Entropy in strongly interacting Fermi gases

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Outline

Ultracold atoms - a testbed for manybody quantum physics

ULTRALOW temperatures down to 50pK

TESTS MANY-BODY THEORY IN NEW REGIMES!

- Superchemistry: Stimulated molecule formation
- Entangled BEC: Spin-squeezing with spinor atoms
- Universality: Strongly interacting fermions
- Lattice gases: Hubbard model and superconductivity
- Spin liquids: Cooling to picoKelvins
- Quantum dynamics: Far from equilibrium

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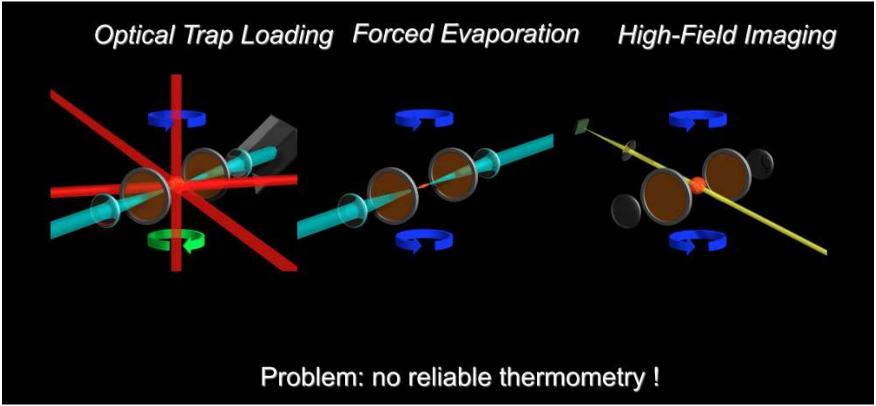
Ultracold Fermi experiments



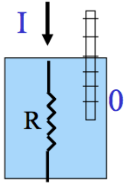
Classical Thermometry

1) known energy input:

$$\Delta E = I^2 R \Delta t$$

2) measure entropy

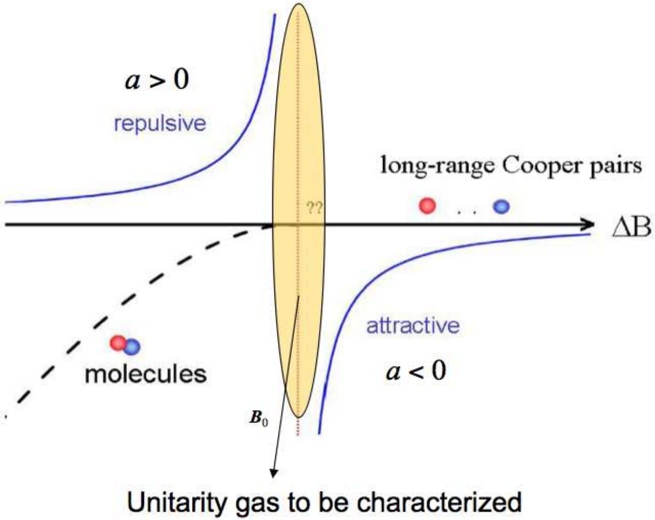
heat capacity



1) Precise energy input
2) Entropy measurement

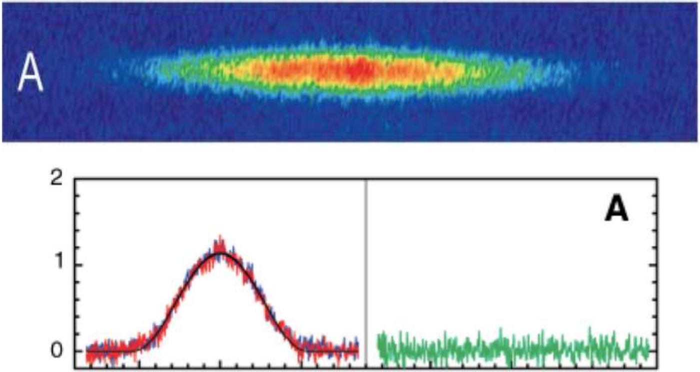
→ Thermodynamics

Experimental Investigations of Thermodynamics



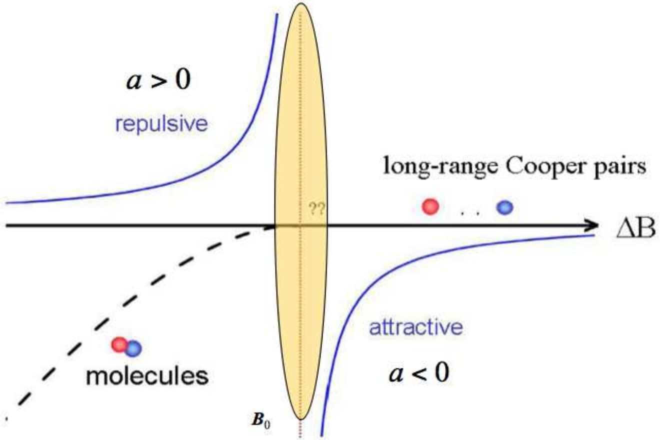
Experimental Energy

Energy from interacting gas



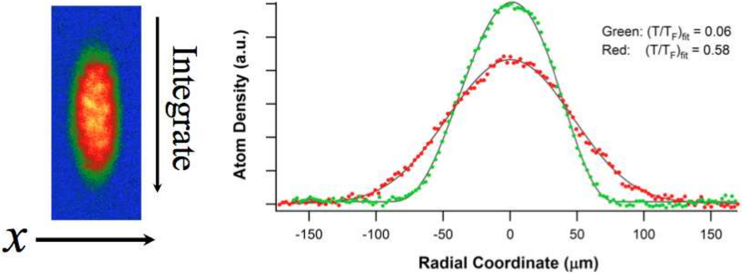
Potential energy is obtained from axial cloud size

Isentropic Thermometry *[Thomas, PRL 98, 080402 (07)]*



Isentropic sweep to the weak coupling BCS limit

Noninteracting Entropy



From Thomas- Fermi Fit:

"true" temperature (entropy) for non-interacting gas

More precise tests

Local pressure $P(\mu(z), T)$ inferred from density profiles

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- Temperature determined using ^{7}Li impurity.
- Chemical potential determined using the local density approximation
- Experimentalists measured a universal function

$$h[\zeta] = P(\mu, T)/P^{(1)}(\mu, T)$$

- $\zeta \equiv \exp(-\mu/k_B T)$
- $P^{(1)}(\mu, T) =$ pressure of ideal two-component Fermi gas

S. Nascimbène, et. al, New J. Phys. 12, 103026 (2010).
M. Horikoshi, et. al., Science 327, 442 (2010).

What are the theories?

The hamiltonian of the system can then be written as,

$$\mathscr{H} = \sum_{\mathbf{k}\sigma} (\varepsilon_{\mathbf{k}} - \mu)\, c^{+}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + U \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} c^{+}_{\mathbf{k}+\mathbf{q}\uparrow} c^{+}_{\mathbf{k}'-\mathbf{q}\downarrow} c_{\mathbf{k}'\downarrow} c_{\mathbf{k}\uparrow}, \tag{1}$$

where $\varepsilon_{\mathbf{k}} = \hbar^2 \mathbf{k}^2/(2m)$ is the fermionic kinetic energy at wave number k, and

$$\frac{1}{U} = \frac{m}{4\pi\hbar^2 a_s} - \sum_{\mathbf{k}} \frac{1}{2\varepsilon_{\mathbf{k}}} \tag{2}$$

is the *bare* contact interaction renormalized in terms of the s-wave scattering length a_s.

