4 = -4/9A_2)$
 $(\eta = 1, A_4 = 0)$
 $(\eta = 3, A_4 = 4A_2)$

Terms beyond the parabolic approximation can be important for astrophysics!

 \rightsquigarrow investigate the expansion in δ :

 $F(T,\rho,\delta) \sim \sum_{n=0}^{N} A_{2n}(T,\rho) \delta^{2n}, \quad \text{with}$

th
$$A_{2n}(T,\rho)$$

$$= \frac{1}{(2n)!} \frac{\partial^{2n} \bar{F}(T,\rho,\delta)}{\partial \delta^{2n}} \bigg|_{\delta = 0}$$

- o convergence behavior of the expansion?
- accuracy of parabolic approximation: how large is $F_{sym}(T, \rho) A_2(T, \rho)$?

Results for Expansion Coefficients $A_{2,4,6}$ (and for $F_{sym} - A_2$)



- dominant contribution to $F_{sym} A_2$ from noninteracting term and 3N interactions
- $A_{2n\geq 4}$ become very large at low $T \rightarrow \text{divergent asymptotic expansion!}$ $\Rightarrow \text{ higher-order parametrizations of } \delta \text{ dependence inhibited at low } T$

Divergent Expansion at Low Temperature

Examine higher-order approximations, e.g., $F_{[4]} := A_0 + A_2 \delta^2 + A_4 \delta^4$



What is the origin of the divergent behavior at low T?

 \rightarrow contributions beyond Hartree-Fock in MBPT, e.g., second-order term:

 $F_{2}(T, \tilde{\mu}^{n}, \tilde{\mu}^{p}) = -\frac{1}{8} \sum_{1234} \bar{V}_{2B}^{12,34} \, \bar{V}_{2B}^{34,12} \, \frac{n_{1}n_{2}\bar{n}_{3}\bar{n}_{4} - \bar{n}_{1}\bar{n}_{2}n_{3}n_{4}}{\varepsilon_{3} + \varepsilon_{4} - \varepsilon_{1} - \varepsilon_{2}}$

T = 0: integrand diverges at boundary of integral, leads to $|A_{2n\geq 4}| \xrightarrow{T \to 0} \infty$

Logarithmic Terms in the Isospin-Asymmetry Dependence at T = 0

Exact results (at second order) with S-wave contact interaction

$$F(T = 0, \rho, \delta) = A_0(0, \rho) + A_2(0, \rho) \,\delta^2 + \sum_{n=2}^{\infty} A_{2n, reg}(\rho) \,\delta^{2n} + \sum_{n=2}^{\infty} A_{2n, log}(\rho) \,\delta^{2n} \ln|\delta|$$

- Logarithmic terms also from third-order terms Holt & Kaiser: 1612.04309 (2016)
- Logarithmic terms also when ladders are resummed (checked numerically)



Influence of higher-order terms (beyond δ^2) on neutron-star properties?

- logarithmic δ terms: only small influence on proton fraction
- influence of using Y parametrizations? (work in progress)

Isospin-Asymmetry Dependence of Nuclear Liquid-Gas Phase Transition

Stability criterion: $\mathcal{F}_{ij} = \frac{\partial^2 F(T, \rho_n, \rho_p)}{\partial \rho_i \partial \rho_i}$ has only positive eigenvalues

- $\delta = 0$: reduces to pure-substance criterion $\partial P/\partial \rho > 0$
- isospin distillation in isospin-asymmetric nuclear matter (binary system!)
- endpoint of critical line ${\cal T}_c(\delta)$ at proton fraction $Y=(1-\delta)/2\simeq 3\cdot 10^{-4}$
- fragmentation temperature $T_{\rm FP}(\delta)$ endpoint at $Y \simeq 0.17$



 \rightarrow at large δ : $T_c(\delta)$ strongly influenced by entropy of mixing $\sim T Y \ln(Y)$ \rightarrow at T = 0: terms $\sim Y^{5/3}$ (also from interaction contributions!)

