Recent Application of Fisher-Hartwig Formula to Quantum Spin Chains

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A CELEBRATION OF STATISTICAL MECHANICS
Looking back, looking forward . . .

△

through prism of Toeplitz determinant

Outline

Toeplitz Matrix

- Entries of $n \times n$ matrix T depends on the difference:

$$T_{kj} = T_{k-j}$$

  Constant along diagonal.
- Convenient parametrisation: generating function $g(\theta)$, can have zeros and phase jumps.

$$T_{k-j} = \frac{1}{2\pi} \int_0^{2\pi} g(\theta) \mathrm{e}^{-\mathrm{i}(k-j)\theta} \mathrm{d}\theta$$

- Asymptotic of $\det T$ for large n is described by Fisher-Hartwig formula.

Fisher-Hartwig Formula: Conditions

- Generating function $g(\theta)$:

$$g(\theta) = \psi(\theta) \prod_{r=1}^{R} t_{\beta_r}(\theta - \theta_r) u_{\alpha_r}(\theta - \theta_r)$$

$\psi(\theta)$ is a smooth non-vanishing function with zero winding number. Each function t_{β_r} and u_{α_r} can be represented as:

$$\begin{aligned} t_\beta(\theta) &= \exp\{i\beta(\theta - \pi \mathrm{sign}\theta)\}, & \frac{1}{2} > \Re\beta > -\frac{1}{2} \\ u_\alpha(\theta) &= [2 - 2\cos(\theta)]^\alpha, & \frac{1}{2} > \Re\alpha > -\frac{1}{2} \end{aligned}$$

Fisher-Hartwig Formula

- The following limit exists :

$$\lim_{n\to\infty} \frac{\det(T)}{\mathcal{F}^n \left[n^{\sum_{r=1}^{R}(\alpha_r^2 - \beta_r^2)} \right]} = E$$

n is the dimension of the matrix

$$\mathcal{F} = \exp\left(\frac{1}{2\pi} \int_0^{2\pi} d\theta \ln\{\psi(\theta)\} \right)$$

the coefficient

Consider Weiner-Hopf factorization of

$$\psi = \mathcal{F}\psi_+ \left(\exp\{i\theta\}\right) \psi_- \left(\exp\{-i\theta\}\right)$$

The coefficient E is

$$E = \mathcal{E}\left[\prod_{r=1}^{R} \frac{G(1+\alpha_r+\beta_r)G(1+\alpha_r-\beta_r)}{G(1+2\alpha_r)}\right] \times$$
$$\left[\prod_{r=1}^{R} \left(\psi_-(\exp\{i\theta_r\}\right)^{-\alpha_r-\beta_r} \left(\psi_+(\exp\{-i\theta_r\}\right)^{-\alpha_r+\beta_r}\right] \times$$
$$\prod_{1\leq k\neq j\leq R} \left[1 - \exp(i\{\theta_k - \theta_j\}\right]^{-(\alpha_k+\beta_j)(\alpha_k+\beta_j)}$$

Barnes

$$\mathcal{E} = \exp\left(\sum_{k=1}^{\infty} k s_k s_{-k}\right)$$

s_k is Fourier coefficient of $\ln \psi(\theta)$.
G is Barnes function: $G(1+z) = G(z)\Gamma(z), \quad G(1) = 1.$

$$G(1+z) = (2\pi)^{\frac{z}{2}} e^{\{-(z+1)z/2-\gamma_E z^2/2\}} \prod_{k=1}^{\infty}\left(1+\frac{z}{k}\right)^k e^{\{-z+z^2/2k\}}$$

$\gamma_E \approx 0.5772156649\ldots$ is Euler constant.