Calculating Perturbation Theory

T-matrix can be schematically represented

$$t(Q) = U + UGGU + UGGUGGU + \cdots,$$

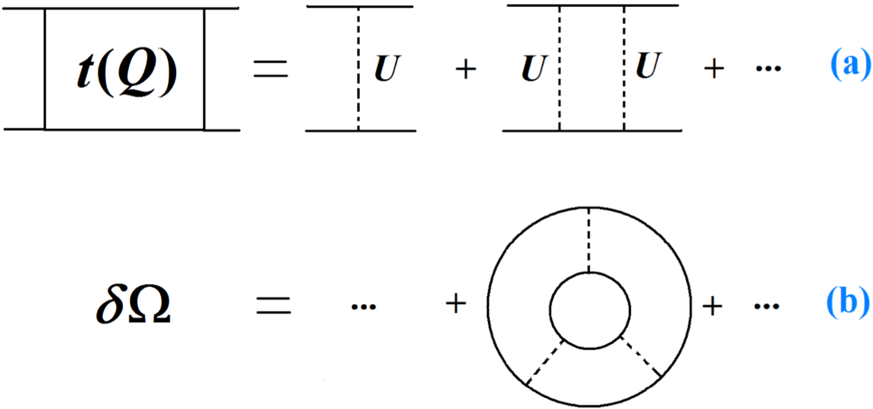
In the *normal* state, the ladder sum is calculated as,

$$t(Q) = \frac{U}{[1 + U\chi(Q)]},$$

Where $Q = (\mathbf{q}, i\nu_n)$, $K = (\mathbf{k}, i\omega_m)$, and $\mathbf{q}$ and $\mathbf{k}$ are wave vectors, while $\nu_n = 2n\pi k_B T$ and $\omega_m = (2n+1)\pi k_B T$ $(n = 0, \pm 1, \pm 2, \cdots)$ are bosonic and fermionic Matsubara frequencies.

Perturbation Theory Diagrams

Solid line = single-particle Green function G , dashed line = interaction U.



GPF ($G_0 G_0$) vs Haussman (GG)

Different T-matrix theories use different Green's functions

$$\chi(Q) = \sum_K G_\alpha(K)\, G_\beta(Q-K),$$

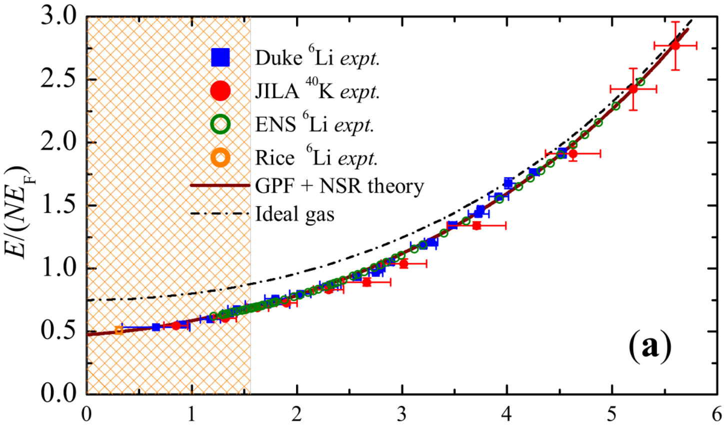
and the self-energy,

$$\Sigma(K) = \sum_Q t(Q)\, G_\gamma(Q-K),$$

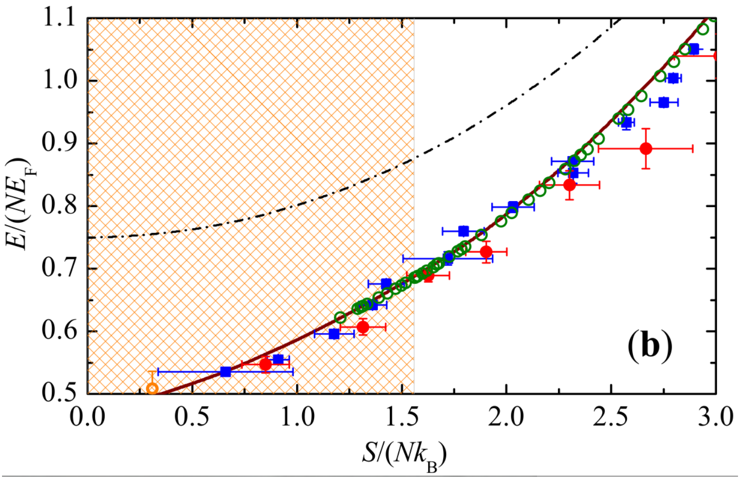
The subscripts α, β, and γ may be "0", indicating a non-interacting Green's function, or be absent, indicating an interacting Green's function, using the Dyson equation,