Thermodynamic Nuclear EoS from Chiral EFT Interactions

- proper finite-temperature MBPT: **canonical** series, cumulants evaluated via Legendre transformation to **grand-canonical ensemble averages**
- \bullet accuracy of parabolic δ approximation decreased for high densities and high temperatures
- δ dependence is nonanalytic at low T, logarithmic terms at T=0
- entropy of mixing $\sim TY \ln(Y)$, terms $Y^{5/3}$ at T = 0

Outlook: Chiral EoS for Astrophysics Applications

- need to extrapolate EoS to higher densities and temperatures
- one approach: construct explicit (ρ, T) parametrizations via fits
 (→ quantify uncertainties of extrapolation via fit ambiguities)
- ho dependence straightforward, but T dependence problematic:
 - extrapolation not well-behaved for many parametrizations (e.g., "Sommerfeld"-polynomial $\sum_{n} \alpha_n \tau^{2n}$)
 - SNM: computed data has tendency towards pressure isotherm crossing
 - PNM: approximately au -independent for $au\lesssim$ 25 MeV and $ho\lesssim$ 2 $ho_{\sf sat}$

Thank you for your attention!

Appendix 1: Isospin-Asymmetry Expansions

A1: Extraction of Maclaurin Coefficients with Finite Differences

General of 2N + 1 point central finite difference approximation for $\bar{A}_{2n}(T, \rho)$

$$\bar{A}_{2n}(T,\rho) \simeq \bar{A}_{2n}^{N,\Delta\delta}(T,\rho) = \frac{1}{(2n)! (\Delta\delta)^{2n}} \sum_{k=0}^{N} \omega_{2n}^{N,k} \bar{F}(T,\rho,k\Delta\delta).$$

Fornberg: Math.Comp 51 (1988)



• stepsize $(\Delta \delta)$ and grid length (N) variations as accuracy checks

• systematically increase precision of numerical integration routine

A2: Extraction of Leading Logarithmic Term at Zero Temperature

• finite differences of zero-temperature logarithmic series ($\sim \delta^{2n \ge 4} \ln |\delta|$):

$$\bar{A}_{4}^{N,\Delta\delta} = \bar{A}_{4,\text{reg}} + C_{1}^{4}(N)\bar{A}_{4,\log} + \bar{A}_{4,\log} \ln(\Delta\delta) + C_{2}^{4}(N)\bar{A}_{6,\log}\Delta\delta^{2} + \mathcal{O}(\Delta\delta^{4}), \qquad (0.1)$$

$$\bar{A}_{6}^{N,\Delta\delta} = \bar{A}_{6,\text{reg}} + C_{1}^{6}(N)\bar{A}_{4,\log}\Delta\delta^{-2} + \bar{A}_{6,\log} \ln(\Delta\delta) + C_{2}^{6}(N)\bar{A}_{6,\log} + \mathcal{O}(\Delta\delta^{2}).$$
(0.2)

• extract leading logarithmic term via:

$$\Xi_{4}(N_{1}, N_{2}) := \frac{\bar{A}_{4}^{N_{1}, \Delta\delta} - \bar{A}_{4}^{N_{2}, \Delta\delta}}{C_{4}^{1}(N_{1}) - C_{4}^{1}(N_{2})} \simeq \bar{A}_{4, \log}, \qquad (0.3)$$

$$\Xi_{6}(N_{1}, N_{2}) := \frac{\bar{A}_{6}^{N_{1}, \Delta \delta} - \bar{A}_{6}^{N_{2}, \Delta \delta}}{C_{6}^{1}(N_{1}) - C_{6}^{1}(N_{2})} \Delta \delta^{2} \simeq \bar{A}_{4, \log}, \qquad (0.4)$$

• benchmark against analytical results for S-wave contact interaction



A3: BCS distribution functions

What about pairing? ightarrow perturbation series about BCS ground state (\sim Bogoliubov)

