Entanglement and correlation in many-electron systems

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Many-Electron States: 4 states/site,

$$\langle n_{i\uparrow}n_{j\uparrow}\rangle$$
, $\langle n_{i\uparrow}n_{j\downarrow}\rangle$

 A fixed number of sites, up spins, down spins
 Distinct Labeled Spatial Part

 Image: Comparison of the system of the syste

Strongly-Correlated States: No Double Occupancy, 3 States/site, On-site Spin Correlations

Spin-Only States: No holes either, Two states/site, Qubits $\langle S_i^z \rangle$, $\langle S_i^z S_j^z \rangle$, $\langle S_i^+ S_j^- \rangle$

$$\left|\psi\right\rangle = \sum_{\{s_i\}} \phi(s_1, s_2..s_N) \left|s_1, s_2..s_N\right\rangle$$

$$\Gamma(r) \approx m^2 + \frac{A}{r^p} + Be^{-\frac{r}{\xi}}$$

Diagonal LRO: Constant m nonzero Long-ranged Correlations: A Nonzero Many-eletcron State:

$$|\psi\rangle = \Pi_k (u_k + v_k c_{k\uparrow}^* c_{-k\downarrow}^*) |0\rangle$$



Double Occupancy

Order Parameter

Strongly-Correlated electron state: Gutzwiller Projection, Inhibit double occupancy

Start from a metallic 'Uncorrelated' State

$$|\psi_g\rangle = \Pi_i |1 - (1 - g)n_{i\uparrow}n_{i\downarrow}| |F\rangle$$

$$d(g) \le \frac{n^2}{4}$$

Projection operator for the site Hilbert Space:

g=0 states with Doubly-occupied sites are projected out.

 $\langle \mathbf{n} | \mathbf{n} \rangle$

g=1 No Correlation, Metallic State, U=0:

 $d = n_{\uparrow} n_{\downarrow}$

g=0 Strong Correlation U=infinity :

$$d=0$$

$$d(g) = \frac{1}{N} \sum_{D} D |\alpha_{D}|^{2} g^{2D} = \frac{1}{2N} \frac{\partial \ln \gamma}{\partial \ln g} \qquad \qquad \alpha_{D} \equiv \langle D | P_{D} | g \rangle$$

$$\gamma(g) \equiv \langle g | g \rangle$$

$$1 - D \quad d(g) = \frac{1}{2} \frac{g^{2}}{(1 - g^{2})^{2}} (ng^{2} - n - \ln[1 - n - ng^{2}]) \qquad \qquad n \leq 1$$

Metzner and Vollhardt (1988)



Quantum Entanglement: Subsystem Entropy, Quantum Correlations, Measures

Entanglement between spatial partitions: Correlated, Superconductor, Metal states

Multi-Species Entanglement: Macroscopic entanglement, Quantum Criticality One-Dimensional Transverse-Ising model

Conclusions



Entanglement between Distinct Partitions



Spatial Partitions



Many-dim Hilbert Space For each Partition Many ways to partition!

u denotes the state of Partition A

$$|\psi\rangle = \sum_{u,v} \psi(u,v) \ |u\rangle_A \ |v\rangle_B$$

Two Species

Label Partition by A and B Type of Particles Both types access full space

u denotes the set of locations occupied by A-type particles

Different Ways of Entanglement

Spin States of Distinct Spatial partitions

 $|\uparrow\rangle_1|\downarrow\rangle_2+\beta|\downarrow\rangle_1|\uparrow\rangle_2$ Spatial parts 1 and 2 entangled

Spatial State of Distinct Spin partitions

 $|1\rangle_{\uparrow}|2\rangle_{\downarrow}+\beta|1\rangle_{\uparrow}|3\rangle_{\downarrow}+\gamma|2\rangle_{\uparrow}|3\rangle_{\downarrow}$ Spin partitions entangled

Entangled Spins + Entangled Spatial Parts

 $|\uparrow_1\downarrow_2\rangle + \beta |\uparrow_1\downarrow_3\rangle + \gamma |\downarrow_2\downarrow_3\rangle$