$$G(K) = G_0(K) / [1 - G_0(K)\Sigma(K)],$$

Evidence for universality: E vs S



Evidence for universality: close-up



Reduced temperature from $h(\zeta)$

Obtaining the reduced temperature

- Need derivative of measured h function:

$$\left(\frac{T_F}{T}\right)^{3/2} = \frac{3\sqrt{\pi}}{4}\left[\tilde{n}^{(1)}(\zeta)\,h(\zeta) - \tilde{P}^{(1)}(\zeta)\,\zeta\frac{dh}{d\zeta}\right],$$

- Dimensionless non-interacting density and pressure,

$$\tilde{n}^{(1)} \equiv \frac{n^{(1)}\lambda^3}{2} = \frac{2}{\sqrt{\pi}}\int_0^\infty \frac{dt\sqrt{t}}{(\zeta e^t + 1)},$$

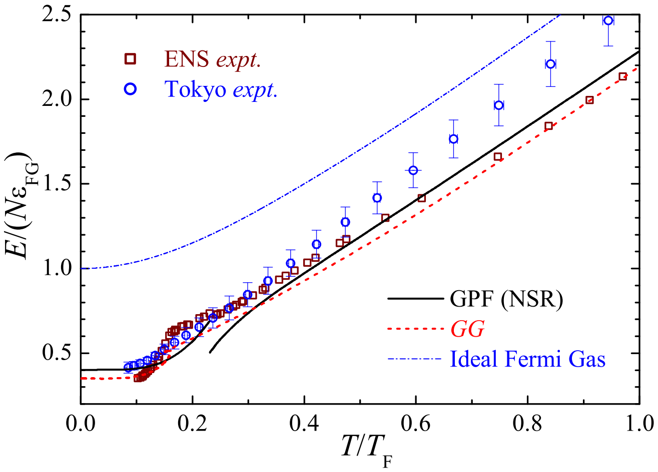
$$\tilde{P}^{(1)} \equiv \frac{P^{(1)}k_B T\lambda^3}{2} = \frac{2}{\sqrt{\pi}}\int_0^\infty dt\sqrt{t}\ln\left(1+\zeta^{-1}e^{-t}\right).$$

Universal Thermodynamic Functions from $h(\zeta)$

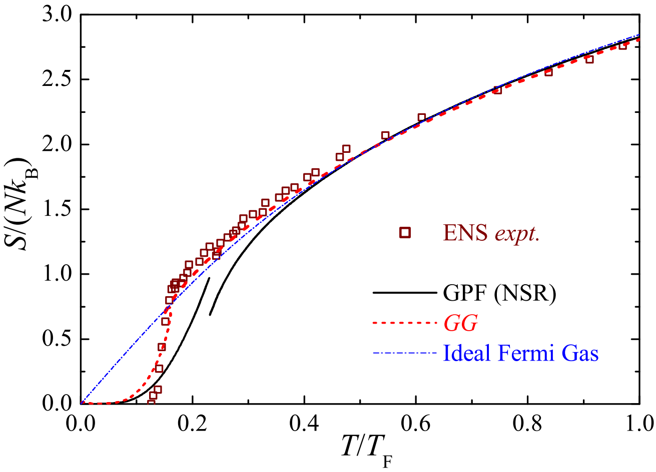
Calculating universal equations of state

$$
\begin{aligned}
\frac{\mu}{\varepsilon_F} &= -\frac{T}{T_F}\ln\zeta, \\
\frac{E}{N\varepsilon_F} &= \frac{9}{4}h(\zeta)\left(\frac{T}{T_F}\right)^{5/2}\int_0^\infty dt\sqrt{t}\ln\left(1+\zeta^{-1}e^{-t}\right), \\
\frac{S}{Nk_B} &= \left(\frac{T_F}{T}\right)\left(\frac{5}{3}\frac{E}{N\varepsilon_F}-\frac{\mu}{\varepsilon_F}\right).
\end{aligned}
$$