BCS distribution functions:

$$n_k^{\text{BCS}} = \frac{1}{2} \Big[1 + \xi_k \big(\Delta_k^2 + \xi_k^2 \big)^{-1/2} \Big], \qquad \bar{n}_k^{\text{BCS}} = \frac{1}{2} \Big[1 - \xi_k \big(\Delta_k^2 + \xi_k^2 \big)^{-1/2} \Big]$$

ightarrow compare with finite-temperature Fermi-Dirac distributions



ightarrow expansion divergent also for BCS perturbation series, similar to low- ${\cal T}$ results

Overall:

- logarithmic terms for $T \to 0 \land \{N, \Omega\} \to \infty \land \Delta_k \to 0$
- divergent asymptotic expansion in the region "close enough" to these limits

A4: Ladder resummation

Logarithmic terms also in self-consistent schemes, e.g., BHF, SCGF ?

 \rightarrow examine δ dependence of EoS from all-order-sum of ladder diagrams with S-wave contact interaction $V_{\text{contact}} = \pi M^{-1}(a_s + 3a_t + (a_t - a_s)\vec{\sigma_1} \cdot \vec{\sigma_2})$

$$\bar{E}_{0,\text{resum}}(k_F^n,k_F^p) = -\frac{24}{\pi M[(k_F^n)^3 + (k_F^p)^3]} \left(\Gamma_{\text{resum}}^{nn}(a_s) + \Gamma_{\text{resum}}^{pp}(a_s) + \Gamma_{\text{resum}}^{np}(a_s) + 3\Gamma_{\text{resum}}^{np}(a_t) \right)$$

where

$$\Gamma_{\text{resum}}^{nn/pp}(a_s) = \int_{0}^{1} ds \, s^2 \, \int_{0}^{\sqrt{1-s^2}} d\kappa \, \kappa \, (k_F^{n/p})^5 \arctan \frac{l(s,\kappa)}{(a_s k_F^{n/p})^{-1} + \pi^{-1} R(s,\kappa)}$$

$$\Gamma_{\text{resum}}^{np}(a_{s/t}) = \int_{0}^{(k_F^n + k_F^p)/2} dP \, P^2 \, \int_{q_{\min}}^{q_{\max}} dq \, q \arctan \frac{\Phi(P,q,k_F^n,k_F^p)}{(a_{s/t})^{-1} + (2\pi)^{-1} \left[k_F^n R(\frac{P}{k_F^n},\frac{q}{k_F^n}) + k_F^p R(\frac{P}{k_F^p},\frac{q}{k_F^p})\right]}$$

The functions $I(s,\kappa)$, $R(s,\kappa)$ and $\Phi(P,q,k_F^n,k_F^p)$ are given by

$$\begin{split} I(s,\kappa) = &\kappa \,\Theta(1-s-\kappa) + \frac{1-s^2-\kappa^2}{2s} \,\Theta(s+\kappa-1), \\ R(s,\kappa) = &2 + \frac{1-(s-\kappa)^2}{2s} \ln \frac{1+s+\kappa}{|1-s-\kappa|} + \frac{1-s^2-\kappa^2}{2s} \ln \frac{1+s-\kappa}{1-s+\kappa} \\ \Phi(P,q,k_F^n,k_F^n) = \begin{cases} q \quad \text{for} \quad P+q < k_F^n \\ \frac{(k_F^n)^2-(P-q)^2}{4P} \quad \text{for} \quad k_F^n < P+q < k_F^n \ \wedge |P-q| < k_F^n \\ \frac{(k_F^n)^2+(k_F^n)^2-2(P^2-q^2)}{4P} \quad \text{for} \quad k_F^n < P+q \ \wedge P^2 + q^2 < \frac{(k_F^n)^2+(k_F^n)^2}{2} \end{cases} \end{split}$$

Ladder resummation: isospin-asymmetry dependence



Finite-difference results:

- quadratic coefficient \bar{A}_2 regular
- quartic coefficient \bar{A}_4 : logarithmic for np-channel, but regular in nn+pp

Interaction contribution to ground-state energy per particle (np-channel):