Two Different Sources of Entanglement

$$|\psi\rangle = \sum_{u,v} \psi(u,v) |u\rangle_A |v\rangle_B \xrightarrow{\text{Uncorrelated}} |x\rangle_A |y\rangle_B \xrightarrow{\text{Uncorrelated}} |y\rangle_B$$

Correlations Between A and B: Wave function not factorizable

Constraint over degrees of freedom: Ex. Number of down spins fixed

$$|\psi\rangle = \sum_{x, u, v} \psi_x(u, v) |x, u\rangle_A |x, v\rangle_B$$

Even if the amplitude factorizes in each sector

$$|\psi\rangle = \sum_{x} \lambda(x) |\tilde{x}\rangle_{A} |\tilde{x}\rangle_{B} \implies \text{Entanglement}$$

Schmidt Form

Spin States:
$$|\psi\rangle = \sum_{\{s_i\}} \phi(s_1, s_2..s_N) |s_1, s_2..s_N\rangle$$



How Entangled Is a Spin State?



 $E_{ij} = -Tr \rho_{ij} \ln \rho_{ij}$ Entropy of the block: Ent. Between ij and rest

Т

$$\varepsilon = 1 - 4m^2$$
 $\frac{1}{2}C_{ij} = |\Gamma_{off-diag}| - \sqrt{(\frac{1}{4} + \Gamma_{diag})^2 - m^2}$

Diagonal Ordering/Correlations Decrease Entanglement

Examples:

Bell State: $|00\rangle + e^{i\phi}|11\rangle \quad \varepsilon = 1 \quad C = 1$ GHZ State: $|000\rangle + |111\rangle \quad \varepsilon = 1 \quad C = 0$ W State: $|001\rangle + |010\rangle + |100\rangle \quad \varepsilon = \frac{8}{9} \quad C = \frac{2}{3}$

 Shor's 9-qubit
 $|0\rangle \equiv |000+111\rangle |000+111\rangle |000+111\rangle$

 Error-correcting Code
 $|1\rangle \equiv |000-111\rangle |000-111\rangle |000-111\rangle$

5-Qubit $|0\rangle \equiv |00000 - (10100 + 11000 + 11110 + 11110 + cycl)\rangle$

 $\varepsilon=1$ For all states in code subspace

How Entangled are Many-Electron States?

Max. Ent. Each Eigenvalue=1/4 d=1/4 $n_{\uparrow}=n_{\downarrow}=1/2$ $\mathcal{E}=1$

Strong Correlations U large d=0 No

Now only 3 states per site

Max. Ent. Each Eigenvalue=1/3 $n_{\uparrow} = n_{\downarrow} = 1/3$

Half-filled Case: No holes either Max. Ent. Each Eigenvalue=1/2

$$n_{\uparrow} = n_{\downarrow} = 1/2$$
 $\varepsilon = 2/3$

 $n = n_{\uparrow} + n_{\downarrow}$

 $\varepsilon = 8/9$

Gutzwiller Projection: Start from a metallic 'Uncorrelated' State

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d=0

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1- D

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Metzner and Vollhardt (1988)

Global Entanglement and electron correlation: d=1 Gutzwiller State

 $|\psi_{g}\rangle = \Pi_{i} |1 - (1 - g)n_{i\uparrow}n_{i\downarrow}| |F\rangle$ VS, Phys. Lett. A374, 3151 (2010)

Entanglement in 1-D Gutzwiller State 1



1 Uncorrelated No projection



Metallic Fermi State
$$|\psi\rangle = \Pi_k (u_k + v_k c_{k\uparrow}^* c_{-k\downarrow}^*) |0\rangle$$

BCS-Superconducting State



Double Occupancy

Order Parameter

Entanglement in the BCS Superconducting State

VS (2010)



Multi-Species Entanglement VS, Quant. Inform. Comp. (2011)

Let u (v) denote the set of sites occupied by A (B) particles

$$|\psi\rangle = \sum_{u,v} \psi(u,v) \ |u\rangle_A \ |v\rangle_B$$

Strong exclusion: B occupies only sites unoccupied by A Half filling: Total number of particles equals the number of Now, v stands for the complement of the set u

$$|\psi\rangle = \sum_{u} \psi(u) \ |u\rangle_A \ |u\rangle_B$$

Schmidt numbers: Eigenvalues of reduced density matrix

$$S_A = -\sum_{u} |\psi(u)|^2 \log |\psi(u)|^2 \quad \varepsilon_{A,B} = \lim_{N \to \infty} \frac{S_A}{N}$$