Uniform Energy vs Experiment: GG vs $G_0 G_0$ (GPF)



Uniform Entropy vs Experiment: GG vs G_0G_0 (GPF)



High Temperature Virial Expansions

Virial expansions use exact two and three-body solutions

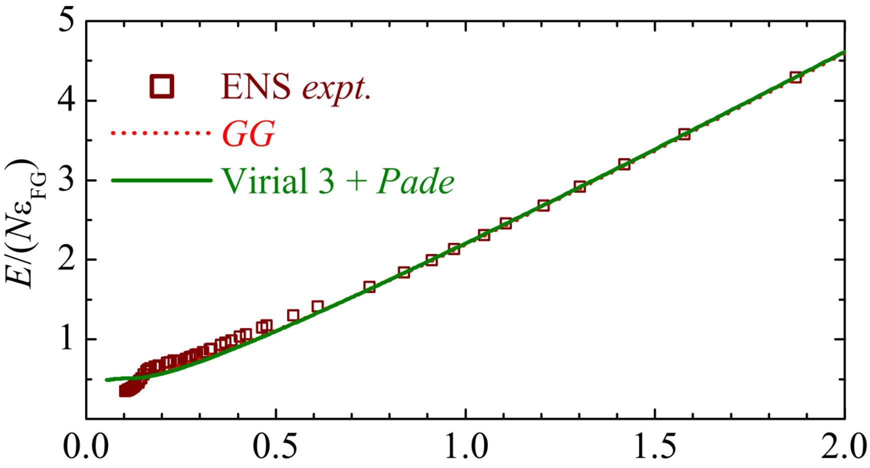
$$\Omega - \Omega^{(1)} = -\frac{2kT}{\lambda^3}\left[\Delta b_2 z^2 + \ldots + \Delta b_n z^n +\right],$$

where,$z = \exp(\mu/kT) = 1/\zeta$, $\Omega^{(1)}$ is the free particle thermodynamic potential

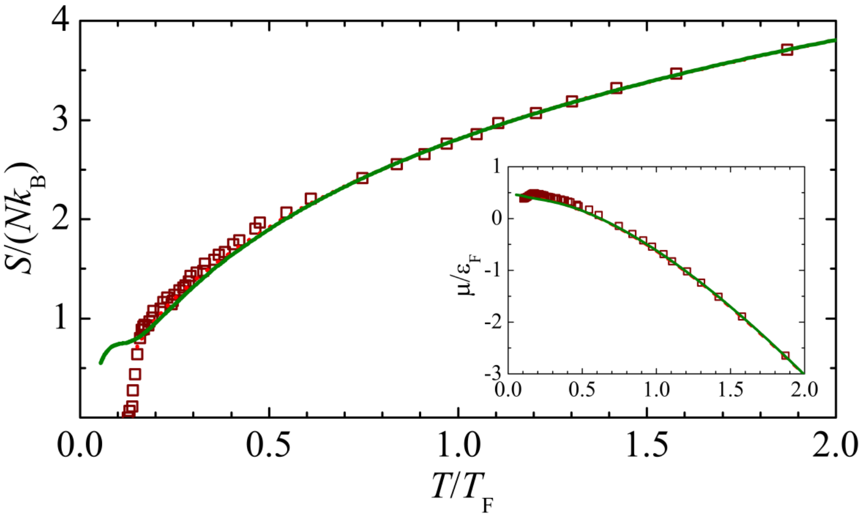
$$h_{pade} = \frac{1 + \left[b_2^{(1)} + \Delta b_2 - \Delta b_3/\Delta b_2\right]\zeta^{-1}}{1 + \left[b_2^{(1)} - \Delta b_3/\Delta b_2\right]\zeta^{-1}}$$

and:$\Delta b_2 = 1/\sqrt{2}$, $\Delta b_3 = -0.355..$
[Liu et al, PRL 102, 160401 (2009)]

Energy vs Experiment: Virial



Entropy vs Experiment: Virial



Calculating entropy from simulations

Entropy: a fundamental measure of information

- Measurable with ultra-cold atoms (John Thomas)
- Hard to check predictions of diagrammatic calculations
- Can we investigate entropic entanglement?
- Paradox - can entropy change with time?