- ullet breakdown of "parabolic law", $ar{F}_{sym} ar{A}_2 \simeq 15.6 8.3$ large
- $\bullet\,$ quartic+log approximation very accurate for $\delta \lesssim$ 0.5, but large deviation in very neutron-rich region
- exact results: maximum at $\delta \gtrsim$ 0.99 (vanishes for larger a), and even a kink?

ightarrow nonanalytic terms should arise also in self-consistent schemes, e.g., BHF, SCGF

Appendix 2: MBPT

Standard Finite-Temperature Perturbation Theory

grand-canonical partition function: $Y = \sum_{p} \langle \Psi_{p} \mid e^{-\beta(\mathcal{H} - \mu \mathcal{N})} \mid \Psi_{p} \rangle = \sum_{p} \langle \Psi_{p} \mid e^{-\beta(\mathcal{T} - \mu \mathcal{N})} \mathscr{U}(\beta) \mid \Psi_{p} \rangle$ Oyson operator: $\mathscr{U}(\beta) = e^{-\beta \mathcal{T}} e^{\beta \mathcal{H}} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_{0}^{\beta} d\beta_n \cdots d\beta_1 \mathcal{P}[\mathcal{V}_{\mathsf{l}}(\beta_n) \cdots \mathcal{V}_{\mathsf{l}}(\beta_1)]$ • change basis $(\Psi_p \to \Phi_p)$, then $\Delta A = A - A$ given by: $\Delta A = -\frac{1}{\beta} \ln \left[\sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \int_{0}^{\beta} d\beta_n \cdots d\beta_1 \left\langle \mathcal{P} \left[\mathcal{V}_{\mathsf{l}}(\beta_n) \cdots \mathcal{V}_{\mathsf{l}}(\beta_1) \right] \right\rangle \right]$ • contraction rules (where $f_i^- = 1/[1 + \exp(\beta(\varepsilon_i - \mu))], f_i^+ = 1 - f_i^-)$: $a_i^{\dagger}a_k = \delta_{ik}f_i^{-}$ (hole) $a_k a_i^{\dagger} = \delta_{jk}f_i^{+}$ (particle) Inked-cluster theorem: $\Delta A = \frac{1}{\beta} \sum_{n=0}^{\infty} (-1)^n \int_{\beta > \beta_n > \ldots > \beta_0 > 0} d\beta_n \cdots d\beta_0 \ \langle \mathcal{V}_1(\beta_n) \cdots \mathcal{V}_1(\beta_0) \rangle_{\text{linked}}$

Note: all this works also for canonical ensemble, but the constraint $\langle \Phi_p | \mathcal{N} | \Phi_p \rangle = N$ implies that single-particle states cannot be summed over independently \Rightarrow useless!

Third-Order Non-Skeletons



- \bullet non-skeletons are insertions: cut articulation lines \rightsquigarrow collection of unlinked clusters
- "self-energy" and anomalous one-loop diagrams related by cyclic vertex permutations ~-> spurious terms in perturbation series

Cumulant Formalism

•
$$\mathcal{G}_{i_{1}\cdots i_{n}}^{k_{1}\cdots k_{m}} = \langle a_{i_{1}}^{\dagger} a_{i_{1}}\cdots a_{i_{n}}^{\dagger} a_{i_{n}} a_{k_{1}} a_{k_{1}}^{\dagger}\cdots a_{k_{m}} a_{k_{m}}^{\dagger} \rangle$$
 has generating function \mathcal{Y} :
 $\mathcal{G}_{i_{1}\cdots i_{n}}^{k_{1}\cdots k_{m}} = \frac{1}{\mathcal{Y}} \frac{\partial}{\partial(-\beta\varepsilon_{i_{1}})}\cdots \frac{\partial}{\partial(-\beta\varepsilon_{i_{n}})} \left(1 - \frac{\partial}{\partial(-\beta\varepsilon_{k_{1}})}\right)\cdots \left(1 - \frac{\partial}{\partial(-\beta\varepsilon_{k_{m}})}\right) \mathcal{Y}$