 \mathbf{C}

Example: Multi-Species Entanglement

 $|\uparrow\rangle_{A}|\uparrow\rangle_{B}+|\uparrow\rangle_{A}|\downarrow\rangle_{B}$

Sites A and B unentangled

$$= |A, B\rangle_{\uparrow} |0\rangle_{\downarrow} + |A\rangle_{\uparrow} |B\rangle_{\downarrow}$$

Up and Down Spins Entangled Multi-Species Entanglement!

$$|\psi\rangle$$
 = $|\uparrow\rangle+|\downarrow\rangle$ = $|O\rangle_{\uparrow}$ $|U\rangle_{\downarrow}+|U\rangle_{\uparrow}$ $|O\rangle_{\downarrow}$

Entanglement for a single Qubit

 $|\psi\rangle$ = $\prod |\uparrow\rangle_i + |\downarrow\rangle_i$ No entanglement in any spatial partitionng

Macroscopic Entanglement betwen Up and Down Spins: N log 2

Spin Systems: States with a given number Spins N, N_{\uparrow} . N_{\downarrow}

$$\left|\psi\right\rangle = \sum_{\{s_i\}} \phi(s_1, s_2..s_N) \left|s_1, s_2..s_N\right\rangle$$

Macroscopic System with Thermodynamic densities $n_{\uparrow} = \lim_{N \to \infty} \frac{N_{\uparrow}}{N}$ $n_{\downarrow} = \lim_{N \to \infty} \frac{N_{\downarrow}}{N}$

$$|\phi[s_i]|^2$$
 Eigenvalue of ρ_{\uparrow}

Macroscopic Entangment Betwen up and down spins

$$\varepsilon_{\uparrow,\downarrow} = \lim_{N \to \infty} \frac{S_{\uparrow}}{N}$$

We will see Multi-Species Entanglement has a Thermodynamic Limit Can display a singularity that are Associated with Quantum Phase Transitions.

In Contrast, entropy of Spatial Partition does not scale with System Size! Block entropy per site does not tend to a limit Transverse Ising Model: Quantum Phase Transition in the ground state

$$\mathcal{H} = -J\sum_{i} \sigma_{i}^{x} \sigma_{i+1}^{x} - h\sum_{i} \sigma_{i}^{z} \quad \ \ \text{-Pauli operators}$$

$$\begin{split} h = 0 \qquad |GS\rangle &= \Pi |\uparrow + \downarrow\rangle \qquad J > 0 \\ &= \Pi |\uparrow + \downarrow\rangle |\uparrow - \downarrow\rangle \quad J < 0 \end{split} \\ \end{split} \label{eq:gs} \mbox{Ordered Phase}$$

 $h \neq 0$ Fluctuations similar to thermal (incoherent) excitations

h=J Quantum critical point, Order parameter vanishes

Nearest-Neighbor
Concurrence
$$\frac{dC(1)}{d\lambda} = \frac{8}{3\pi^2} \ln|\lambda - \lambda_c| + \text{const} \qquad \lambda = |J/h|$$

Osterloh et al, Nature, 416, 608 (2002)

Transverse Ising.... $\mathcal{H} = -J\sum_{i}\sigma_{i}^{x}\sigma_{i+1}^{x} - h\sum_{i}\sigma_{i}^{z}$

Spin Operators acting at different sites behave like bose operators

Spin Operators acting at one site behave like fermi operators

 $[\sigma_i^x, \sigma_j^y] = 0$ $\{\sigma_i^x, \sigma_j^y\} = 2i\sigma_i^z$

Jordan-Wigner Transform to Fermi Operators, but nonlocal phase-factor tags

Impose Periodic Boundary Conditions, Even and Odd Sectors have different Effective Fermion Hamiltonians, States with either Even or Odd number of particles