How can we simulate this directly?

Types of entropy

Shannon or von Neumann entropy

- $S = -Tr\left(\widehat{\rho}\ln\widehat{\rho}\right)$

Renyi entropy

- The Renyi entropy is: $S_2 = -\ln Tr\left(\widehat{\rho}^2\right)$

Phase-space expansions

Phase-space representations

$$\widehat{\rho} = \int P(\boldsymbol{\lambda})\widehat{\Lambda}(\boldsymbol{\lambda})d\boldsymbol{\lambda} \ ,$$

where:

- $P(\boldsymbol{\lambda})$ is a probability density
- $\boldsymbol{\lambda}$ is a vector parameter in a general phase-space,
- $\widehat{\Lambda}(\boldsymbol{\lambda})$ is an operator basis.

Sampled Renyi entropy

Sampled distribution

- $\widehat{\rho} \approx \widehat{\rho}_S = \frac{1}{N} \sum_{j=1}^{N} \widehat{\Lambda}(\boldsymbol{\lambda}_j)$.

Sampled RENYI entropy

- $S_2 \approx -\ln \left[\sum_{i,j=1}^{N} Tr \left(\widehat{\Lambda}(\boldsymbol{\lambda}_i) \widehat{\Lambda}(\boldsymbol{\lambda}'_j) \right) / N^2 \right]$.

Bose and Fermi Representations

What are the common phase-space representations?

Property: **Repn.**	Ordering	***Particle Statistics***	**Phase-space Dimension**
P	Normal	Bose	Classical
W	Symmetric	Bose	Classical
Q	Antinormal	Bose	Classical
+P	Normal	Bose	Classical×2
G	**Normal**	**Any**	**(Classical)^2**

Gaussian phase-space distributions

Gaussian phase-space

- Gaussian basis, $\widehat{\Lambda}(\boldsymbol{\lambda}) =: \exp\left[-\delta\hat{a}^{\dagger}\underline{\boldsymbol{\mu}}\delta\hat{a}\right] : /\mathscr{N}$
- $\underline{\boldsymbol{\mu}}$ is a complex $M \times M$ matrix so that $\boldsymbol{\lambda} = \left[\boldsymbol{\alpha}, \boldsymbol{\beta}^{\dagger}, \underline{\boldsymbol{\mu}}\right]$,
- **Positive distribution always exists**
  Corney & PDD, PRB 73,125112 (06)
- **Best current method for 2D Hubbard**
  Aimi & Imada, J.Phys. Soc. Jpn 76, (07)

What are the Gaussian parameters physically?

How do we map observables to Gaussian parameters?

- Bosons $\underline{\boldsymbol{\mu}} = \left(\underline{I} + \underline{n}^{T}\right)^{-1}$
- $\left\langle \widehat{a}_i^{\dagger} \widehat{a}_j \right\rangle = \left\langle \beta_i^{*} \alpha_j + n_{ij} \right\rangle_P$
- Fermions $\underline{\boldsymbol{\mu}} = \left(\underline{I} - \underline{n}^{T}\right)^{-1} - 2\underline{\mathrm{I}}$
- $\left\langle \widehat{a}_i^{\dagger} \widehat{a}_j \right\rangle = \left\langle n_{ij} \right\rangle_P$

Example: Glauber-Sudarshan Phase-space

Definition using coherent states

$$\widehat{\rho} = \int P(\alpha) \left|\alpha\right\rangle \left\langle\alpha\right| d^2\alpha$$

Generates normal-ordered operator products

- Maps quantum states into 2M real coordinates: $\alpha = p + ix$,
- Advantage: No UV vacuum divergence
- Problem: Singular for entangled states