Brief History

- Discovery:

  M E Fisher, R E & Hartwig *Adv. Chem. Phys.* **15** 333, 1968
- Proof:
  G. Szegő, H.Widom, E. Basor, A. Böttcher, B Silbermann
- Extensive research: P. Deift, A. Its, C. Tracy, P. Bleher
- *Toeplitz determinants have multiple applications :*
  Ising correlations E.W. Montroll, R.B. Potts, J.C. Ward, L.P.Kadanoff, B.McCoy, T.T. Wu . . .
  approximation of determinant of Fredholm integral operators with sin kernel by F.Dyson.

example important for spin chains

generating function $g(\theta)$ is equal to $\lambda - 1$ on interval $-k_F < \theta < k_F$ and $\lambda + 1$ on the compliment. Factorization:

$$g(\theta) = \psi(\theta) t_{-\beta(\lambda)}(\theta - k_F) t_{\beta(\lambda)}(\theta + k_F)$$

has two jumps at $\theta = \pm k_F \implies$ E.L. Basor

$$\psi(\theta) = (\lambda + 1)\left(\frac{\lambda + 1}{\lambda - 1}\right)^{-k_F/\pi}, \qquad \beta(\lambda) = \frac{1}{2\pi i} \ln \frac{\lambda + 1}{\lambda - 1}$$

Here λ is a spectral parameter of XY spin chain.

$$\det T = (2 - 2\cos(2k_F))^{-\beta^2(\lambda)} \times$$
$$\{G(1 + \beta(\lambda))G(1 - \beta(\lambda))\}^2 \left((\lambda + 1)\{\tfrac{\lambda+1}{\lambda-1}\}^{-k_F/\pi}\right)^n n^{-2\beta^2(\lambda)}$$

Application to XX Model

- Spin chain

$$H_{XX} = -\sum_{n=-\infty}^{\infty} \sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y + h\sigma_n^z, \qquad |h| \leq 2$$

- Lieb , Schultz & Mattis 1961
- The $|gs\rangle$ is unique
- Entanglement of a block of L sequential spins with the rest of the ground state [environment].

Entanglement

- $|gs\rangle = |B \cup E\rangle$
- density matrix of the ground state state

$$\rho = |gs\rangle\langle gs|$$

- Density matrix of the block

$$\rho_B = \mathrm{Tr}_E\, \rho$$

Quantum Entanglement

Measures of entanglement

- Von Neumann Entropy

$$S(\rho_B) = -\mathrm{Tr}_B\left(\rho_B \ln \rho_B\right)$$

- Rényi Entropy

$$S(\rho_B, \alpha) = \frac{\ln\left(\mathrm{Tr}_B \rho_B^\alpha\right)}{1-\alpha}$$

α is a paramer.

Calculation of Entropy

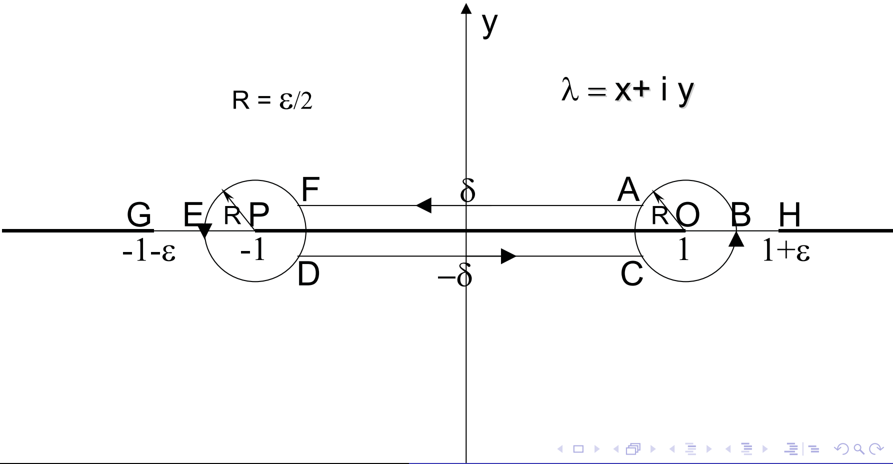
- Contour integral representation: Jin, Korepin 2004:

$$S(\rho_B) = \lim_{\epsilon \to 0^+} \lim_{\delta \to 0^+} \frac{1}{2\pi \mathrm{i}} \oint_{c(\epsilon,\delta)} e(1+\epsilon, \lambda) \mathrm{d} \ln D_L(\lambda)$$

$$e(x, \lambda) = -\frac{x+\lambda}{2} \ln\left(\frac{x+\lambda}{2}\right) - \frac{x-\lambda}{2} \ln\left(\frac{x-\lambda}{2}\right)$$