Nearest-Neighbor interaction absorbs phases, effectively a quadratic Hamiltonian

Fourier transform, followed by a Bogoliubov transform, yields all eigenstates

Spin-Spin Correlation functions easy to find, though entropy/entanglement tough

Lieb Schultz Mattis, Ann. Phys (1961) Pfeuty, Ann. Phys (1970)

Exact Solution: Jordan-Wigner Fermions Fermion Occupation--> Up Spin

$$\begin{split} \sigma_l^z &= 2n_l - 1, \quad \sigma_l^+ = e^{i\pi\sum_{j=1}^{l-1}n_j}c_l^\dagger \\ c_q &= \frac{1}{\sqrt{N}}\sum c_l \ e^{-iql} \quad \text{Modes} \quad q = \pm \frac{\pi}{N}, \pm \frac{3\pi}{N}...\pm \frac{(N-1)\pi}{N} \\ \text{Ground State} \qquad & \left|G\right\rangle = \prod_{q>0}\left(a_q|0\right) + b_q|\phi_q\rangle\right) \\ |\phi_q\rangle &\equiv c_q^\dagger c_{-q}^\dagger |0\rangle \quad \left|a_q|^2 = \frac{1}{2}\left(1 - \frac{h+J\cos q}{\sqrt{h^2 + J^2 + 2Jh\cos q}}\right)\right] \end{split}$$

Label components of Superposition by u (set of q values occupied by Up Spins) Corresponding amplitude is product of b's and a's (Schmidt Numbers)

$$\rho_{\uparrow} = \prod a_q^2 |0\rangle \langle 0| + \sum_q b_q^2 \prod_{q' \neq q} a_{q'}^2 |0, 0..\phi_q..0\rangle \langle 0, 0..\phi_q..0| + ..$$

Eigenvalues of
$$\mathcal{P}_{\uparrow}$$
 $\lambda_{0} = \prod |b_{q_{i}}|^{2} \lambda_{1} = \lambda_{0} \frac{|a_{Max}|^{2}}{1 - |a_{Max}|^{2}}$
 $\lambda(\eta_{1}, \eta_{2}, \cdot) = \Pi |a_{q_{i}}|^{2\eta_{i}} |b_{q_{i}}|^{2(1-\eta_{i})}$
 $S_{\uparrow} = -\sum_{i} |a_{q_{i}}|^{2} \log |a_{q_{i}}|^{2} + |b_{q_{i}}|^{2} \log |b_{q_{i}}|^{2}$
 $S_{\uparrow} = \sum_{i} H(p_{i}) H(p) = -p \log p - (1-p) \log(1-p)$
Shannon Binary Entropy
 $\varepsilon(x) = \frac{1}{N} \sum_{i=1}^{N/2} H(p_{i}) = \int_{0}^{1} dp \ g(p, x) \log \frac{1-p}{p}$
 $g(p, x) = \frac{1}{N} \sum_{i} \theta(p - p_{i}(x))$ Integrated Density $x = J/h$

Macroscopic limit, Large N Mode eigenvalues as x=J/h is varied Gap between Two bands stays Within one Band continuous +++'+ + +' + × '× × ×'× ××× Location 0.95 + \times \times \times \times \times \times N=20 ++++++++++|x|0.9+ \times \times \times \times \times Λ 0.85 $\times \times \times \times \times \times$ 0.4 0.20.6 0.8 1 $a_{q_i}^2$ $b_{q_i}^2$ $\Delta \approx (1-|x|)$ near |x| \approx]

Integrated Eigenvalue Density



Counting only lower Of the two eigenvalues For every mode

Contribution for entropy From the other eigenvalue Taken care of by Shannon Binary Entropy



$$\varepsilon(x \to \infty) = \frac{\log 2}{2} - \frac{1}{2} \sum_{\text{even } n} \frac{1}{n(n-1)2^n} C_{\frac{n}{2}} \approx 0.19$$

Jump-discontinuity in the derivative of Entanglement



Conclusions

Entanglement useful: Measures aplenty tracking how entangled is a state

Different Sources of Entanglement: Correlations between partitions, Constraints

Different ways of entanglement: Multipartite, Spatial partitions, Multi Species

Multi-Species Entanglement: Macroscopic Entanglement Scales with Size Exists in the Thermodynamic Limit, Can Display Singularities

Transverse-field Ising Model: Macroscopic Entanglement between ↑, ↓ Capable of tracking quantum phase transition and critical behaviour.