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Glauber-Sudarshan Phase-space

Inner product of two basis elements

$$Tr\left(\widehat{\Lambda}_1(\boldsymbol{\alpha})\widehat{\Lambda}_1(\boldsymbol{\alpha}')\right) = \exp\left[-\left|\boldsymbol{\alpha}-\boldsymbol{\alpha}'\right|^2\right]$$

Example

- Thermal case: $P(\alpha) = exp\left[-|\alpha|^2/n_{th}\right]$
- Free Bose gas entropy: $S_2 = \ln(1+2n_{th})$

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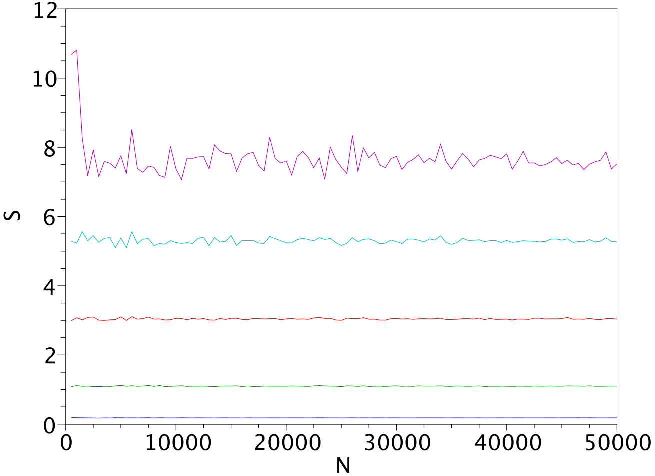
Sampled Renyi Entropy ($n_{th} = 0.1, 1, \ldots 1000$)



Trace of fermionic Gaussian operator products

Define an un-normalized fermionic Gaussian operators,

$$\hat{\Lambda}_u\left(\underline{\boldsymbol{\mu}}\right) =: e^{-\hat{a}^\dagger \underline{\boldsymbol{\mu}} \hat{a}} :$$

Trace of two un-normalized fermionic Gaussian operators

- $F\left(\underline{\boldsymbol{\mu}}, \underline{\boldsymbol{\nu}}\right) = Tr\left[\hat{\Lambda}_u\left(\underline{\boldsymbol{\mu}}\right)\hat{\Lambda}_u\left(\underline{\boldsymbol{\nu}}\right)\right] = Tr\left[: e^{-\hat{a}^\dagger \underline{\boldsymbol{\mu}} \hat{a}} :: e^{-\hat{a}^\dagger \underline{\boldsymbol{\nu}} \hat{a}} :\right]$
- How do we evaluate this for arbitrary matrices $\underline{\boldsymbol{\mu}}$ and $\underline{\boldsymbol{\nu}}$?

Grassmann Identities

Expand in Grassmann coherent states

- $|\boldsymbol{\alpha}\rangle$ is a Grassmann coherent state iff $\hat{a}|\boldsymbol{\alpha}\rangle = \boldsymbol{\alpha}|\boldsymbol{\alpha}\rangle$
- $\boldsymbol{\alpha}$ are a set of anticommuting Grassmann variables
- $Tr[\hat{O}] = \int d^{2M}\boldsymbol{\alpha}\langle -\boldsymbol{\alpha}|\hat{O}|\boldsymbol{\alpha}\rangle,$
- Identity operator: $\int d^{2M}\boldsymbol{\alpha}|\boldsymbol{\alpha}\rangle\langle\boldsymbol{\alpha}| = 1.$
- See: *Cahill and Glauber, PRA59, 1538 (1999).*

Grassmann Eigenvalues

Therefore:

$$F\left(\underline{\boldsymbol{\mu}},\underline{\boldsymbol{\nu}}\right) = \frac{1}{\pi^{2M}}\int d\boldsymbol{\alpha} d\boldsymbol{\beta} \left\langle -\boldsymbol{\alpha}\right| : e^{-\hat{a}^{\dagger}\underline{\boldsymbol{\mu}}\hat{a}} : \left|\boldsymbol{\beta}\right\rangle \times \times \left\langle \boldsymbol{\beta}\right| : e^{-\hat{a}^{\dagger}\underline{\boldsymbol{\nu}}\hat{a}} : \left|\boldsymbol{\alpha}\right\rangle .$$