- $D_L = \det T$ is a Toeplitz determinant. Dimension of the matrix is n is the same as the size of the block L.

contour



Von Neumann Entropy

- Asymptotic $L \to \infty$ from Fisher-Hartwig formula:

$$S(\rho_A) = \frac{1}{3}\ln L + \frac{1}{6}\ln\left[1 - \left(\frac{h}{2}\right)^2\right] + \frac{1}{3}\ln 2 + \Upsilon_1$$

  $\ln L$ term agrees with Holzhey, Larsen, Wilczek 1994 and Cardy, Calabrese 2004

- Sub-leading terms B.-Q. Jin, V.E. Korepin 2004

$$\Upsilon_1 = -\int_0^\infty \mathrm{d}t \left\{ \frac{\mathrm{e}^{-t}}{3t} + \frac{1}{t\sinh^2(t/2)} - \frac{\cosh(t/2)}{2\sinh^3(t/2)} \right\} \approx 0.495$$

Rényi Entropy

Asymptotic of Rényi entropy is

$$S(\rho_A, \alpha) \to \left(\frac{1 - \alpha^{-1}}{6} \right) \ln \left(2L \sqrt{1 - \left(\frac{h}{2} \right)^2} \right) + \Upsilon^{\{\alpha\}}$$

Constant $\Upsilon^{\{\alpha\}}$ was evaluated by B.-Q. Jin, V.E. Korepin 2004

XY model

$$H_{XY} = -\sum_{n=-\infty}^{+\infty} (1+\gamma)\sigma_n^x \sigma_{n+1}^x + (1-\gamma)\sigma_n^y \sigma_{n+1}^y + h\sigma_n^z$$

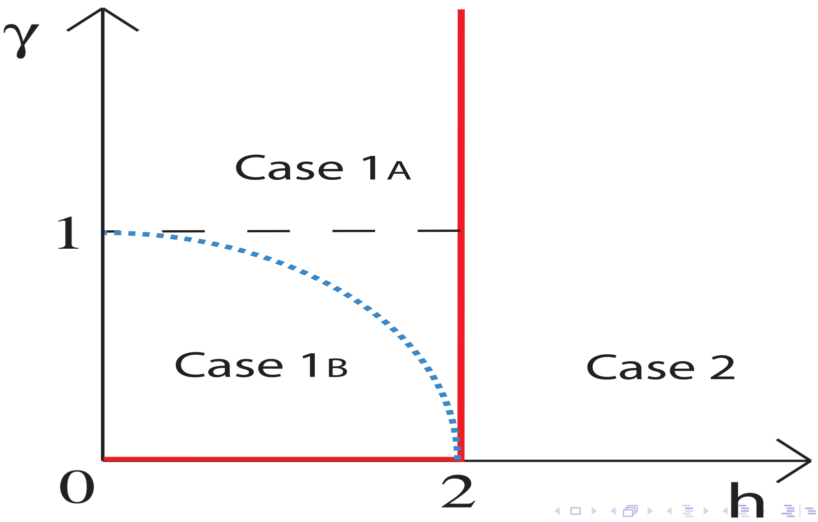
- Lieb , Schultz & Mattis 1961
- Abraham, Barouch, Gallavotti and Martin-Löf, 1970
- Phases

  1a. Moderate field: $2\sqrt{1-\gamma^2} < h < 2$

  1b. Weak field: $0 \leq h < 2\sqrt{1-\gamma^2}$

  2. Strong field: $h > 2$

Phase diagram



Boundary between 1a and 1b

Barouch-McCoy circle $h = 2\sqrt{1-\gamma^2}$

$$|GS\rangle = |GS_1\rangle + |GS_2\rangle$$

$$\begin{aligned} |GS_1\rangle &= \prod_{n \in \text{lattice}} [\cos(\theta)|\uparrow_n\rangle + \sin(\theta)|\downarrow_n\rangle] \ , \\ |GS_2\rangle &= \prod_{n \in \text{lattice}} [\cos(\theta)|\uparrow_n\rangle - \sin(\theta)|\downarrow_n\rangle] \end{aligned}$$