Thank You For Your Attention

Superconducting State...

$$|\psi\rangle = \prod_{k} (u_{k} + v_{k} c^{*}_{k} \uparrow c_{-k}) |0\rangle$$
 $u^{2} + v^{2} = 1$ every k

$$\langle n_{k\uparrow} \rangle = \langle 0 | (u_k + v_k c_{-k\downarrow} c_{k\uparrow}) n_{k\uparrow} (u_k + v_k c^*_{k\uparrow} c^*_{-k\downarrow}) | 0 \rangle = v_k^2$$

 $\langle c_{-k\downarrow} c_{k\downarrow} \rangle = u_k v_k$

Pairing stabilized by attractive interaction

$$D(E) \equiv \frac{1}{\Omega} \sum_{k} \delta(E - \varepsilon_{k})$$

$$V(q) = -V_0 |\varepsilon_q - E_F| < \hbar \omega_D$$

$$\Rightarrow \Delta_k = \Delta_0$$

$$n_{\uparrow} = \Sigma n_{k\uparrow}$$
 $\frac{n}{2} \varsigma \equiv \left\langle c_{i\downarrow} c_{i\uparrow} \right\rangle$ Off-diag element Of Density matrix

$$n_{\uparrow} = \frac{n}{2} = \int d\varepsilon \, D(\varepsilon) v^2(\varepsilon) \qquad \qquad \frac{n}{2} \varsigma = \int d\varepsilon \, D(\varepsilon) \, u(\varepsilon) v(\varepsilon)$$

Pair-Entanglement Distributions

$$|\Psi\rangle = \sum_{i} \varphi_{i} |\uparrow\uparrow \cdot\uparrow\downarrow\downarrow\uparrow\cdot\rangle$$
$$p(c) = \begin{cases} (1/\pi)K_{0}(c/2) & (\text{GOE})\\ cK_{0}(c) & (\text{GUE}) \end{cases}$$

TR Breaking --> More Ent.Sharin Ave. Ent. Related to Localization





Kicked-Transverse Ising Chain Global Entanglement Generation AL & VS, Phys. Rev. A65, 052304 (2003)

AL & VS, Phys. Rev. A71, 062324 (2005)

Heisenberg Antiferromagnet GS: S=0 Spatially Uniform

VS (2004)

Kagome and Triangular: $C_{ij} = 0$ No pair concurrences!

Average Site Mixedness $\varepsilon = 1$ for all lattices!

One-Magnon State
$$|\psi
angle = \Sigma \phi_l |l
angle$$
 - Location of Down Spin

$$C_{ave} = \frac{2}{N} (\frac{2}{\pi})$$
 Time Reversal Invariant
 AL,VS (2003)
 $= \frac{2}{N} (\frac{\pi}{4})$ No Time Reversal

Entropy: Independent mode contributions: $p_i = |a_{q_i}|^2$ x = J/h

$$\varepsilon(x) = \frac{1}{N} \sum_{i=1}^{N/2} H(p_i) = \int_0^1 dp \ g(p, x) \log \frac{1-p}{p}$$

 $g(p,x) = rac{1}{N}\sum\limits_{i} heta(p-p_i(x))$ Integrated Eigenvalue Density

$$\varepsilon(x) = \frac{1}{4\pi} \int_0^1 d\zeta \log \frac{1+\zeta}{1-\zeta} \left(\Phi_- - \Phi_+\right) \theta(x^2 + \zeta^2 - 1)$$

$$\cos \Phi_{\pm} = \frac{-1 + \zeta^2 \pm |\zeta| \operatorname{Sgn}(x) \sqrt{\zeta^2 + x^2 - 1})}{x}$$

$$\frac{\partial \Phi_{-}}{\partial x} = -\frac{1 - x}{|1 - x|} \frac{\sqrt{1 - \zeta^2}}{\zeta} \qquad \qquad \frac{\partial^2 \Phi_{-}}{\partial x^2} \approx \frac{1}{|x - 1|} \frac{\sqrt{1 - \zeta^2}}{\zeta}$$