• evaluate in terms of cumulants $\mathcal{K}_{i_1...i_n} = \frac{\partial^n \ln \mathcal{Y}}{\partial(-\beta \varepsilon_{i_1}) \cdots \partial(-\beta \varepsilon_{i_n})}$:

$$\mathcal{G}_{i_{1}\cdots i_{n}}^{k_{1}\cdots k_{m}} = \sum_{P\subset\{1,\dots,m\}} (-1)^{|P|} \mathcal{G}_{i_{1}\cdots i_{n}\prod_{\nu\in P}k_{\nu}}, \qquad \mathcal{G}_{i_{1}\cdots i_{n}} = \sum_{\substack{P\in \text{ partitions } I\in P\\ \text{ of } \{1,\dots,n\}}} \prod_{I\in P} \mathcal{K}_{\prod_{\nu\in I}i_{\nu}}$$

- skeletons unchanged: $\mathcal{K}_{i_1\cdots i_n} = \mathcal{G}_{i_1\cdots i_n}$ for $i_1 \neq i_2 \neq \ldots \neq i_n$
- self-energy diagrams:

$$\mathcal{G}_{i_1\cdots i_naa}^{k_1\cdots k_m} \sim \mathcal{K}_a\mathcal{K}_a + \mathcal{K}_{aa} = f_a^- f_a^- + f_a^- f_a^+ = f_a^-$$

$$\mathcal{G}_{i_1\cdots i_naaa}^{k_1\cdots k_m} \sim \mathcal{K}_a\mathcal{K}_a\mathcal{K}_a + 3\mathcal{K}_{aa}\mathcal{K}_a + \mathcal{K}_{aaa} = f_a^- f_a^- f_a^- + 3f_a^- f_a^+ + f_a^- f_a^+ (f_a^+ - f_a^-) = f_a^-$$

$$\vdots$$

• no contributions from anomalous diagrams:

$$\mathcal{G}^{\mathfrak{a}\cdots\mathfrak{a}}_{i_{1}\cdots i_{n}\mathfrak{a}\cdots\mathfrak{a}} = \sum_{\mathbf{P}\subset\{1,\dots,l\}} (-1)^{|\mathbf{P}|} \mathcal{G}_{i_{1}}\cdots i_{n}\mathfrak{a}\cdots\mathfrak{a}\prod_{\nu\in\mathbf{P}}\mathfrak{a}_{\nu} = \sum_{\mathbf{P}\subset\{1,\dots,l\}} (-1)^{|\mathbf{P}|} \mathcal{G}_{i_{1}}\cdots i_{n}\mathfrak{a} = 0$$

Anomalous Contributions via Simply-Connected Diagrams

expansion of logarithm yields

$$\Delta \mathbf{A} = \sum_{n=0}^{\infty} \sum_{k} \sum_{\{\mathbf{a}_i\}, \{\mathbf{b}_i\}} \beta^{\mathbf{b}_1 + \ldots + \mathbf{b}_k - 1} {\binom{\mathbf{b}_1 + \ldots + \mathbf{b}_k}{\mathbf{b}_1, \ldots, \mathbf{b}_k}} \frac{(\mathbf{A}_{\mathbf{a}_1})^{\mathbf{b}_1} \cdots (\mathbf{A}_{\mathbf{a}_k})^{\mathbf{b}_k}}{\mathbf{b}_1 + \ldots + \mathbf{b}_k} \Big|_{\mathbf{a}_1 \mathbf{b}_1 + \ldots + \mathbf{a}_k \mathbf{b}_k = n}$$