$$\cos^2(2\theta) = (1-\gamma)/(1+\gamma)$$

Von Neumann Entropy

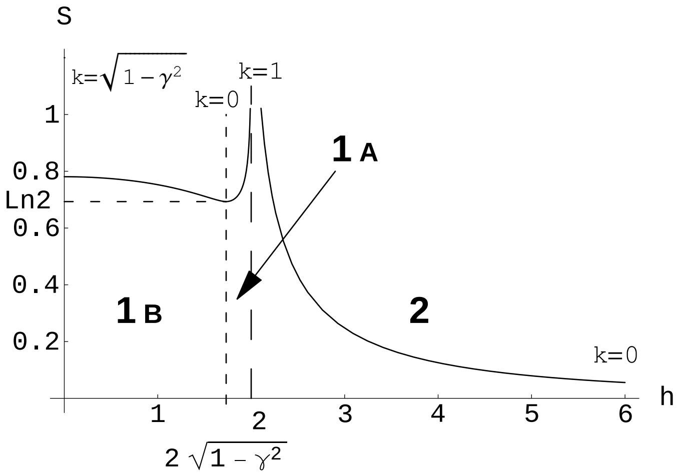
- Entropy of a large block has a limit: Its, Jin, Korepin 2004. Result of calculations for weak magnetic field [case 1b]:

$$S(\rho_A) = \frac{1}{2}\int_1^\infty \ln\left(\frac{\theta_3\left(\beta(\lambda)+\frac{\tau}{2}\right)\theta_3\left(\beta(\lambda)-\frac{\tau}{2}\right)}{\theta_3^2\left(\frac{\sigma\tau}{2}\right)}\right)\mathrm{d}\lambda$$

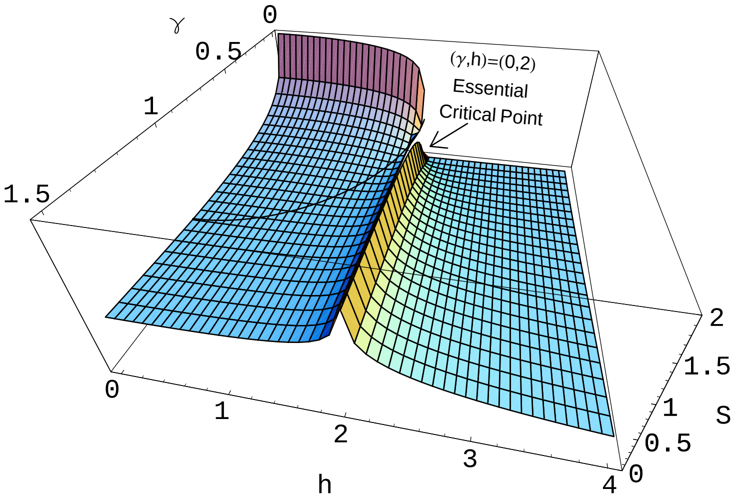
$$\beta(\lambda) = \frac{1}{2\pi\mathrm{i}}\ln\frac{\lambda+1}{\lambda-1}, \quad \tau = \mathrm{i}\frac{I(k')}{I(k)}, \quad k = \sqrt{\frac{1-(h/2)^2-\gamma^2}{1-(h/2)^2}}$$

- θ_3 the Jacobi theta-function; $\quad (k')^2 + k^2 = 1$
- Entropy is constant on the ellipsis: $\quad k = const$
- Complete elliptic integral of the first kind $I(k) = \int_0^1 \frac{\mathrm{d}x}{\sqrt{(1-x^2)(1-x^2k^2)}}$

Plot of Entropy at Constant Anisotropy $\gamma = \frac{1}{2}$



3-D Plot of Entropy



Rényi Entropy

- Limiting entropy in the region $0 < h < 2$ is:
  $S(\rho_B, \alpha) = \frac{1}{6}\frac{\alpha}{1-\alpha}\ln\left(\frac{k'}{k^2}\right) + \frac{1}{3}\frac{1}{1-\alpha}\ln\left(\frac{\theta_2(0,q^\alpha)\theta_4(0,q^\alpha)}{\theta_3^2(0,q^\alpha)}\right) + \frac{1}{3}\ln 2$

$$\tau = \mathrm{i}\frac{I(k')}{I(k)} \equiv \mathrm{i}\tau_0, \qquad q = e^{\pi \mathrm{i}\tau}$$