Using $\hat{a}\left|\boldsymbol{\alpha}\right\rangle = \boldsymbol{\alpha}\left|\boldsymbol{\alpha}\right\rangle$

$$F\left(\underline{\boldsymbol{\mu}},\underline{\boldsymbol{\nu}}\right) = \int d\boldsymbol{\gamma} e^{\boldsymbol{\alpha}^{\dagger}\underline{\boldsymbol{\mu}}\boldsymbol{\beta}-\boldsymbol{\beta}^{\dagger}\underline{\boldsymbol{\nu}}\boldsymbol{\alpha}-\boldsymbol{\alpha}^{\dagger}\boldsymbol{\beta}+\boldsymbol{\beta}^{\dagger}\boldsymbol{\alpha}^{\dagger}-\left(\boldsymbol{\alpha}^{\dagger}\boldsymbol{\alpha}+\boldsymbol{\beta}^{\dagger}\boldsymbol{\beta}\right)}$$

Gaussian integral over $2M$ Grassmann coordinates

Introducing double-dimension Grassmann vector :

$$\boldsymbol{\gamma} = \begin{bmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\beta} \end{bmatrix},$$

$$F\left(\underline{\boldsymbol{\mu}}, \underline{\boldsymbol{\nu}}\right) = \int d\boldsymbol{\gamma} e^{-\boldsymbol{\gamma}^{\dagger}\underline{\boldsymbol{\Gamma}}\boldsymbol{\gamma}} = \det\left[\underline{\boldsymbol{\Gamma}}\right]$$

Here we introduced

$$\underline{\boldsymbol{\Gamma}} = \begin{bmatrix} \underline{I} & \underline{I} - \underline{\boldsymbol{\mu}} \\ \underline{\boldsymbol{\nu}} - \underline{I} & \underline{I} \end{bmatrix}$$

Therefore: $F\left(\underline{\boldsymbol{\mu}}, \underline{\boldsymbol{\nu}}\right) = \det\left[\mathrm{I} + \left(\underline{I} - \underline{\boldsymbol{\mu}}\right)\left(\underline{I} - \underline{\boldsymbol{\nu}}\right)\right]$

Stochastic Green's functions

Normalized Gaussian operators in terms of Green's functions

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- Stochastic Green's functions: $n_{ij} = Tr\left[\widehat{\Lambda}(\mathbf{n})\hat{a}_i^\dagger \hat{a}_j\right] = G_{ij}$
- Hole Green's functions: $\underline{\tilde{\mathbf{n}}} = [\underline{\mathrm{I}} - \underline{\mathbf{n}}]$,

Normalized inner product:

,

- $Tr\left[\widehat{\Lambda}(\mathbf{m})\widehat{\Lambda}(\mathbf{n})\right] = \det\left[\underline{\tilde{\mathbf{n}}\tilde{\mathbf{m}}} + \underline{\mathbf{nm}}\right]$

Sampled Fermion Entropy

Direct way to calculate fermionic Renyi entropy

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- $\hat{\rho} = \frac{1}{N}\sum_{i=1}^{N}\widehat{\Lambda}(n_i)$.

Normalized inner product:

,

- $S_2 = -\ln\left[\frac{1}{N^2}\sum_{i,j=1}^{N}\det\left[\underline{\tilde{\mathbf{n}}\tilde{\mathbf{n}}}' + \underline{\mathbf{nn}}'\right]\right]$.

SUMMARY

Entropy is measurable, challenging to compute

- Sensitive measure for different strong-coupling theories
- Current data requires differentiation - can we improve this?

Gaussian phase-space provides a newmethodology

- Maps **quantum field evolution** into c-number equations
- Renyi entropy directly calculable via sampling

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CAOUS People