• each term A_{a_i} has linked and unlinked contributions $A_{n,unlinked} = \left[\frac{1}{\beta} \frac{1}{\alpha_1! \cdots \alpha_\nu!} (\Gamma_{n_1})^{\alpha_1} \cdots (\Gamma_{n_\nu})^{\alpha_\nu}\right]_{n_{\alpha}^{\alpha_1} + \dots + n_{\nu}^{\alpha_\nu} = n}$

by factorization theorem the only terms that survive are simply-connected in terms of higher cumulants, e.g.,
 (Γ_{2,normal})ⁱⁱ_{kl}(Γ₁)_{ab}: [𝔅ⁱⁱ_{kl}→^l_{kl}]_{kl} = 2² × δ_{ia}𝔅_{ii}𝔅_j𝔅_bκ̄_lκ̄_k − 2² × δ_{ka}𝔅_{kk}𝔅_i𝔅_bκ̄_l



resummation of insertions \rightsquigarrow renormalization of distribution functions $f_a^{\pm}[S] = \sum_{m=0}^{\infty} \frac{1}{m!} (S(a))^m \frac{\partial^m}{\partial \varepsilon_a^m} f_a^{\pm} = \frac{1}{1 + \exp\left(\pm\beta\left(\varepsilon_a + S(a) - \mu\right)\right)}$

Canonical-Ensemble Perturbation Theory

Correlation-Bond Formalism

• start with standard perturbation series for $\Delta F = F - F$:

$$\Delta F = \sum_{n=0}^{\infty} \sum_{k} \sum_{\{a_i\}, \{b_i\}} \beta^{b_1 + \ldots + b_k - 1} {\binom{b_1 + \ldots + b_k}{b_1, \ldots, b_k}} \frac{\left(F_{a_1}\right)^{b_1} \cdots \left(F_{a_k}\right)^{b_k}}{b_1 + \ldots + b_k} \bigg|_{a_1 b_1 + \ldots + a_k b_k = n}$$

• the cumulants are now given by $\mathcal{K}_{i_1...i_n} = \frac{\partial^n \ln \mathcal{Z}}{\partial [-\beta \varepsilon_{i_1}] \cdots \partial [-\beta \varepsilon_{i_n}]}$; evaluate using $\ln \mathcal{Z}(\mathcal{T}, \tilde{\mu}, \Omega) = \ln \mathcal{Y}(\mathcal{T}, \tilde{\mu}, \Omega) - \tilde{\mu} \frac{\partial \ln \mathcal{Y}(\mathcal{T}, \tilde{\mu}, \Omega)}{\partial \tilde{\mu}}$

where $\tilde{\mu}$ is given by $N(\mathcal{T}, \tilde{\mu}, \Omega) = \sum_i \tilde{t}_i^-$; since N is regarded fixed, $\tilde{\mu}$ is a functional of the spectrum $\{\varepsilon_\alpha\}$, i.e., as implicit equation:

$$\mathcal{J}(\tilde{\mu}, \{\varepsilon_{\alpha}\}) = \sum_{\alpha} \tilde{f}_{\alpha}^{-} - N = 0$$

R. Brout & F. Englert, PR 120 (1960)

This method effectively "shifts" the constraint $\langle \Phi_p | \mathcal{N} | \Phi_p \rangle = N$ to the level of diagrams, resulting in new simply-connected contributions ("correlation bonds"), e.g., $\mathcal{K}_{ia} \sim \mathcal{K}_{ia} + \delta_{ia} \mathcal{K}_{ii}$, with

$$\mathcal{K}_{i_1i_2} = \left(\frac{\partial \mathcal{K}_{i_1}}{\partial [-\beta \varepsilon_{i_2}]}\right)_{\mathcal{J}} = \frac{\partial \mathcal{K}_{i_1}}{\partial [\beta \tilde{\mu}]} \left(\frac{\partial [\beta \tilde{\mu}]}{\partial [-\beta \varepsilon_{i_2}]}\right)_{\mathcal{J}} = -\frac{\tilde{t}_{i_1}^- \tilde{t}_{i_1}^+ \tilde{t}_{i_2}^- \tilde{t}_{i_2}^+}{\sum_{\alpha} \tilde{t}_{\alpha}^- \tilde{t}_{\alpha}^+}$$

Resummation of correlation bonds renormalizes auxiliary chemical potential $ilde{\mu}$