- Dependence on h and γ similar to von Neumann.
  It is a modular function of α.

$$\tau \to \tau + 2, \qquad \tau \to -1/\tau$$

Spectrum of the density matrix of very large block

p_m are eigenvalues of the limiting density matrix. They form exact geometric sequence converging to zero:

$$p_m = p_0 \mathrm{e}^{-\pi \tau_0 m}, \quad m = 0, 1, 2, \ldots \infty, \quad \tau_0 = \frac{I(k')}{I(k)} > 0$$

The maximum eigenvalue

$$p_0 = (kk'/4)^{1/6} \exp\left[\frac{\pi}{12}\tau_0\right] \qquad \text{is unique}$$

$$\text{Degeneracy} \rightarrow \left(192^{-1/4}\right) \left(\mathrm{m}^{-3/4}\right) \mathrm{e}^{\pi\sqrt{\mathrm{m}/3}}, \qquad \mathrm{m} \rightarrow \infty$$

Toeplitz determinants vs Fredholm determinants

- Toeplitz determinants were used for evaluation of correlation functions in Ising model: E.W. Montroll, R.B. Potts, J.C. Ward, L.P.Kadanoff, B.McCoy, T.T. Wu.
- Toeplitz determinants were used for approximation of Fredholm determinants: F. Dyson

$$\det(I+\hat{K}), \qquad K(\lambda,\mu)=\frac{\sin[x(\lambda-\mu)])}{\lambda-\mu}$$

- Another relation of Toeplitz $\rightarrow$ Fredholm: P.Deift . Integrable integral operators:

$$D_L(\lambda)=\det(I+\hat{V}), \qquad V(\lambda,\mu)=\frac{\sum_j e_j(\lambda)E_j(\mu)}{\lambda-\mu}$$

- Correlation functions $\rightarrow$ Fredholm determinant $\det(I+\hat{V})$

XX Correlation are Fredholm determinants of integrable integral operators

$$H_{XX} = -\sum_{n=-\infty}^{\infty} \sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y + h\sigma_n^z \ ;$$

$$g(n,t) = \frac{\mathrm{Tr}\left\{ \mathrm{e}^{-\frac{H_{XX}}{T}} \sigma_{n_2}^{+}(t_2)\sigma_{n_1}^{-}(t_1) \right\}}{\mathrm{Tr}\{e^{-\frac{H_{XX}}{T}}\}}, \quad n = n_2 - n_1, \quad t = t_2 - t_1$$

$$g(n,t) \to \exp\left\{ \frac{1}{2\pi} \int_{-\pi}^{\pi} \mathrm{d}p |n - 4t \sin p| \ln \left| \tanh\left(\frac{h - 2\cos p}{T} \right) \right| \right\}.$$

As space and time separation $n \to \infty$ and $t \to \infty$ correlation function **g** exponentially decay. Its, Izergin, Korepin. Slavnov, PRL, 1993

XXZ Model challenge for the future

- More complicated spin chains:

$$H_{XXZ} = -\sum_{n=-\infty}^{\infty} \sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y + \Delta \sigma_n^z \sigma_{n+1}^z$$

- Phases

$\Delta > 1$:	ferromagnetic
$-1 < \Delta < 1$:	critical
$\Delta < -1$:	gapped & anti-ferromagnetic

Open Problems

- Calculation of von Neumann entropy & Rényi entropy of large block of spins for anti-ferromagnetic case with a gap. Dependence of limiting entropy on Δ.
- Calculation of space-time-temperature dependent correlation functions in critical region $|\Delta| < 1$. The rate of exponential decay for large time intervals.
- Determinant representation $\Longrightarrow$ Eßler , Frahm , Izergin , Korepin,1995 *CMP* .

Conclusion

Toeplitz determinants
were used since 1960s for calculations of Ising correlations;
now they are used for evaluation of entropy;
further research will reveal closer relation of Toeplitz matrices to the theory of quantum completely integrable models

For Further Reading I

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  Integro-Difference Equation for a correlation function of the spin-$\frac{1}{2}$ Heisenberg XXZ chain *Nucl. Phys.* B **446** 448-460
- Frahm H, Its A R & Korepin V E 1994
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